

Impurity effect and vortex cluster phase in mesoscopic type-1.5 superconductors

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Abstract

Based on two-band time-dependent Ginzburg-Landau theory, we study the electromagnetic properties of two-band mesoscopic superconductors. We perform the numerical simulations with the finite element method, and determine the minimum sample size L_c for the existence of the type-1.5 superconductivity from the obtained phase diagram in the absence of impurity. Meanwhile in the presence of an isotropic impurity, our numerical results reveal that the vortex cluster state induced by the attractive defect potential will gradually appear in the mesoscopic system with the sample size $L < L_c$, and the critical defect strength is about 0.2 in the T_c disorder model. In addition, we also investigate the effect of anisotropic defect structures and multiple correlated disorders on the patterns of magnetic vortex distributions. Our theoretical study thus indicates that the diversity of impurity depositions has a significant influence on the semi-Meissner state in mesoscopic type-1.5 superconductors.

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17 **1 Introduction**

18 Over the past two decades, two-band superconductivity has become an important research
19 subject in condensed matter physics. This field started from the discovery of superconductivity
20 in MgB₂ [1], where the existence of two distinct superconducting gaps reveals the complexity
21 of Fermi surface topology in this system. Since then, extensive theoretical and experimental
22 studies have been performed to provide novel insights into unconventional superconducting
23 pairing mechanisms and physical properties in these materials. For example, the multi-gap
24 superconductivity signals a new pathway to achieve more superconducting pairing modes,
25 which can induce phase competition or coexistence between multiple bands by adjusting the
26 external magnetic field or impurity distribution. Furthermore, the magnetic vortex behavior
27 can be optimized through rational design of multi-band structures and its interaction with
28 impurities can improve the overall performance of superconducting devices [2, 3].

29 As we know, each condensate in two-band superconductors is predicted to support vortex
30 excitation with fractional quantum flux [4]. Due to the interband Josephson coupling, the
31 vortices from different condensates are bounded together with the string interaction and their
32 normal cores will be locked to form a composite vortex with the standard integer quantum
33 flux in the ground state. Recently in a series of experiments of iron-based superconductors,
34 the fractional vortices with a magnitude that varies continuously with temperature have been
35 clearly observed in some special locations [5–7]. In general, the physics of composite vortices
36 in the two-band system will be influenced by the coherence lengths ξ_1 and ξ_2 as well as the
37 magnetic field penetration depth λ . When the particular condition $\xi_1 < \sqrt{2}\lambda < \xi_2$ is satisfied,
38 there may exhibit a new superconducting state that combines characteristics of both type-1
39 and type-2 superconductors. This so-called semi-Meissner phase or vortex cluster phase is
40 formed due to the interaction of long-range attraction and short-range repulsion between
41 composite vortex excitations [8–10]. The existence of this novel vortex pattern was first vi-
42 sualized by Bitter decorations on high quality MgB₂ single crystal in 2009 [11]. Thereafter,
43 zero-field muon spin experiments have also revealed the presence of this type-1.5 supercon-
44 ducting state in unconventional superconductors Sr₂RuO₄ [12, 13] and LaPt₃Si [14, 15].

45 In the present paper, we study the electromagnetic effect of type-1.5 superconductors
46 based on the time-dependent Ginzburg-Landau (TDGL) theory. With the COMSOL Multi-
47 physics software and the finite element method, we first obtain the $L - \kappa_1$ phase diagram of
48 the two-band superconductor in the absence of impurity, with L the sample size and κ_1 the
49 GL parameter. Our numerical results demonstrate that there exists a critical sample size L_c
50 for this two-band system, and the semi-Meissner state induced by long-range vortex attrac-
51 tion disappears below L_c . Then in the presence of an isotropic impurity, we show the $g - \kappa_1$
52 phase diagram with the sample size below L_c , where g represents the disorder strength in this
53 system. For $|g| > 0.22$, we can directly observe the crossover of this mesoscopic system from
54 the diamagnetic Meissner state to the vortex cluster phase, and ultimately to the Abrikosov
55 lattice phase. Furthermore, we also discuss the possible patterns of vortex cluster induced by
56 the anisotropic defect structures and multiple correlated disorders in this superconductor. All
57 of our theoretical results indicate that the diversity of impurity depositions has a significant
58 influence on the collective behaviors of magnetic vortices in the type-1.5 superconducting

59 system.

60 The rest of this article is organized as follows. In Section 2, we introduce the two-band
61 TDGL theory and apply this formalism to the type-1.5 superconductors. In Section 3, we give
62 the procedure of numerical simulations based on the finite element method. Then in Section
63 4, we systematically investigate the impurity effect and vortex cluster phase in the mesoscopic
64 system. Finally, Section 5 gives the conclusion of the paper.

65 2 Model and formalism

66 The simplest GL free energy functional of two-gap superconductors can be written as [16–20]
67

$$F = \sum_i \left[\frac{1}{2m_i} \left| \left(-i\hbar\nabla - \frac{2e}{c}\mathbf{A} \right) \Psi_i \right|^2 - \alpha_i |\Psi_i|^2 + \frac{\beta_i}{2} |\Psi_i|^4 \right] + \frac{\mathbf{B}^2}{8\pi}. \quad (1)$$

68 Here Ψ_i ($i = 1, 2$) represents the superconducting order parameter and m_i is the effective
69 mass for each band. The coefficient α_i is a function of temperature, while β_i is independent
70 of temperature. $\mathbf{B} = \nabla \times \mathbf{A}$ is the magnetic induction and \mathbf{A} is the vector potential. Starting
71 from the seminal works of Thuneberg [21, 22], two main disorder models have been proposed
72 to describe the effect of nonmagnetic impurities on the superconducting system in the frame-
73 work of the GL theory [23, 24]. The first one is the T_c disorder model with T_c the critical
74 temperature, which is characterized by altering the GL free energy coefficient $\alpha_i \rightarrow \alpha_{i0}g(\mathbf{r})$
75 in Eq. (1) [25]. The other one is the l disorder model with l the mean free path, achieved by
76 modifying the effective mass $1/m_i \rightarrow (1/m_i)h(\mathbf{r})$ in Eq. (1), where $h(\mathbf{r}) = l/l_m < 1$ repre-
77 sents the ratio of the mean free path inside and outside the well-defined pinning area [26].

78 If the superconductor is driven out of equilibrium, the order parameter should relax back
79 to its equilibrium value. It is well known that this deviation of superconducting materials
80 can be conveniently described by the TDGL theories. The single-band TDGL equations were
81 first proposed by Schmid [27] and derived from the microscopic BCS theory by Gor'kov and
82 Éliashberg [28]. The extension of TDGL equations to the multi-component superconducting
83 system can be written as [29–32]

$$-\Gamma_i \frac{\partial \Psi_i}{\partial t} = \frac{\delta F}{\delta \Psi_i^*} \quad \text{and} \quad -\sigma_n \frac{\partial \mathbf{A}}{\partial t} = \frac{\delta F}{\delta \mathbf{A}} \quad (2)$$

84 where Γ_i is the relaxation time of order parameters and σ_n represents the electrical conduc-
85 tivity of the normal sample in the two-band case. Therefore, minimization of the free energy
86 F with respect to Ψ_i and \mathbf{A} leads to the following dimensionless TDGL equations in the zero-
87 electrostatic potential gauge

$$-\Gamma_1 \frac{\partial \Psi_1}{\partial t} = - \left[g(\mathbf{r}) - |\Psi_1|^2 \right] \Psi_1 + h(\mathbf{r}) (-i\nabla - \mathbf{A})^2 \Psi_1, \quad (3)$$

$$-\Gamma_2 \frac{\partial \Psi_2}{\partial t} = - \left[\frac{\alpha_{20}}{\alpha_{10}} g(\mathbf{r}) - \frac{\beta_2}{\beta_1} |\Psi_2|^2 \right] \Psi_2 + \frac{m_1}{m_2} h(\mathbf{r}) (-i\nabla - \mathbf{A})^2 \Psi_2 \quad (4)$$

89 and

$$-\frac{\partial \mathbf{A}}{\partial t} = \kappa_1^2 \nabla \times \nabla \times \mathbf{A} - \mathbf{J}_s \quad (5)$$

90 with the supercurrent

$$\mathbf{J}_s = h(\mathbf{r}) \left\{ \left[\frac{i}{2} (\Psi_1 \nabla \Psi_1^* - \Psi_1^* \nabla \Psi_1) - |\Psi_1|^2 \mathbf{A} \right] + \frac{m_1}{m_2} \left[\frac{i}{2} (\Psi_2 \nabla \Psi_2^* - \Psi_2^* \nabla \Psi_2) - |\Psi_2|^2 \mathbf{A} \right] \right\}. \quad (6)$$

91 Here in the clean limit with the impurity function $g = h = 1$, we at first introduce the co-
 92 herence length $\xi_i^2 = \hbar^2/(2m_i\alpha_{i0})$, the London penetration depth $\lambda^{-2} = \lambda_1^{-2} + \lambda_2^{-2}$ with
 93 $\lambda_i^{-2} = 4\pi e^2\Psi_{i0}^2/(m_i c^2)$ and $\Psi_{i0} = \sqrt{\alpha_{i0}/\beta_i}$, and the GL parameter $\kappa_1 = \lambda_1/\xi_1$. We then take
 94 the coordinate \mathbf{r} in units of ξ_1 , the time t in units of $t_0 = m_1\sigma_n/(4e^2\Psi_{10}^2)$, Γ_i in units of
 95 $\alpha_{10}t_0$ and the order parameter Ψ_i in units of Ψ_{10} . We also set the magnetic induction \mathbf{B} in
 96 units of $H_0 = \Phi_0/(2\pi\xi_1^2)$ with the flux quantum $\Phi_0 = \pi\hbar c/e$ and the vector potential \mathbf{A} in
 97 units of $A_0 = H_0\xi_1$.

