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In multiband systems, such as iron-based superconductors, the superconducting states with locking and antilocking of the interband phase differences are usually considered as mutually exclusive. For example, a dirty two-band system with interband impurity scattering undergoes a sharp crossover between the $s_{\pm}$ state (which favors phase antilocking) and the $s_{++}$ state (which favors phase locking). We discuss here that the situation can be much more complex in the presence of an external field or superconducting currents. In an external applied magnetic field, dirty two-band superconductors do not feature a sharp $s_{\pm} \rightarrow s_{++}$ crossover but rather a washed-out crossover to a finite region in the parameter space where both $s_{\pm}$ and $s_{++}$ states can coexist for example as a lattice or a microemulsion of inclusions of different states. The current-carrying regions such as the regions near vortex cores can exhibit an $s_{\pm}$ state while it is the $s_{++}$ state that is favored in the bulk. This coexistence of both states can even be realized in the Meissner state at the domain’s boundaries featuring Meissner currents. We demonstrate that there is a magnetic-field-driven crossover between the pure $s_{\pm}$ and the $s_{++}$ states.

I. INTRODUCTION

It is widely accepted that in iron-based superconductors, the pairing between electrons is produced by interband electron-electron repulsion [1–3]. In such a situation, the superconducting state, which features a sign inversion between the two $s$-wave gap functions, is called $s_{\pm}$, in contrast to the $s_{++}$ state, which has no sign inversion. The presence of disorder is known to potentially lead to a crossover from the $s_{\pm}$ to the $s_{++}$ state [4]. In the absence of an external magnetic field, the crossover is sharp and has basically no thermodynamic features. It was however recently demonstrated that the crossover line is accompanied by a nontrivial transition in the core structure of vortices [5]. More precisely the vortices, in the vicinity of the crossover line, can acquire a circular nodal line around the singular point in one of the superconducting components [5]. This singular nodal line, which in three dimensions extends to a cylindrical nodal surface surrounding the vortex line, results in the formation of a peculiar “moat”-like profile in the subdominant component of the superconducting gap. As a result, the inner region of the vortex core shows a $\pi$ relative phase between the gaps while it is zero in the outer region. This means that these moat-core vortices consist of an $s_{\pm}$ phase inclusion in the vortex core, which is separated from the bulk $s_{++}$ phase by the nodal line. Here we investigate the consequences of this physics on the phase diagram of such dirty two-band superconductors, in an external magnetic field. In a low applied external field the lattices and liquids of such moat-core vortices represent a phase coexistence or a microemulsion of such $s_{\pm}$ inclusions inside the bulk $s_{++}$ state. At elevated fields this results in a field-induced transition between the $s_{\pm}$ and $s_{++}$ states.

We start our investigation, in Sec. II, by deriving a two-band Ginzburg-Landau model (including the gradient terms) from the microscopic Usadel theory of dirty two-band superconductors and discuss the essential properties of the phase diagram. Next, Sec. III is devoted to the investigation of the physical properties of the elementary topological excitations (the vortices) and their core structure in that model. There, we show that across the $s_{\pm}/s_{++}$ crossover line there is a structural transition in the core of topological excitations, and we further construct the diagram where such solutions occur, as a function of the system’s microscopic parameters. In Sec. IV we investigate the consequences for the phase diagram in an applied external magnetic field, and finally our conclusions are presented in Sec. V.

II. THEORETICAL FRAMEWORK

Within a weak-coupling approximation, two-band superconductors with a high concentration of impurities can be described by a system of two Usadel equations, coupled by interband impurity-scattering terms (see, e.g., [6]):

$$\omega_n f_i = \frac{D_i}{2} (g_i \nabla^2 f_i - f_i \nabla^2 g_i) + \Delta_i g_i + \sum_{j \neq i} \gamma_{ij} (g_i f_j - g_j f_i).$$

(1)

Here $\omega_n = (2n + 1)\pi T$ (with $n \in \mathbb{Z}$) are the Matsubara frequencies, $T$ is the temperature, $D_i$ are the electron diffusivities, and $\gamma_{ij}$ are the interband scattering rates. The quasiclassical propagators $g_i$ and $f_i$ are respectively the anomalous and normal Green’s functions in each band, which obey the normalization condition $|f_i|^2 + g_i^2 = 1$. The components of the order parameter $\Delta_j = |\Delta_j| e^{i\theta_j}$ are determined by the
The coefficients of gradient terms are given by [5]

\[ \Delta_i = 2\pi T \sum_{n=0}^{N_d} \sum_j \lambda_{ij} f_j(o_n), \]  

for the Green’s functions that satisfy Eq. (1). Here, \( N_d = \Omega_d/(2\pi T) \) is the summation cutoff by Debye frequency \( \Omega_d \).