98 Following Ref. [8], multi-component systems allow a type of superconductivity that is dis-
 99 tinct from type-1 or type-2 superconductor. With the condition $\xi_1 < \sqrt{2}\lambda < \xi_2$, the type-1.5
 100 superconducting state will originate from a peculiar vortex interaction which exhibits short-
 101 range repulsion and long-range attraction characteristics. The short-range repulsion prevents
 102 adjacent vortices from overlapping, while the long-range attraction facilitates the clustering
 103 of composite vortices. Consequently, this state is different from type-1 superconductors that
 104 completely repel magnetic flux and type-2 superconductors which allow considerable mag-
 105 netic flux penetration and the formation of vortex lattice. In the ideal sample, the constraint
 106 mentioned above can be specifically expressed as

$$\sqrt{\frac{1}{2} \left(1 + \frac{m_1 \alpha_{20} \beta_1}{m_2 \alpha_{10} \beta_2} \right)} < \kappa_1 < \sqrt{\frac{1}{2} \left[\frac{m_1 \alpha_{10}}{m_2 \alpha_{20}} + \left(\frac{m_1}{m_2} \right)^2 \frac{\beta_1}{\beta_2} \right]}. \quad (7)$$

107 In this circumstance, the magnetic composite vortices will form vortex clusters and coexist
 108 with domains of the two-component Meissner state in the framework of the GL theory.

109 In order to perform systematic numerical simulations, we need to specify appropriate
 110 boundary conditions of the superconducting sample. We use the following superconductor-
 111 insulator (or vacuum) boundary conditions in the zero-electrostatic potential gauge (see Ap-
 112 pendix A for the detailed derivation) [33–35]

$$\nabla\Psi_i \cdot \mathbf{n} = 0, \quad \mathbf{A} \cdot \mathbf{n} = 0 \quad \text{and} \quad \nabla \times \mathbf{A} = \mathbf{H} \quad (8)$$

113 where \mathbf{n} is the outward unit vector normal to the boundary and the external applied mag-
 114 netic field is set as $\mathbf{H} = H\hat{\mathbf{z}}$. The first two conditions just indicate that any current passing
 115 through the interface between a superconducting domain and vacuum/insulator would be
 116 nonphysical for each band. The third equation represents the continuity of magnetic field
 117 across the boundary. The partial differential equations (3)-(5) will be solved numerically for
 118 the mesoscopic geometry in the two-dimensional space. The initial conditions at $t = 0$ are
 119 taken as $|\Psi_i| = 1$ and $\mathbf{A} = (0, 0)$ on the xy -plane, corresponding to the Meissner state and
 120 zero magnetic field inside the superconductor.

121 3 Finite element method and numerical computations

122 Based on the COMSOL Multiphysics software platform [36], we will describe the procedure
 123 of the numerical simulations on the TDGL equations in this section. We first split the order
 124 parameters into the real and imaginary parts, i.e. $\Psi_1 = u_1 + iu_2$ and $\Psi_2 = u_3 + iu_4$. The mag-
 125 netic potential is also written in component form as $\mathbf{A} = (u_5, u_6)$. In order to implement the
 126 boundary conditions, we will introduce an auxiliary variable $u_7(x, y, t)$ for reasons explained
 127 below. In the procedure of simulations, we set $\Gamma_1 = \Gamma_2 = 5$ and $m_1 = 2m_2$. To stabilize the
 128 semi-Meissner state, we also take $\alpha_{10} = \alpha_{20}$ and $\beta_1 = \beta_2$ in the calculations.

129 In this way, we can transform the TDGL equations into the general form of partial differ-

130 ential equations in this software package

$$\sum_k \mu_{jk} \frac{\partial u_k}{\partial t} + \sum_l \partial_l v_{jl} = \eta_j. \quad (9)$$

131 Here we have $j, k = 1, 2, \dots, 7$, $l = 1, 2$ and $(\partial_1, \partial_2) = (\partial_x, \partial_y)$. The 7×7 matrix μ_{jk} and the
132 7×2 column vector v_{jl} take the form

$$\mu_{jk} = \begin{bmatrix} 5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (10)$$

133 and

$$v_{jl} = \begin{bmatrix} -h(\mathbf{r})u_{1x} & -h(\mathbf{r})u_{1y} \\ -h(\mathbf{r})u_{2x} & -h(\mathbf{r})u_{2y} \\ -2h(\mathbf{r})u_{3x} & -2h(\mathbf{r})u_{3y} \\ -2h(\mathbf{r})u_{4x} & -2h(\mathbf{r})u_{4y} \\ 0 & \kappa_1^2 (u_{6x} - u_{5y} - H) \\ \kappa_1^2 (u_{5y} - u_{6x} + H) & 0 \\ u_5 & u_6 \end{bmatrix}. \quad (11)$$

134 Noting that the subscript x or y denotes the partial derivative with respect to the correspond-
135 ing variable here. Meanwhile, the driving force η_j contains all other terms in the TDGL
136 equations except the left handed side of Eq. (9), and detailed calculations will give all the
137 components explicitly as

$$\eta_1 = [g(\mathbf{r}) - (u_1^2 + u_2^2)] u_1 - h(\mathbf{r}) [(u_5^2 + u_6^2) u_1 - (u_{5x} + u_{6y}) u_2 - 2(u_{2x} u_5 + u_{2y} u_6)], \quad (12)$$

$$\eta_2 = [g(\mathbf{r}) - (u_1^2 + u_2^2)] u_2 - h(\mathbf{r}) [(u_5^2 + u_6^2) u_2 + (u_{5x} + u_{6y}) u_1 + 2(u_{1x} u_5 + u_{1y} u_6)], \quad (13)$$

$$\eta_3 = [g(\mathbf{r}) - (u_3^2 + u_4^2)] u_3 - 2h(\mathbf{r}) [(u_5^2 + u_6^2) u_3 - (u_{5x} + u_{6y}) u_4 - 2(u_{4x} u_5 + u_{4y} u_6)], \quad (14)$$

$$\eta_4 = [g(\mathbf{r}) - (u_3^2 + u_4^2)] u_4 - 2h(\mathbf{r}) [(u_5^2 + u_6^2) u_4 + (u_{5x} + u_{6y}) u_3 + 2(u_{3x} u_5 + u_{3y} u_6)], \quad (15)$$

$$\eta_5 = h(\mathbf{r}) [(u_{2x} u_1 - u_{1x} u_2) + 2(u_{4x} u_3 - u_{3x} u_4) - (u_1^2 + u_2^2 + 2u_3^2 + 2u_4^2) u_5], \quad (16)$$

$$\eta_6 = h(\mathbf{r}) [(u_{2y} u_1 - u_{1y} u_2) + 2(u_{4y} u_3 - u_{3y} u_4) - (u_1^2 + u_2^2 + 2u_3^2 + 2u_4^2) u_6], \quad (17)$$

$$\eta_7 = u_{5x} + u_{6y} + u_7. \quad (18)$$

138

139 Now we can examine the boundary conditions in this formalism. With the normal vector
140 $\mathbf{n} = (n_1, n_2)$ and the column vector v_{jl} , the boundary conditions in Eq. (8) can be simply

141 casted into the compact form as

$$\sum_l n_l v_{jl} = 0 \quad (19)$$

142 which is best suited to the COMSOL Multiphysics simulations. We also note that from the last
143 equation ($j = 7$) in (9), our manipulations will give a trivial solution $u_7 = 0$ for this auxiliary
144 variable and it insures the self-consistency of our problem.

145 COMSOL Multiphysics is a simulation platform based on the finite element method wide-
146 ly employed in solving coupled physical problems in engineering and fundamental research.
147 The software numerically resolves partial differential equations by discretizing the continuous
148 computational domain into a mesh composed of finite elements [37–39]. In two-dimensional
149 geometries, triangular elements are generally adopted due to their adaptability to irregu-
150 lar boundaries and complex shapes. Based on this discretization, a local function space is
151 constructed to approximate the field variables, typically using piecewise polynomial basis
152 functions to maintain the continuity and stability across element interfaces [40]. To handle
153 time-dependent problems with high accuracy and robustness, COMSOL utilizes implicit time-
154 stepping schemes and often incorporates stable integration methods such as the backward
155 Euler formulation. In our numerical calculations, we take the time step $\Delta t = 0.5t_0$ and treat
156 a simulation as converged when the relative variations of the order parameter $|\Psi_1|$ between
157 two sequential steps are smaller than 10^{-8} . We also set the snapshot time at $t = 10^4 t_0$, which
158 will be justified from two perspectives in Appendix B.

159 4 Results and discussions

160 In this section, we will set the external magnetic field $H = 0.8H_0$ and systematically explore
161 the effects of sample boundary and impurities on various vortex excitations. Based on the
162 TDGL theory (3)-(5), we first perform the numerical calculations to obtain the $L - \kappa_1$ and
163 $g - \kappa_1$ phase diagrams in the two-band superconductor. Then, we investigate the effect of
164 anisotropic defect structures and multiple correlated disorders on the patterns of magnetic
165 vortex distributions in the mesoscopic sample.