The diagonal elements \( \lambda_{ii} \) of the coupling matrix \( \lambda \) in the self-consistency equation (2) describe the intraband pairing, while the interband interaction is determined by the off-diagonal terms \( \lambda_{ij} \) \( (j \neq i) \). The interband coupling parameters and impurity scattering amplitudes satisfy the symmetry relation [6]

\[ \lambda_{ij} = -\lambda_{ji}/N_i \text{ with } j \neq i, \text{ and } \gamma_{ij} = \Gamma N_j, \]  

where \( \lambda, \Gamma > 0 \), and \( N_{1,2} \) are the partial densities of states in the two bands.

In order to investigate the physical properties of dirty two-band superconductors in the external field, we consider a Ginzburg-Landau (GL) model that is derived from the microscopic Usadel theory of dirty superconductors. The Ginzburg-Landau free energy functional for multiband models is obtained as an expansion in several small parameters: small gaps and gradients (not to be confused with a symmetry-based GL expansion that uses a single small parameter \( \tau \); see also remark [7]). The resulting expression, including gradient terms, reads as [5]

\[ \mathcal{F} = \frac{2}{\mathcal{F}_0} \left( \frac{k_{ij}}{2} [\mathbf{\Pi} \Delta_j]^2 + a_{ij}|\Delta_j|^2 + \frac{b_{ij}}{2} |\Delta_j|^4 \right) \]  

\[ + \frac{k_{ij}}{2} \left( [\mathbf{\Pi} \Delta_i]^2 [\mathbf{\Pi} \Delta_j] + [\mathbf{\Pi} \Delta_j]^2 [\mathbf{\Pi} \Delta_i] \right) \]  

\[ + 2(a_{ij} + c_{ij}|\Delta_i|^2 + c_{ij}|\Delta_j|^2) \text{Re}(\gamma_{ij} \Delta_i \Delta_j) \]  

\[ + (b_{ij} + c_{ij} \cos \theta_{ij}) [\mathbf{\Pi} \Delta_i]^2 |\Delta_j|^2 + \frac{B^2}{2}, \]  

Here, the complex fields \( \Delta_j = |\Delta_j| e^{i\phi} \) represent the superconducting gaps in the different bands, and \( \theta_{ij} = \theta_1 - \theta_2 \) stands for the relative phase between them. The two gaps in the different bands are electromagnetically coupled by the vector potential \( \mathbf{A} \) of the magnetic field \( \mathbf{B} = \nabla \times \mathbf{A} \), through the gauge derivative \( \mathbf{\Pi} \equiv \nabla + i q \mathbf{A} \), and the coupling constant \( q \) parameterizes the penetration depth of the magnetic field.

The coefficients of the Ginzburg-Landau functional \( a_{ij}, b_{ij}, c_{ij}, \) and \( k_{ij} \) are calculated from a given set of input parameters \( \lambda_{ij}, D_i, T, \) and \( \Gamma \) of the microscopic self-consistent equation. First, the coefficients of gradient terms are given by [5]

\[ k_{ii} = 2\pi T N_i \sum_{n=0}^{N_d} D_i(o_n + \gamma_{ji})^2 \gamma_{ij} \gamma_{ji} D_j(o_n + \gamma_{ij} + \gamma_{ji})/o_n(o_n + \gamma_{ij} + \gamma_{ji}), \]  

\[ k_{ij} = 2\pi T N_i \gamma_{ij} \sum_{n=0}^{N_d} D_i(o_n + \gamma_{ji}) + D_j(o_n + \gamma_{ij})/o_n(o_n + \gamma_{ij} + \gamma_{ji}), \]  

with \( j \neq i \). Next, the coefficients of the potential terms are

\[ a_{ij} = \frac{N_i \lambda_{ij}}{\det(\lambda)} - 2\pi T \sum_{n=0}^{N_d} \frac{\gamma_{ij} N_i}{o_n(o_n + \gamma_{ij} + \gamma_{ji})}. \]
as a function of temperature and interband scattering amplitude $\gamma$. Although the physics of the subdominant gap $\Delta_1$, which is the crossover between $s_\pm$ and $s_{++}$ states. The vertical line shows a field-cooling path realized later for a simulation in the external field.