166 Before the detailed numerical simulations, we would like to briefly discuss the method
167 of determining the critical points of the phase transitions in the two-gap superconducting
168 system. Following Ref. [41], we can identify the phase separation lines in $L - \kappa_1$ and $g - \kappa_1$
169 phase diagrams from the dependence of magnetization M on the GL parameter κ_1 in our
170 investigations. For the type-2 superconductor, at small κ_1 the system will stay at the Meissner
171 phase and give the magnetization $-4\pi M = H - \langle B \rangle \approx 0.8H_0$ due to the perfect diamagnetism,
172 where $\langle B \rangle = \langle u_{6x} - u_{5y} \rangle$ describes the average magnetic induction over the sample area S .
173 While at large κ_1 , the magnetic field penetrates the superconductor to form the Abrikosov
174 vortex lattice and the magnetization will reduce gradually in a broad range of κ_1 . Thus, with
175 the definition of $M' = dM/d\kappa_1$, it will show a discontinuous jump at the critical κ_1 of the
176 phase transition from the perfect diamagnetic state to the vortex lattice state. For the type-
177 1.5 superconductor, at small κ_1 the sample remains in the Meissner state and M is still close
178 to $0.8H_0$. With the increase of κ_1 , the system first enters the vortex cluster phase and the
179 magnetization will decrease linearly in a narrow range of κ_1 exactly as in the case of the
180 intermediate state of type-1 superconductors. As κ_1 is further raised, we will observe the
181 vortex lattice phase, and the decline in M will exhibit a significant deceleration compared to
182 the vortex cluster phase due to the dominance of short-range repulsive intervortex interaction.
183 In this circumstance, M' will display two discontinuous jumps at the critical points of the phase
184 transitions from the perfect diamagnetic state to the vortex cluster state, and ultimately to the
185 vortex lattice state. We note that the identification method discussed above is still applicable

186 to systems with a relatively small number of vortices.

187 4.1 $L - \kappa_1$ phase diagram in the clean limit

188 In this subsection, we first investigate the $L - \kappa_1$ phase diagram of the $L \times L$ two-band super-
 189 conductor in the absence of impurity. As an example, we choose $15\xi_1 \times 15\xi_1$ and $50\xi_1 \times 50\xi_1$
 190 superconducting samples to determine the critical κ_1 in the phase transitions. We then plot the
 191 variations of M and its derivative with κ_1 at $t = 10^4 t_0$ in Fig. 1. From Fig. 1, we can observe
 192 that the $15\xi_1 \times 15\xi_1$ system exhibits the type-2 magnetic behavior. At small κ_1 , the super-
 193 conductor stays at the Meissner phase and the perfect diamagnetism leads to $-4\pi M \approx 0.8H_0$.
 194 While at large κ_1 , the sample enters the vortex lattice phase and M reduces gradually in a
 195 broad range of κ_1 . On the contrary, we can also see from Fig. 1 that the $50\xi_1 \times 50\xi_1$ system
 196 shows the type-1.5 superconducting properties. At small κ_1 , the superconductor remains at
 197 the Meissner state and M is still close to $0.8H_0$. With the increase of κ_1 , the magnetic field
 198 starts to penetrate the sample and the flux lines will exist in the form of the magnetic cluster
 199 due to the long-range attractive interaction between vortices, which induces a linear decrease
 200 of the magnetization in a narrow range of κ_1 . As κ_1 is further raised, the number of vortices
 201 in the system continues to increase and eventually forms the stable Abrikosov flux lattice. In
 202 this circumstance, the rate of increase in vortex density will significantly slow down compared
 203 to the vortex cluster phase due to the dominance of short-range repulsive intervortex interac-
 204 tion. In order to accurately determine the critical points of the phase transitions, we further
 205 calculate the first-order derivative M' as a function of κ_1 in the inset of Fig. 1. It can be
 206 clearly observed that for the $15\xi_1 \times 15\xi_1$ superconductor, M' exhibits a discontinuous jump
 207 at $\kappa_1 = 1.48$, which denotes the transition of the system from the Meissner state to the vortex
 208 lattice state. For the $50\xi_1 \times 50\xi_1$ superconductor, M' shows two discontinuous jumps and the
 209 sample enters the vortex cluster phase at $\kappa_1 = 1.28$, then transfers to the vortex lattice phase
 210 at $\kappa_1 = 1.67$.

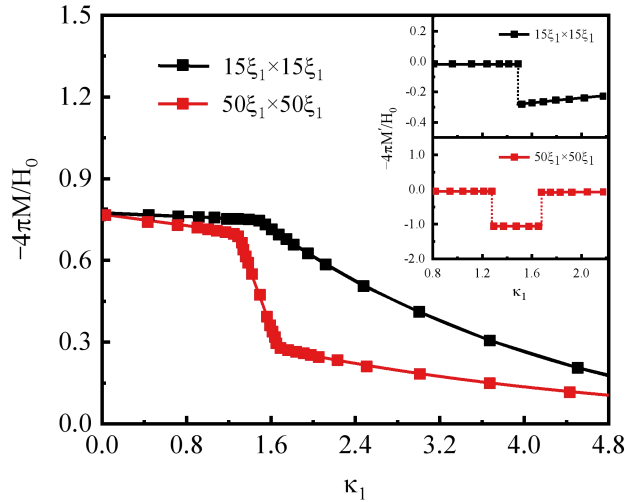


Figure 1: Variations of magnetization M (main) and its first-order derivative M' (inset) with GL parameter κ_1 for the $L \times L$ two-band superconductor in the absence of impurity. We set the external magnetic field $H = 0.8H_0$ in the numerical simulations.

211 With this approach, we can further calculate the critical κ_1 for arbitrary value of L and
 212 obtain the $L - \kappa_1$ phase diagram as shown in Fig. 2. It can be seen from Fig. 2 that with
 213 the decrease of L , the vortex cluster phase produced by the long-range attractive interaction

214 between vortices gradually vanishes. Meanwhile, we also notice the critical sample size L_c for
 215 the disappearance of this cluster state is $32\xi_1$. Thus, the superconducting system will stay in
 216 the type-1.5 regime above L_c and the type-2 regime below L_c in the absence of impurity.

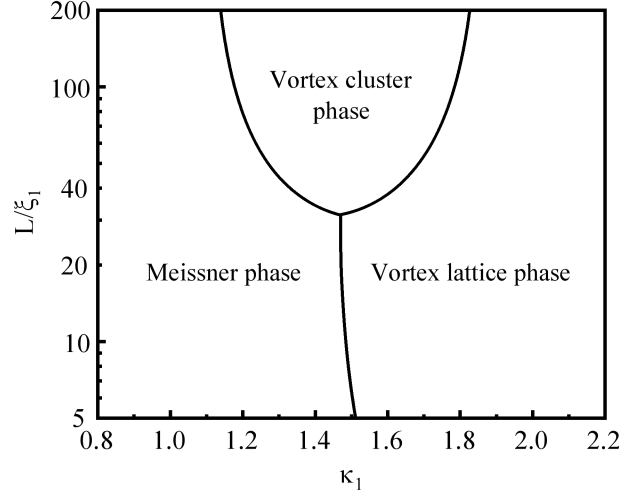


Figure 2: The $L - \kappa_1$ phase diagram of the $L \times L$ two-band superconductor in the absence of impurity. We set the external magnetic field $H = 0.8H_0$ in the numerical simulations, and plot the sample size L on a logarithmic scale.

217 As we know, the type-1.5 superconductor originates from a peculiar vortex interaction that
 218 exhibits short-range repulsion and long-range attraction characteristics. The obtained critical
 219 L_c is consistent with the characteristic length scale (about 30ξ) of the crossover from the
 220 attractive to repulsive intervortex interaction [9]. For the sample size $L > L_c$, the long-range
 221 attractive potential between vortices will dominate at the external magnetic field $H = 0.8H_0$
 222 and the system is allowed to spontaneously form the stable vortex cluster. However for $L < L_c$,
 223 the repulsive intervortex interaction will prevail in the mesoscopic superconductor and the
 224 vortex cluster phase can only be induced by other effects such as impurities.

225 In addition to the superconducting square discussed above, we further examine the tran-
 226 sition behaviors of mesoscopic samples with the aspect ratio different from 1 in the absence of
 227 impurity. As a simple example, we choose the $15\xi_1 \times 20\xi_1$ superconducting sample with each
 228 side length below L_c . We plot the magnetic induction $B = u_{6x} - u_{5y}$ in units of H_0 and the
 229 order parameter of the first condensate $|\Psi_1| = \sqrt{u_1^2 + u_2^2}$ in units of Ψ_{10} at $t = 10^4 t_0$ in Fig. 3.
 230 With the increase of the GL parameter κ_1 , we can see the direct transition of this system from
 231 the perfect diamagnetic state to the Abrikosov lattice phase as shown in Fig. 3. All of these
 232 numerical results thus suggest that the vortex cluster phase will be excluded for arbitrary
 233 mesoscopic sample with the characteristic scale less than L_c in the absence of impurity.

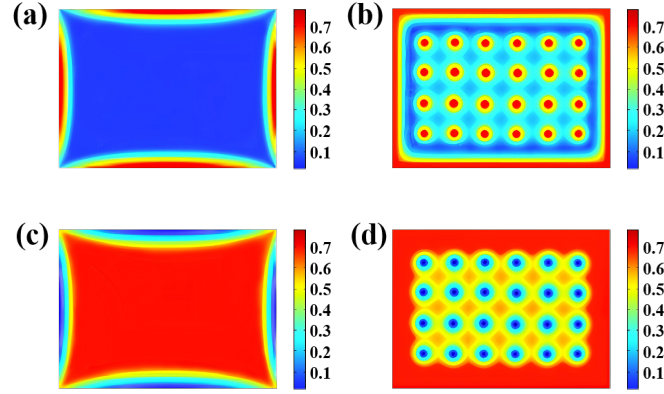


Figure 3: Transition of the magnetic induction B (a,b) and the order parameter of the first condensate $|\Psi_1|$ (c,d) for the $15\xi_1 \times 20\xi_1$ type-2 superconductor. The snapshots show the Meissner phase (a,c) and vortex lattice phase (b,d) at the GL parameter $\kappa_1 = 0.70$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

234 4.2 Effect of an isotropic impurity in the T_c and l disorder models

235 Now, we try to explore the possible generation of the vortex cluster phase in the mesoscopic
 236 superconducting system with $L < L_c$ due to the impurity effect. As an example, we introduce
 237 an isotropic impurity with the radius $0.5\xi_1$ at the center of the $15\xi_1 \times 15\xi_1$ superconducting
 238 sample here. With the T_c disorder model, the defect function $g(\mathbf{r})$ will be characterized by
 239 the disorder strength g inside the impurity and $h(\mathbf{r}) = 1$. We set the value of g as -0.1 and
 240 -0.5 , and then plot the variations of M and its derivative with κ_1 at $t = 10^4 t_0$ in Fig. 4.
 241 From Fig. 4, we can observe that for $g = -0.1$, this mesoscopic system exhibits the type-
 242 2 magnetic behavior. With the transition of the superconductor from the Meissner state to
 243 the vortex lattice state, the magnetization reduces gradually from the perfect diamagnetism
 244 $-4\pi M \approx 0.8H_0$. Meanwhile, we can also see from Fig. 4 that for $g = -0.5$, the sample shows
 245 the type-1.5 superconducting properties. In the process of the transitions from the perfect
 246 diamagnetic state to the vortex cluster state, and ultimately to the vortex lattice state, the
 247 magnetization curve first remains close to $0.8H_0$, then decreases linearly in a narrow range
 248 of κ_1 and finally reduces with a relatively small extent compared to its neighboring phase.
 249 Furthermore, we can clearly observe from the inset of Fig. 4 that for $g = -0.1$, the phase
 250 transition from the Meissner state directly to the vortex lattice state appears at $\kappa_1 = 1.38$. For
 251 $g = -0.5$, the magnetic flux lines in this mesoscopic superconductor condense into the vortex
 252 cluster at $\kappa_1 = 1.08$ and further form the Abrikosov vortex lattice at $\kappa_1 = 1.58$.

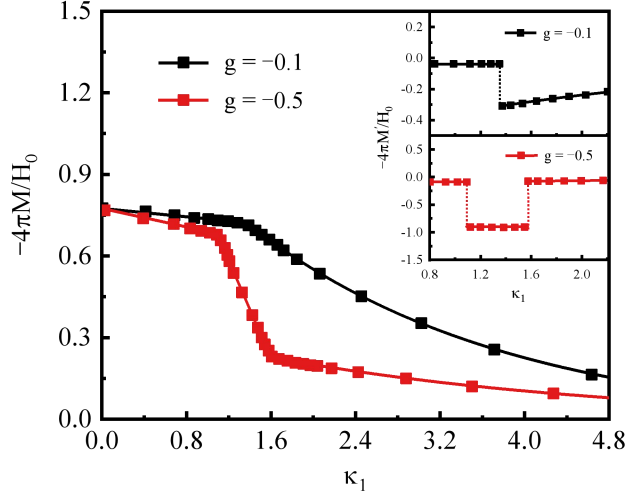


Figure 4: Variations of magnetization M (main) and its first-order derivative M' (inset) with GL parameter κ_1 for the $15\xi_1 \times 15\xi_1$ two-band superconductor in the presence of an isotropic impurity. We set the external magnetic field $H = 0.8H_0$ in the numerical simulations.

253 With this approach, we can calculate the critical κ_1 for arbitrary value of g and obtain the
 254 $g - \kappa_1$ phase diagram as shown in Fig. 5. It can be seen from Fig. 5 that with the increase
 255 of the absolute value of g , the vortex cluster phase induced by the attractive interaction from
 256 the impurity will gradually appear in the system. Meanwhile, we also see that there exists
 257 a critical impurity strength $g_c \approx -0.22$ for the generation of the vortex cluster state in this
 258 sample. Thus, the $15\xi_1 \times 15\xi_1$ mesoscopic superconductor will stay in the type-1.5 regime for
 259 $|g| > |g_c|$ in the presence of an isotropic impurity. Furthermore, it is clearly observed that for
 260 $|g| > |g_c|$, with the increase of $|g|$ the system transfers from the Meissner phase to the vortex
 261 cluster phase at a smaller critical κ_1 , and then enters the vortex lattice phase at a larger κ_1
 262 value.

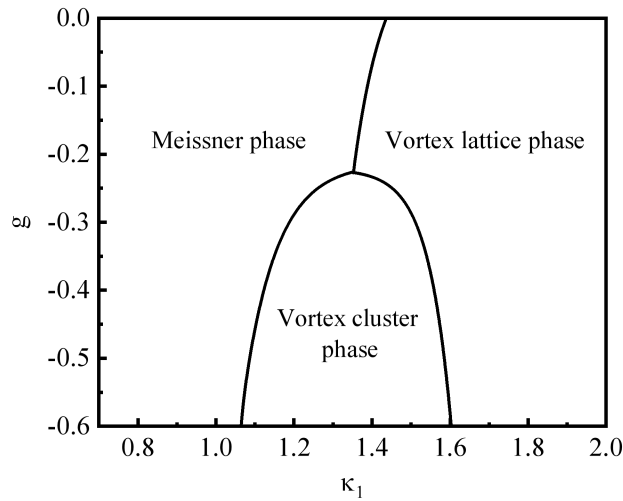


Figure 5: The $g - \kappa_1$ phase diagram of the $15\xi_1 \times 15\xi_1$ two-band superconductor in the presence of an isotropic impurity. We set the external magnetic field $H = 0.8H_0$ in the numerical simulations.

263 At this point, in order to demonstrate the robustness of vortex cluster phase induced by
 264 the localized impurity in the type-1.5 superconductor, we compare the numerical results com-
 265 puted from two types of disorder models, i.e., the T_c disorder model and the l disorder model.
 266 For the T_c disorder model, we choose the impurity function g to take the phenomenological
 267 form [25]

$$g(\mathbf{r}) = \begin{cases} -0.5, & \text{if } |\mathbf{r} - \mathbf{r}_0| < 0.5\xi_1 \\ 1, & \text{otherwise} \end{cases} \quad (20)$$

268 with $|g| > |g_c|$ inside the impurity. It is easy to see that this circular defect is centered at
 269 $\mathbf{r}_0 = (x_0, y_0)$. For simplicity, we insert this pinning site at the center of the $15\xi_1 \times 15\xi_1$
 270 superconducting square. We plot the magnetic induction B and the order parameter of the
 271 first condensate $|\Psi_1|$ at $t = 10^4 t_0$ in Fig. 6. With the GL parameter κ_1 taken as 0.70, 1.30
 272 and 2.10 sequentially, we can clearly observe the transitions of this type-1.5 system from the
 273 perfect diamagnetism state to the vortex cluster phase, and ultimately to the Abrikosov lattice
 274 phase. Our numerical simulations also show that the cluster phase presents the vortex pattern
 275 with octagonal symmetry and appears in the region of $1.08 < \kappa_1 < 1.58$. Moreover, it can be
 276 seen from Fig. 6(c,f) that the isotropic defect induces the localized distortion of the Abrikosov
 277 flux lattice, but will still preserve the C_4 rotational symmetry of the superconducting system.

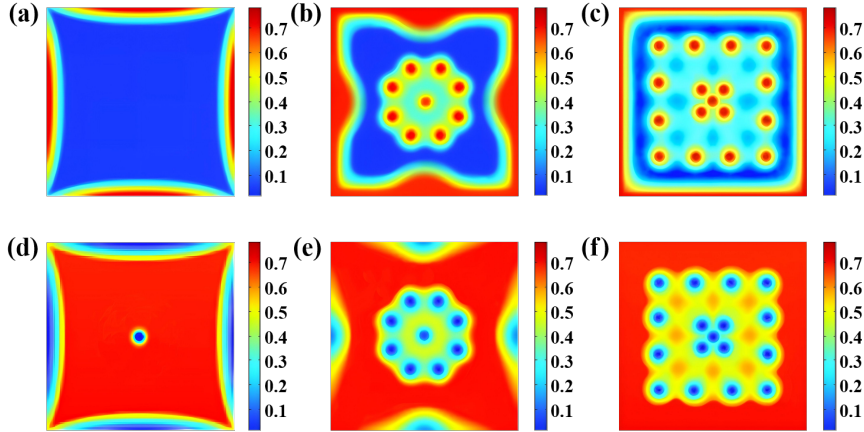


Figure 6: Transitions of the magnetic induction B (a-c) and the order parameter of the first condensate $|\Psi_1|$ (d-f) for the T_c disorder model at the presence of an isotropic defect in the $15\xi_1 \times 15\xi_1$ type-1.5 superconductor. The snapshots show the Meissner phase (a,d), vortex cluster phase (b,e) and vortex lattice phase (c,f) at the GL parameter $\kappa_1 = 0.70, 1.30$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