Another interesting transition between the $s_{++}$ and the $s_\pm$ phases is possible. Indeed, as a results of the presence of impurities, a possibility for an additional phase appears. This extra phase, where the interband phase difference $\theta_{12} = \theta_2 - \theta_1$ is either zero not $\pi$, is termed the $s + is$ state. The fact that the interband phase difference can be such that $\theta_{12} \neq 0, \pi$ follows from the existence of phase-locking terms $\propto \cos \theta$ in (4c) and the others that are $\propto \cos 2\theta$ in (4c). The competition between those terms is responsible for the existence of the impurity-induced $s + is$ state [10]. The $s$-wave states that spontaneously break the time-reversal symmetry have been a subject of much interest in recent years; see, e.g., [9–17].

In this work, we focus on the physics of the direct $s_\pm$ to the $s_{++}$ impurity-induced crossover in an external magnetic field (denoted by the solid black line on Fig. 1). Although the physics of vortices in, and in the vicinity of, the $s + is$ is very rich, it is beyond the scope of the current work and its detailed study will be addressed in a subsequent work [18].

Below, we discuss that in an external applied magnetic field, dirty two-band superconductors do not feature a sharp $s_\pm \rightarrow s_{++}$ crossover but there appears a finite region in the parameter space where both $s_\pm$ and $s_{++}$ states can coexist in a peculiar way.

### III. STRUCTURAL TRANSITION OF VORTEX CORES

When going from the $s_{++}$ to $s_\pm$ state, there is a transition in the vortex core structure: the vortices there can develop an additional circular nodal line around the singular point in one of the superconducting components [5]. Thus these vortices consist of an $s_\pm$ phase inclusion in the vortex core, which is separated from the bulk $s_{++}$ phase by the nodal line.

In order to investigate the properties of single-vortex solutions, the vector potential $A$ and the gap functions $\Delta_{1,2}$ are discretized using a finite-element framework [19]. Starting with an initial configuration where both components have the same phase winding (i.e., at large distances $\Delta_2 \propto e^{i\theta}$ where $\theta$ is the polar angle relative to the vortex center), the Ginzburg-Landau free energy (4) is then minimized using a nonlinear conjugate gradient algorithm. We begin by simulating the vortex solutions in zero external field. For that purpose, the vortices are induced only by the initial configuration of the phase winding. For further details on the numerical methods employed here, see for example the related discussion in [20].

Figure 2 shows the numerically calculated (isolated) vortex solutions in the vicinity of the impurity-induced crossover, in the case of a two-band superconductor with nearly degenerate bands and weak repulsive interband pairing interaction. Deep in the $s_{++}$ and $s_\pm$ regimes (in the first and fourth column), the vortices have multilayer structure where both components exhibit a vortex profile with different sizes of conventional cores, determined by the fundamental length scales. The vortex profiles of the minority component $\Delta_1$ become very different when approaching the crossover line. On the $s_\pm$ side of the crossover, the minority component exhibits a strong overshoot near the core. The density overshoot effect, although much
smaller, was also reported in the microscopic model with one clean and one dirty band [21].

The very unconventional feature of vortices in this model of dirty two-band superconductors is the appearance of an additional circular nodal line of the minority component in addition to the usual point singularity at the center of the vortex [5]. While the bulk relative phase is zero (the $s_{++}$ state) far from the vortex center, due to the competition between gradient and potential terms, it is more favorable to achieve a $\theta_{12} = \pi$ relative phase ($s_{\pm}$ state) in the vicinity of the core singularity. The transition between the “core” states with $\theta_{12} = \pi$ and the asymptotic state $\theta_{12} = 0$ is realized by nullifying the minority component at a given distance of the core, when the potential terms dominate over the gradient term. This can be seen in the third column of Fig. 2. Analytical explanation of such behavior was given in the previous work Ref. [5].

The existence of the circular nodal line results in the formation of a peculiar “moat”–like profile in the subdominant component of the superconducting gap. Note that the total superconducting order parameter does not vanish there; rather it is the subdominant gap (here $\Delta_1$) that vanishes exactly at this nodal line. Indeed, since it separates regions with $\theta$ from regions with zero phase difference, it has to be exactly zero somewhere. This can be viewed as a real-space counterpart of the crossover on the phase diagram. Namely, the line of direct crossover that separates the $s_{++}$ state from the $s_{\pm}$ phase is that where the subdominant gap vanishes.