278 For the l disorder model, we set $g(\mathbf{r}) = 1$ and the impurity function h as [26]

$$h(\mathbf{r}) = \begin{cases} 0.2, & \text{if } |\mathbf{r} - \mathbf{r}_0| < 0.5\xi_1 \\ 1, & \text{otherwise} \end{cases} \quad (21)$$

279 with $h < h_c$ inside the impurity. Here h_c stands for the critical disorder strength for the for-
 280 mation of the vortex cluster state in the l disorder model, which is estimated as 0.6 from our
 281 numerical simulations. Then, we also insert this pinning site at the center of the $15\xi_1 \times 15\xi_1$
 282 mesoscopic sample. The magnetic induction B and the order parameter of the first conden-
 283 sate $|\Psi_1|$ at $t = 10^4 t_0$ are plotted in Fig. 7. For the GL parameter $\kappa_1 = 1.30$ and 2.10 , we

284 can observe a vortex cluster pattern with octagonal symmetry in Fig. 7(b,e) and the locally
 285 distorted flux lattice with C_4 rotational symmetry in Fig. 7(c,f) respectively. For this particu-
 286 lar disorder model, the vortex cluster phase is generated around the pinning site within the
 287 range $1.06 < \kappa_1 < 1.59$. Based on the numerical results mentioned above, we can conclude
 288 that within the framework of the GL theory, the T_c and l disorder models are qualitatively
 289 equivalent in describing the local effect of the impurity on collective vortex distributions for
 290 the type-1.5 superconductor.

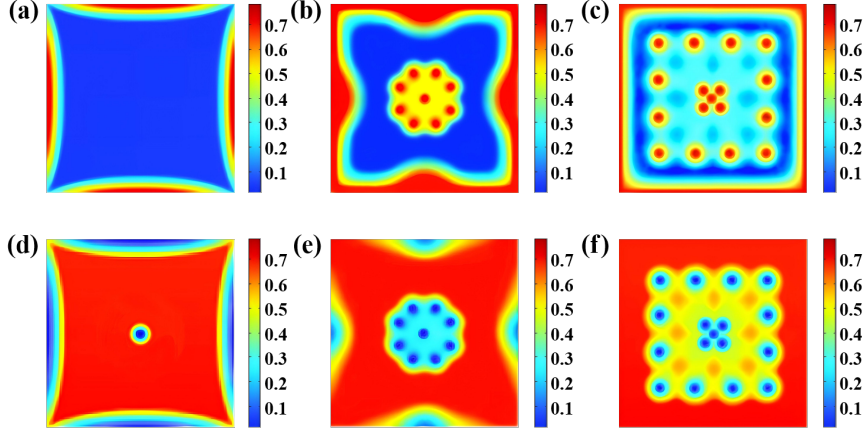


Figure 7: Transitions of the magnetic induction B (a-c) and the order parameter of the first condensate $|\Psi_1|$ (d-f) for the l disorder model at the presence of an isotropic defect in the $15\xi_1 \times 15\xi_1$ type-1.5 superconductor. The snapshots show the Meissner phase (a,d), vortex cluster phase (b,e) and vortex lattice phase (c,f) at the GL parameter $\kappa_1 = 0.70, 1.30$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

291 At the same time, in the type-2 regime, we take the defect strength $g = -0.1$ for the T_c
 292 disorder model and $h = 0.8$ for the l disorder model inside each isotropic impurity. We still
 293 insert this pinning site at the center of the $15\xi_1 \times 15\xi_1$ superconducting square. We plot the
 294 magnetic induction B and the order parameter of the first condensate $|\Psi_1|$ at $t = 10^4 t_0$ in Fig.
 295 8 and Fig. 9. With the GL parameter κ_1 taken as 0.70 and 2.10 sequentially, we can observe
 296 the direct transition of this type-2 system from the perfect diamagnetic state to the Abrikosov
 297 lattice phase in Fig. 8 and Fig. 9. Based on the numerical calculations mentioned above, we
 298 can see that both the T_c and l disorder models give the similar results for the type-2 systems.

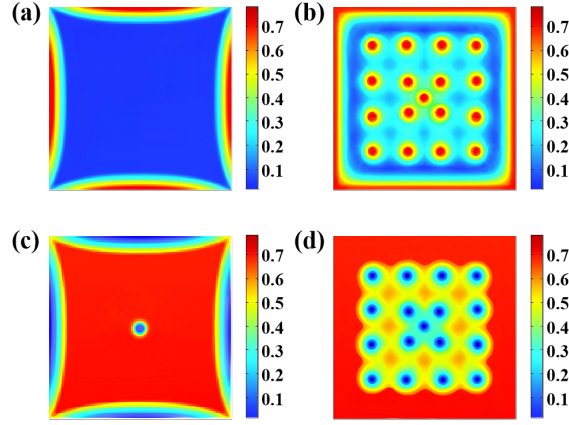


Figure 8: Transition of the magnetic induction B (a,b) and the order parameter of the first condensate $|\Psi_1|$ (c,d) for the T_c disorder model at the presence of an isotropic defect in the $15\xi_1 \times 15\xi_1$ type-2 superconductor. The snapshots show the Meissner phase (a,c) and vortex lattice phase (b,d) at the GL parameter $\kappa_1 = 0.70$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

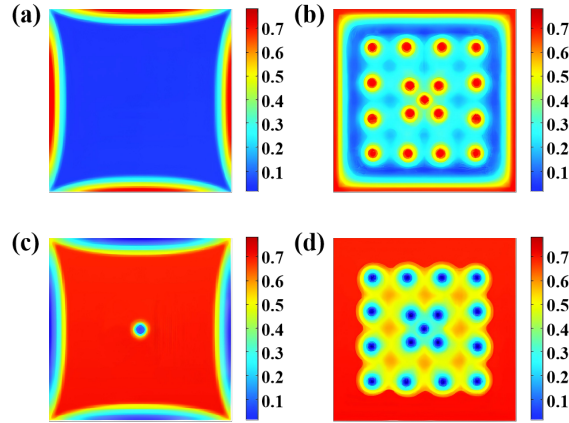


Figure 9: Transition of the magnetic induction B (a,b) and the order parameter of the first condensate $|\Psi_1|$ (c,d) for the l disorder model at the presence of an isotropic defect in the $15\xi_1 \times 15\xi_1$ type-2 superconductor. The snapshots show the Meissner phase (a,c) and vortex lattice phase (b,d) at the GL parameter $\kappa_1 = 0.70$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

299 4.3 Vortex cluster phase in the presence of an anisotropic impurity

300 In addition to the isotropic impurity discussed above, we will investigate the effect of trian-
 301 gular and square defect configurations on the vortex cluster phase in the T_c disorder model.
 302 The triangular or square impurity is with a side length of ξ_1 and placed at the center of the
 303 $15\xi_1 \times 15\xi_1$ mesoscopic superconducting system. We also set the impurity function $g = -0.5$
 304 inside the impurity. Then, we plot the magnetic induction B and the order parameter of the
 305 first condensate $|\Psi_1|$ at $t = 10^4 t_0$ for triangular and square defect configurations in Fig. 10
 306 and Fig. 11 respectively. With the GL parameter κ_1 taken as 0.70 , 1.30 and 2.10 sequentially,
 307 we can clearly observe the transitions of this system from the perfect diamagnetism state to
 308 the vortex cluster phase, and ultimately to the vortex lattice phase. For the triangular (or

309 square) impurity case, the peculiar vortex cluster is generated around the pinning site within
 310 the range $1.15 < \kappa_1 < 1.52$ (or $1.03 < \kappa_1 < 1.62$). It can be seen from Fig. 10(b,e) that the
 311 introduction of triangular defect breaks the C_4 rotational symmetry of the mesoscopic system
 312 and will form a distorted cluster in this circumstance. In contrast, the presence of square im-
 313 purity ensures that the vortex pattern will still preserve the C_4 rotational symmetry, as shown
 314 in Figs. 11(b,e) and 11(c,f).