In order to understand how generic are such solutions, we further investigate numerically their existence on various phase diagrams. We find that the existence of these kinds of “moat-core” vortices does not depend on the specific values of the pairing coefficients. By that statement we mean that we have been able to identify regions of the $(T,\Gamma)$ diagram where “moat-core” vortices do form. This can be heuristically addressed with the following criterion that the condition for the transition of the vortex core structure is that the mixed-gradient energy (4b) dominates the Josephson energy (4c). This was discussed analytically in Ref. [5]. The investigation of the vortex solutions, for various parameter sets, rather shows that the moat-core is a common feature in the vicinity of the crossover line. The region of their existence is shown in Fig. 3. It is clearly visible that the region with moat-core vortex solutions shrinks close to $T_c$ and is eventually suppressed [panel (a) and (b)]. This is to be expected because near critical temperature, the solutions are dominated by a critical mode (see corresponding analytical estimates in [5]). For the investigated regimes, the width (in terms of impurities $\delta\Gamma$) of the regions where moat-core vortices exist increases with increasing the band disparity $\lambda_{ii}$ [compare for example panels (b) and (d)]. By comparing panels (a), (b), and (c), it can also be seen that the width of the moat “region” increases with the interband coupling $\lambda_{12}$.

IV. PHASE COEXISTENCE IN EXTERNAL FIELD AND MAGNETIC-FIELD-DRIVEN Crossover

In this section, we consider the effect in the presence of intervortex interactions and its implication for states of dirty two-band superconductors in an external magnetic field. First of all the existence of these moat-core vortices, where both $s_{\pm}$ and $s_{++}$ phases coexist, implies that a lattice of such vortices would represent a special kind of phase coexistence and that, in an external field, the sharp crossover found in the ground state is rather washed out to a finite region in the parameter space.

In order to investigate the response to an applied external magnetic field $\mathbf{H} = H\mathbf{e}_z$, perpendicular to the plane, the Gibbs free energy $\mathcal{G} = \mathcal{F} - B \cdot \mathbf{H}$ is minimized, with requiring that $\nabla \times \mathbf{A} = B_{y,z}$ on the boundary (for details, see a related discussion in Ref. [20]).

Figure 4 demonstrates the external-magnetic-field-driven crossover between the $s_{\pm}$ and $s_{++}$ states. The coupling parameters are those of Fig. 2, and the temperature and the strength of the interband impurity scattering place the system in the bulk $s_{++}$ state, close to the crossover line. The computations are thus performed for parameters where the single-vortex solutions have a circular nodal line similar to that shown in the third column in Fig. 2. In zero and low external fields, the preferred phase locking in the bulk is $\theta_{12} = 0$ (the $s_{++}$ state). Upon increasing the external field, vortices start to enter the domain, introducing small inclusions of state with $\theta_{12} = \pi$ in their core. When the density of vortices becomes significant, the
cores of the subdominant component start to overlap until the whole system shows the \( \theta_{12} = \pi \) phase locking everywhere. Thus the crossover here is driven by the external magnetic field.

We find that even in a low applied field, below the first critical field, the Meissner state also exhibits the unusual property of coexistence of both \( s_{++} \) and \( s_{\pm} \) states. Indeed, the \( s_{\pm} \) state can be realized near the boundaries while in the bulk, it is the \( s_{++} \) state. That is, as can be seen from the first column of Fig. 4, the region carrying Meissner currents shows a \( \theta_{12} = \pi \) phase locking (thus an \( s_{\pm} \) state near boundaries), while the bulk is in the \( s_{++} \) state (with \( \theta_{12} = 0 \)). This current-carrying region with \( \theta_{12} = \pi \) is separated from the \( \theta_{12} = 0 \) bulk by a nodal line of the subdominant component. That nodal line originates in the competition between phase-locking kinetic terms favoring a \( \theta_{12} = \pi \) relative phase in the current-carrying regions, and potential terms that favor zero phase difference. The reversal of the phase locking in the current-carrying region is thus in some sense similar to that occurring in vortex cores in the vicinity of the crossover [5].

As illustrated in Fig. 4, the magnetization properties in the vicinity of the \( s_{\pm} / s_{++} \) crossover are rather unusual. It is also interesting to consider the case of a field-cooled simulation close to the impurity-induced crossover. Figure 5 displays a simulation of a field-cooled experiment at a constant applied field that starts at temperatures placing the system above the crossover line in the \( s_{\pm} \) phase, and that ends in the \( s_{++} \) phase. This field-cooled path is denoted by the vertical line displayed in the phase diagram of Fig. 1. Sufficiently far from the crossover, the relative phase corresponds to that of the bulk properties in zero field, i.e., the \( s_{++} \) phase for temperatures above the crossover line and \( s_{++} \) below the crossover. However, unlike the zero-field case, there is no sharp crossover between both states. As can be seen in the third column, after the crossover, the vortex-carrying regions remain mostly with the \( s_{\pm} \) phase because the cores of the subdominant component still overlap. When going away from the crossover, that is, when further decreasing the temperature, the cores in the subdominant component \( \Delta_1 \) do not overlap anymore. Still the vortices with zero nodal line feature inclusion of the \( \theta_{12} = \pi \) state while the intervortex spaces have relative phase \( \theta_{12} = 0 \). That situation of a lattice (or liquid) of moat-core vortices thus represents a phase coexistence or a microemulsion of \( s_{\pm} \) inclusions inside the \( s_{++} \) state.

V. CONCLUSION

We considered a two-band superconducting system that has an impurity-driven \( s_{\pm} / s_{++} \) crossover line. We generalize...
FIG. 5. A field-cooled state simulation for a dirty two-band superconductor, in the vicinity of the impurity induced crossover line. The displayed quantities are the same as in Fig. 4. The preferred phase locking at high temperatures is $\theta_{12} = \pi$ (the $s^\pm$ state), while it is $\theta_{12} = 0$ (the $s^{++}$ state) at low temperatures. Decreasing the temperatures drives the system across the crossover line. After the crossover, vortices still carry inclusions of $\theta_{12} = \pi$ in their core. Only far below the crossover temperature, vortices do not carry different phase locking in their core anymore, and the whole system shows a $\theta_{12} = 0$ phase locking everywhere.

the zero-field phase diagram to the case where the system is subjected to external magnetic field. We report that it is a rather generic feature that on the $s^{++}$ side of this crossover, the vortex solutions are unconventional, featuring a circular nodal line that segregates the $s^\pm$ phase inclusions in the cores from the bulk $s^{++}$ phase. Further, we demonstrated that as a consequence of such vortex solutions, the behavior of dirty two-band superconductors in the vicinity of the crossover is also rich in an external field. Indeed, in contrast to the zero-field picture of a sharp crossover, the lattice and liquids of moatcore vortices represent a lattice or a “micromulsion” of $s^\pm$ inclusions inside the $s^{++}$ state. Moreover, as the vortex density raises in increasing field, there is also a field-induced crossover from $s^{++}$ to the $s^\pm$, which can be resolved in local phase-sensitive probes [22–24]. We also pointed out that in these systems in an applied external field, the superconducting state near the Meissner current carrying boundary can be $s^\pm$ while it is $s^{++}$ in the bulk. This result has direct implications for local probes of superconducting states, such as the one proposed in Refs. [22–24], and for Josephson junction experiments. The coexistence state will manifest itself in the existence of signatures of both the $s^\pm$ and $s^{++}$ states depending on the probe’s position. The formation of nodal lines was also found in a different phenomenological clean three-band model where it arises for a different reason due to frustrated Josephson terms [13] rather than originating from competition between mixed-gradient and potential terms. That suggests that the phenomenon is rather generic and applies also to other models featuring a crossover from the $s^\pm$ to $s^{++}$ state.

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APPENDIX: Ginzburg-Landau Coefficients

Table I shows the actual values of the coefficients entering the Ginzburg-Landau functional that were used for the various simulations throughout the paper.
TABLE I. Coefficients of the Ginzburg-Landau free energy functional (4), which correspond to the various numerical simulations reported in the main text of the theory. They are calculated using the formulas (5), (6), (7), and (8), derived consistently from the microscopic Usadel theory (1). The last column shows the effective Josephson coupling $J_{\text{eff}} = 2(a_{12} + c_{11} |\Delta_1|^2 + c_{22} |\Delta_2|^2)$. Positive (resp. negative) values of $J_{\text{eff}}$ denote the $s_+ \rangle$ (resp. $s_+$) phase, while $J_{\text{eff}} = 0$ exactly at the crossover.

| Control parameter | $k_{11} = k_{22}$ | $k_{12}$ | $a_{11}$ | $a_{22}$ | $c_{11} = c_{22}$ | $c_{12}$ | $J_{\text{eff}}$ |
|------------------|--------------------|--------|---------|---------|------------------|---------|--------------|
| $\Gamma = 0.253$ | 4.57854            | 0.37352| 3.46285 | -2.29089| 0.1615           | 0.741321| -2.80412   |
| $\Gamma = 0.256$ | 4.58081            | 0.37838| 3.46165 | -2.29209| -0.86902         | 0.742242| -2.83503   |
| $\Gamma = 0.257$ | 4.58157            | 0.380002| 3.46123| -2.29251| -1.10501         | 0.742549| -2.84532   |
| $\Gamma = 0.260$ | 4.58386            | 0.384875| 3.45997| -2.29377| -1.81332         | 0.743474| -2.87614   |
| $\Gamma = 0.263$ | 4.55512            | 1.06235| 8.70857 | 2.95483 | 3.982549         | 3.439215| 3.32965    |

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