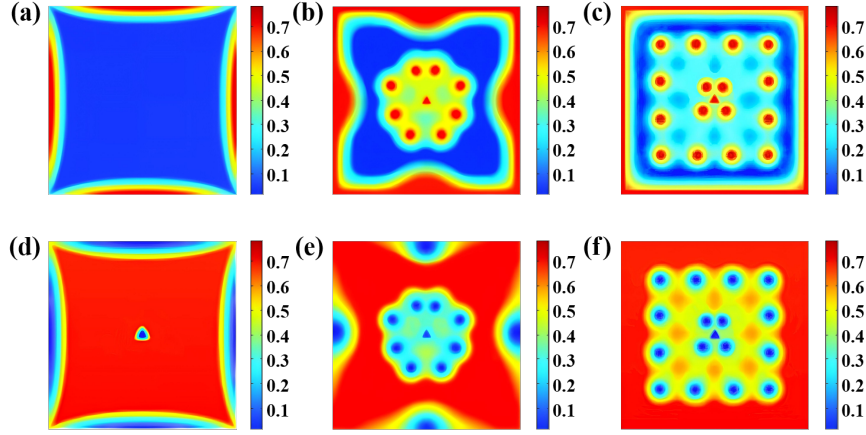


Figure 10: Transitions of the magnetic induction B (a-c) and the order parameter of the first condensate $|\Psi_1|$ (d-f) at the presence of a triangular defect in the $15\xi_1 \times 15\xi_1$ type-1.5 superconductor. The snapshots show the Meissner phase (a,d), vortex cluster phase (b,e) and vortex lattice phase (c,f) at the GL parameter $\kappa_1 = 0.70, 1.30$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

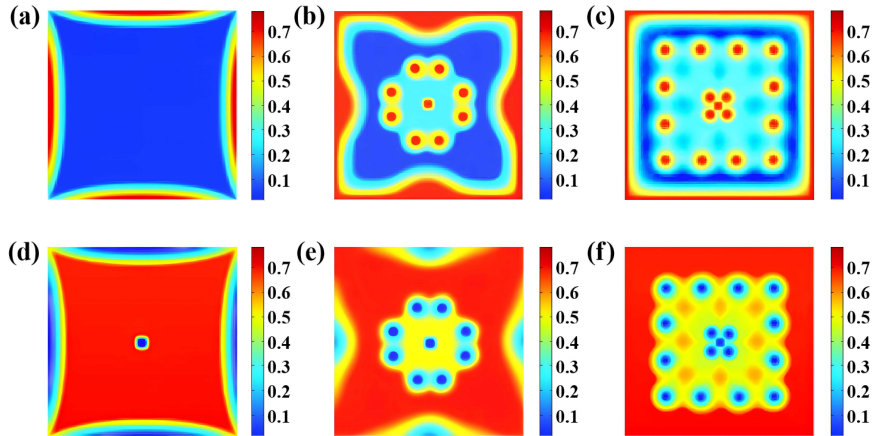


Figure 11: Transitions of the magnetic induction B (a-c) and the order parameter of the first condensate $|\Psi_1|$ (d-f) at the presence of a square defect in the $15\xi_1 \times 15\xi_1$ type-1.5 superconductor. The snapshots show the Meissner phase (a,d), vortex cluster phase (b,e) and vortex lattice phase (c,f) at the GL parameter $\kappa_1 = 0.70, 1.30$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

315 4.4 Uncorrelated and correlated disorder systems

316 In this subsection, we set the disorder strength $|g| > |g_c|$ at the impurity sites in the T_c
 317 disorder model, and discuss the effects of multiple uncorrelated and correlated defects on
 318 vortex cluster patterns in the $15\xi_1 \times 15\xi_1$ mesoscopic superconductor. In the uncorrelated
 319 case, we choose the impurity function $g(\mathbf{r})$ to take the phenomenological form

$$g(\mathbf{r}) = \prod_{n=1}^N g_n(\mathbf{r}) \quad \text{with} \quad g_n(\mathbf{r}) = \begin{cases} -0.5, & \text{if } |\mathbf{r} - \mathbf{r}_{0n}| < 0.5\xi_1 \\ 1, & \text{otherwise} \end{cases}. \quad (22)$$

320 It is easy to see that the isotropic impurity is centered at $\mathbf{r}_{0n} = (x_{0n}, y_{0n})$ with $n = 1, 2, \dots, N$.
 321 For simplicity, we take the impurity number $N = 2$ and select the pinning centers at $(\pm 3\xi_1, 0)$
 322 in $15\xi_1 \times 15\xi_1$ superconducting sample, which ensures the uncorrelation between these two
 323 defects. We plot the magnetic induction B and the order parameter of the first condensate
 324 $|\Psi_1|$ at $t = 10^4 t_0$ in Fig. 12. Different from the single impurity case, multiple vortex clusters
 325 are generated around the pinning sites within $0.87 < \kappa_1 < 1.77$. With the GL parameter
 326 $\kappa_1 = 1.30$, we can see from Fig. 12(b,e) that each vortex cluster exhibits the identical pattern
 327 with hexagonal symmetry. Meanwhile for $\kappa_1 = 2.10$, as shown in Fig. 12(c,f), we can clearly
 328 observe the localized distortions around the pinning positions in the flux lattice due to the
 329 attraction of vortices by impurities.

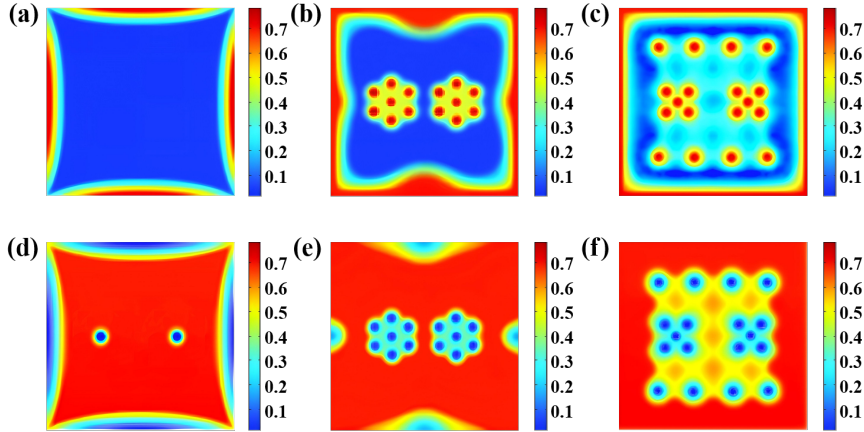


Figure 12: Transitions of the magnetic induction B (a-c) and the order parameter of the first condensate $|\Psi_1|$ (d-f) at the presence of two uncorrelated defects in the $15\xi_1 \times 15\xi_1$ type-1.5 superconductor. The snapshots show the Meissner phase (a,d), vortex cluster phase (b,e) and vortex lattice phase (c,f) at the GL parameter $\kappa_1 = 0.70, 1.30$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

330 In order to take into account the spatial correlation between these impurities, we choose
 331 the following continuous pinning function [42, 43]

$$g(\mathbf{r}) = \prod_{n=1}^N g_n(\mathbf{r}) \quad \text{with} \quad g_n(\mathbf{r}) = \tanh\left(\frac{|\mathbf{r} - \mathbf{r}_{0n}| - R}{R_0}\right). \quad (23)$$

332 We take $R = 0.5\xi_1$ and $R_0 = 1.5\xi_1$ in Eq. (23), and then perform numerical simulations
 333 in the $15\xi_1 \times 15\xi_1$ mesoscopic superconductor. For comparison with the uncorrelated case,
 334 we still choose the defect centers at $(\pm 3\xi_1, 0)$. We plot the magnetic induction B and the

335 order parameter of the first condensate $|\Psi_1|$ at $t = 10^4 t_0$ in Fig. 13. Note that with this new
 336 impurity function, we can obtain the stable vortex cluster phase within $0.92 < \kappa_1 < 1.71$.
 337 For $\kappa_1 = 1.30$, it is shown in Fig. 13(b,e) that two vortex clusters induced by uncorrelated
 338 disorders in Fig. 12(b,e) are fused into a single larger cluster here. Meanwhile with $\kappa_1 = 2.10$,
 339 we can find a vortex lattice pattern with local distortions around the impurities in Fig. 13(c,f).

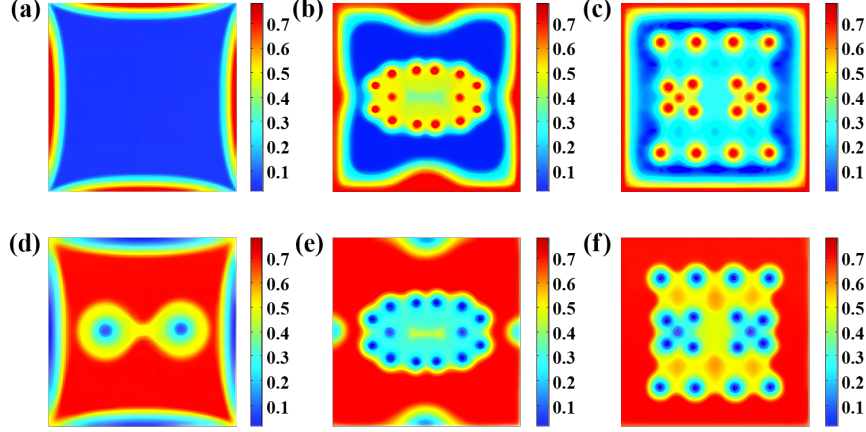


Figure 13: Transitions of the magnetic induction B (a-c) and the order parameter of the first condensate $|\Psi_1|$ (d-f) at the presence of two correlated defects in the $15\xi_1 \times 15\xi_1$ type-1.5 superconductor. The snapshots show the Meissner phase (a,d), vortex cluster phase (b,e) and vortex lattice phase (c,f) at the GL parameter $\kappa_1 = 0.70, 1.30$ and 2.10 respectively. The magnetization only has the component perpendicular to the superconducting plane.

340 5 Conclusion

341 Based on two-band TDGL theory, we explore the impurity effect on the vortex collective be-
 342 haviors in the mesoscopic type-1.5 superconductor. With the finite element method, the in-
 343 vestigations suggest that the vortex cluster phase will be excluded for arbitrary mesoscopic
 344 sample with the characteristic scale less than L_c in the absence of impurity. In the presence
 345 of an isotropic impurity, our numerical results give the direct evidence for the existence of
 346 semi-Meissner state at $|g| > |g_c|$ due to the attractive defect interaction. We also discuss the
 347 effect of anisotropic defect structures and multiple correlated disorders on the possible pat-
 348 terns of magnetic vortex distributions. We hope that our theoretical results will inspire further
 349 research on better understanding novel vortex dynamics and transport properties in two-band
 350 superconductors.

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 356 J.L. and H.H.; investigation, T.H., G.W., J.L. and H.H.; resources, H.H.; data curation, T.H.,
 357 G.W., J.L. and H.H.; writing-original draft preparation, T.H., G.W. and H.H.; writing-review

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 360 manuscript.

361 A Zero electric potential gauge and boundary conditions

362 In this Appendix, we will discuss a particular gauge choice of the boundary conditions and
 363 present a microscopic derivation of the dimensionless boundary condition $(\nabla - i\mathbf{A})\Psi_i \cdot \mathbf{n} = 0$.
 364 Firstly, we try to show that in the zero electric potential gauge, the dimensionless boundary
 365 conditions will take the form

$$\nabla\Psi_i \cdot \mathbf{n} = 0, \quad \mathbf{A} \cdot \mathbf{n} = 0 \quad \text{and} \quad \nabla \times \mathbf{A} = \mathbf{H} \quad (\text{A.1})$$

366 as adopted in Eq. (8).

367 We start from the following gauge invariant boundary conditions between a two-band
 368 superconductor and an insulator (or vacuum)

$$(\nabla - i\mathbf{A})\Psi_i \cdot \mathbf{n} = 0, \quad \left(\frac{\partial \mathbf{A}}{\partial t} + \nabla\varphi \right) \cdot \mathbf{n} = 0 \quad \text{and} \quad \nabla \times \mathbf{A} = \mathbf{H}. \quad (\text{A.2})$$

369 Here φ is defined as the electric potential. Given an arbitrary function χ , the gauge transfor-
 370 mation takes the form as

$$\Psi_i \rightarrow \Psi_i e^{i\chi}, \quad \mathbf{A} \rightarrow \mathbf{A} + \nabla\chi \quad \text{and} \quad \varphi \rightarrow \varphi - \frac{\partial \chi}{\partial t}. \quad (\text{A.3})$$

371 It is easy to show that the boundary conditions in Eq. (A.2) maintain the gauge invariance.
 372 Then with the zero electric potential gauge, we can get from the transformation in Eq. (A.3)

$$\frac{\partial \chi}{\partial t} = \varphi. \quad (\text{A.4})$$

373 Plugging this condition into the second equation of the boundary conditions (A.2), it leads to

$$\frac{\partial \mathbf{A}}{\partial t} \cdot \mathbf{n} = 0 \quad (\text{A.5})$$

374 in this new gauge. This equation can be integrated to give $\mathbf{A} \cdot \mathbf{n} = 0$, which transforms the
 375 boundary condition $(\nabla - i\mathbf{A})\Psi_i \cdot \mathbf{n} = 0$ into the form $\nabla\Psi_i \cdot \mathbf{n} = 0$. Based on the analysis above,
 376 we can see that the boundary conditions in Eq. (A.1) are simply the result of a particular gauge
 377 choice.

378 Secondly, we would like to give a microscopic derivation of the dimensionless boundary
 379 condition $(\nabla - i\mathbf{A})\Psi_i \cdot \mathbf{n} = 0$ which is presented in Eq. (A.2). We try to show that at the
 380 interface of two-band superconductor and insulator (or vacuum), this boundary condition
 381 is applicable not only for the simple $U(1) \times U(1)$ symmetric model studied here but also the
 382 two-component GL models in general. In this process, we will follow the procedure in the
 383 single-band case suggested by de Gennes [44].

384 Based on the work of Zhitomirsky and Dao [45], we write the Hamiltonian of a two-band
 385 superconductor as

$$H = \sum_{i\sigma} c_{i\sigma}^\dagger(\mathbf{r}) \hat{h}(\mathbf{r}) c_{i\sigma}(\mathbf{r}) - \sum_{ii'} g_{ii'} c_{i\uparrow}^\dagger(\mathbf{r}) c_{i\downarrow}^\dagger(\mathbf{r}) c_{i'\downarrow}(\mathbf{r}) c_{i'\uparrow}(\mathbf{r}). \quad (\text{A.6})$$

386 Here, $i, i' = 1, 2$ are the band indices and $\sigma = \uparrow, \downarrow$ is the spin index. $\hat{h}(\mathbf{r})$ is the single par-
 387 ticle Hamiltonian of the normal metal, and $g_{ii'}$ are the effective electron-electron interaction
 388 constants with $g_{12} = g_{21}$.

389 We can introduce the gap functions

$$\Delta_i(\mathbf{r}) = - \sum_{i'} g_{ii'} \langle c_{i'\downarrow}(\mathbf{r}) c_{i'\uparrow}(\mathbf{r}) \rangle \quad (\text{A.7})$$

390 and transform the Hamiltonian into the mean field form

$$H_{\text{eff}} = \sum_{i\sigma} c_{i\sigma}^\dagger(\mathbf{r}) \hat{h}(\mathbf{r}) c_{i\sigma}(\mathbf{r}) + \sum_i \left[\Delta_i(\mathbf{r}) c_{i\uparrow}^\dagger(\mathbf{r}) c_{i\downarrow}^\dagger(\mathbf{r}) + \text{H.c.} \right]. \quad (\text{A.8})$$

391 This effective Hamiltonian can be diagonalized by means of the Bogoliubov transformation
392 with b and b^\dagger the annihilation and creation operators of quasi-particle excitations

$$c_{i\uparrow}(\mathbf{r}) = \sum_{\mathbf{k}} \left[u_{i\mathbf{k}}(\mathbf{r}) b_{i\mathbf{k}\uparrow} - v_{i\mathbf{k}}^*(\mathbf{r}) b_{i\mathbf{k}\downarrow}^\dagger \right] \quad (\text{A.9})$$

393 and

$$c_{i\downarrow}(\mathbf{r}) = \sum_{\mathbf{k}} \left[u_{i\mathbf{k}}(\mathbf{r}) b_{i\mathbf{k}\downarrow} + v_{i\mathbf{k}}^*(\mathbf{r}) b_{i\mathbf{k}\uparrow}^\dagger \right] \quad (\text{A.10})$$

394 where \mathbf{k} is the wave vector. With the anti-commutation relations between the fermion opera-
395 tors and the equation of motion for $c_{i\sigma}(\mathbf{r})$, we can obtain the Bogoliubov-de Gennes equations
396 for a two-band superconductor

$$\begin{pmatrix} \hat{h} & \Delta_i(\mathbf{r}) \\ \Delta_i^*(\mathbf{r}) & -\hat{h}^* \end{pmatrix} \begin{pmatrix} u_{i\mathbf{k}}(\mathbf{r}) \\ v_{i\mathbf{k}}(\mathbf{r}) \end{pmatrix} = E_{i\mathbf{k}} \begin{pmatrix} u_{i\mathbf{k}}(\mathbf{r}) \\ v_{i\mathbf{k}}(\mathbf{r}) \end{pmatrix} \quad (\text{A.11})$$

397 where $E_{i\mathbf{k}}$ is the energy of the excitation. Then with Eq. (A.7), we can transform the self-
398 consistent gap equations into

$$\Delta_i(\mathbf{r}) = \sum_{i'\mathbf{k}} g_{ii'} v_{i'\mathbf{k}}^*(\mathbf{r}) u_{i'\mathbf{k}}(\mathbf{r}) [1 - 2f(E_{i'\mathbf{k}})] \quad (\text{A.12})$$

399 with $f(E_{i\mathbf{k}}) = [1 + \exp(E_{i\mathbf{k}}/k_B T)]^{-1}$ and T the temperature.

400 In the analogy with the single-band case, for small gap functions Δ_i , we can obtain the
401 linearized form of self-consistency conditions from Eqs. (A.11) and (A.12) as

$$\Delta_i(\mathbf{r}) = \sum_{i'} \int K_{ii'}(\mathbf{r}, \mathbf{r}') \Delta_{i'}(\mathbf{r}') d\mathbf{r}' \quad (\text{A.13})$$

402 with the kernel

$$K_{ii'}(\mathbf{r}, \mathbf{r}') = \frac{g_{ii'}}{2} \sum_{\mathbf{k}\mathbf{k}'} \frac{\tanh\left(\frac{\varepsilon_{i'\mathbf{k}}}{2k_B T}\right) + \tanh\left(\frac{\varepsilon_{i'\mathbf{k}'}}{2k_B T}\right)}{\varepsilon_{i'\mathbf{k}} + \varepsilon_{i'\mathbf{k}'}} \Phi_{i'\mathbf{k}}^*(\mathbf{r}') \Phi_{i'\mathbf{k}'}^*(\mathbf{r}') \Phi_{i'\mathbf{k}}(\mathbf{r}) \Phi_{i'\mathbf{k}'}(\mathbf{r}). \quad (\text{A.14})$$

403 Here $\Phi_{i'\mathbf{k}}(\mathbf{r})$ and $\varepsilon_{i'\mathbf{k}}$ are defined as the normal-state eigenfunction and eigenvalue of the
404 electron with $\hat{h}\Phi_{i'\mathbf{k}} = \varepsilon_{i'\mathbf{k}}\Phi_{i'\mathbf{k}}$.

405 We now assume the small spatial variations in the vector potential \mathbf{A} . Then the eigenfunc-
406 tions $\Phi_{i'\mathbf{k}}$ in the normal metal in the presence of \mathbf{A} will differ from the eigenfunctions $w_{i'\mathbf{k}}$ in
407 the absence of \mathbf{A} by only a phase factor, i.e.,

$$\Phi_{i'\mathbf{k}}^*(\mathbf{r}') \Phi_{i'\mathbf{k}}(\mathbf{r}) \rightarrow w_{i'\mathbf{k}}^*(\mathbf{r}') w_{i'\mathbf{k}}(\mathbf{r}) \exp \left[\frac{i}{2} \mathbf{A} \cdot (\mathbf{r} - \mathbf{r}') \right]. \quad (\text{A.15})$$

408 Plugging into Eq. (A.13), it will lead to

$$\Delta_i(\mathbf{r}) = \sum_{i'} \int \bar{K}_{ii'}(\mathbf{r}, \mathbf{r}') \Delta_{i'}(\mathbf{r}') \exp [i\mathbf{A} \cdot (\mathbf{r} - \mathbf{r}')] d\mathbf{r}' \quad (\text{A.16})$$

409 with the kernel in the absence of external magnetic field

$$\bar{K}_{ii'}(\mathbf{r}, \mathbf{r}') = \frac{g_{ii'}}{2} \sum_{kk'} \frac{\tanh\left(\frac{\varepsilon_{i'k}}{2k_B T}\right) + \tanh\left(\frac{\varepsilon_{i'k'}}{2k_B T}\right)}{\varepsilon_{i'k} + \varepsilon_{i'k'}} w_{i'k}^*(\mathbf{r}') w_{i'k'}^*(\mathbf{r}') w_{i'k}(\mathbf{r}) w_{i'k'}(\mathbf{r}). \quad (\text{A.17})$$

410 Thus from Eq. (A.16), we can write

$$\Delta_i(\mathbf{r}) = \bar{\Delta}_i(\mathbf{r}) \exp(i\mathbf{A} \cdot \mathbf{r}) \quad (\text{A.18})$$

411 with $\bar{\Delta}_i(\mathbf{r})$ the superconducting gap function in the absence of \mathbf{A} . Then we have

$$\bar{\Delta}_i(\mathbf{r}) = \sum_{i'} \int \bar{K}_{ii'}(\mathbf{r}, \mathbf{r}') \bar{\Delta}_{i'}(\mathbf{r}') d\mathbf{r}'. \quad (\text{A.19})$$

412 Now, we can examine the behavior of the superconducting gap functions near the
413 superconductor-insulator interface. Following the procedure pioneered by de Gennes, we
414 suppose that the gap functions close to the surface behaves as

$$\bar{\Delta}_i(s) = \bar{\Delta}_{i0} + \left(\sum_{i'} \frac{\xi_1}{b_{ii'}} \bar{\Delta}_{i'0} \right) s. \quad (\text{A.20})$$

415 Here s measures the normal distance from the boundary in units of ξ_1 and $s > 0$ is defined
416 in the superconductor. For simplicity, we set the cross section of the boundary as 1. $\bar{\Delta}_{i0}$ rep-
417 represents the gap function at the boundary and $b_{ii'}$ denotes the intraband or interband surface
418 extrapolation length for the two-band superconductor. From Eq. (A.20), we can establish the
419 boundary condition between the two-band superconductor and the insulator (or vacuum) at
420 $s = 0$

$$\frac{d\bar{\Delta}_i}{ds} = \sum_{i'} \frac{\xi_1}{b_{ii'}} \bar{\Delta}_{i'} \quad (\text{A.21})$$

421 in the absence of external magnetic field.

422 Meanwhile, with the explicit expressions of the kernels in the bulk system and the addition
423 of nonlinear terms to the gap equations, we can obtain the two-band GL equations from Eq.
424 (A.19) as [45]

$$-\alpha_1 \bar{\Delta}_1 + \beta_1 |\bar{\Delta}_1|^2 \bar{\Delta}_1 - \gamma_1 \nabla^2 \bar{\Delta}_1 - R_{12} \bar{\Delta}_2 = 0 \quad (\text{A.22})$$

425 and

$$-\alpha_2 \bar{\Delta}_2 + \beta_2 |\bar{\Delta}_2|^2 \bar{\Delta}_2 - \gamma_2 \nabla^2 \bar{\Delta}_2 - R_{12} \bar{\Delta}_1 = 0, \quad (\text{A.23})$$

426 with the GL parameters

$$\alpha_{1,2} = N_{1,2} \left[\frac{1}{\lambda_{\max}} - \frac{\lambda_{22,11}}{\lambda} + \ln\left(\frac{T_{c0}}{T}\right) \right], \quad \beta_i = \frac{7 \zeta(3) N_i}{16 \pi^2 (k_B T_{c0})^2}, \quad (\text{A.24})$$

$$\gamma_i = \frac{7 \zeta(3) \hbar^2 N_i v_{Fi}^2}{16 \pi^2 (k_B T_{c0})^2} \quad \text{and} \quad R_{12} = \frac{N_1 \lambda_{12}}{\lambda} = \frac{N_2 \lambda_{21}}{\lambda}.$$

427 Here $\lambda_{ii'} = g_{ii'} N_{i'}$ with $N_{i'}$ the density of states at the Fermi level for each band,
428 $\lambda = \lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21}$ and $\lambda_{\max} = \frac{1}{2} \left[(\lambda_{11} + \lambda_{22}) + \sqrt{(\lambda_{11} - \lambda_{22})^2 + 4 \lambda_{12} \lambda_{21}} \right]$ the largest
429 eigenvalue of λ -matrix. T_{c0} is the bulk critical temperature and v_{Fi} is the average Fermi
430 velocity for each band.

431 In the spatially homogeneous case, we can neglect the gradient γ -terms. Eqs. (A.22) and
 432 (A.23) yield the gap equation at $T = T_{c0}$

$$\begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix} \begin{pmatrix} \bar{\Delta}_1 \\ \bar{\Delta}_2 \end{pmatrix} = \lambda_{\max} \begin{pmatrix} \bar{\Delta}_1 \\ \bar{\Delta}_2 \end{pmatrix}, \quad (\text{A.25})$$

433 which obviously gives the consistent result.

434 Now, we try to determine the coefficients $b_{ii'}$ in Eq. (A.21) by solving the linearized gap
 435 equation (A.19) in absence of external magnetic field. If we introduce $\bar{K}_{ii'}^0(s, s')$ as the kernel
 436 of gap functions in the superconducting bulk system, we can transform Eq. (A.19) into

$$\bar{\Delta}_i(s) - \sum_{i'} \int \bar{K}_{ii'}^0(s, s') \bar{\Delta}_{i'}(s') ds' = - \sum_{i'} \int [\bar{K}_{ii'}^0(s, s') - \bar{K}_{ii'}(s, s')] \bar{\Delta}_{i'}(s') ds' \equiv - \sum_{i'} H_{ii'}(s). \quad (\text{A.26})$$

437

438 From Eqs. (A.22) and (A.23) with the higher order β -terms omitted, also noting that
 439 $\bar{K}_{ii'}^0(s, s') = \bar{K}_{ii'}^0(s - s')$ due to the translational symmetry, we can read out the Laplace trans-
 440 formation of $\bar{K}_{ii'}^0$ as

$$\bar{K}_{ii'}^0(p) = \frac{\lambda_{ii'}}{\lambda_{\max}} + \frac{\lambda_{ii'} \gamma_{i'}}{N_{i'} \xi_1^2} p^2. \quad (\text{A.27})$$

441 Plugging Eq. (A.27) into (A.26), we can get

$$\bar{\Delta}_i(p) - \sum_{i'} \left(\frac{\lambda_{ii'}}{\lambda_{\max}} \right) \bar{\Delta}_{i'}(p) - \sum_{i'} \left(\frac{\lambda_{ii'} \gamma_{i'}}{N_{i'} \xi_1^2} \right) p^2 \bar{\Delta}_{i'}(p) = - \sum_{i'} H_{ii'}(p). \quad (\text{A.28})$$

442 Here $\bar{\Delta}_i(p)$ and $H_{ii'}(p)$ are the Laplace transformations of $\bar{\Delta}_i(s)$ and $H_{ii'}(s)$ respectively. Since
 443 the first two terms of the left-handed side in Eq. (A.28) can be cancelled out according to Eq.
 444 (A.25), we then have

$$\sum_{i'} \left(\frac{\lambda_{ii'} \gamma_{i'}}{N_{i'} \xi_1^2} \right) p^2 \bar{\Delta}_{i'}(p) = \sum_{i'} H_{ii'}(p). \quad (\text{A.29})$$

445 We can see that both sides in Eq. (A.29) take the main contribution from the boundary region.

446 Notice that the Laplace transformation of the gap function in Eq. (A.20) takes the form

$$\bar{\Delta}_i(p) = \frac{\bar{\Delta}_{i0}}{p} + \sum_{i'} \frac{\xi_1 \bar{\Delta}_{i'0}}{b_{ii'} p^2}. \quad (\text{A.30})$$

447 Then at $p \rightarrow 0$, we will obtain from Eq. (A.29)

$$\sum_{i' i''} \left(\frac{\lambda_{ii'} \gamma_{i'}}{N_{i'} \xi_1 b_{ii''}} \right) \bar{\Delta}_{i''0} = \sum_{i'} H_{ii'}(p=0). \quad (\text{A.31})$$

448 Parallel to de Gennes' analysis, we have the sum rules

$$\int \bar{K}_{ii'}^0(s, s') ds' = \frac{\lambda_{ii'}}{\lambda_{\max}} \quad \text{and} \quad \int \bar{K}_{ii'}(s, s') ds' = \frac{\lambda_{ii'} N_{i'}(s)}{\lambda_{\max} N_{i'}} \quad (\text{A.32})$$

449 with $N_{i'}(s)$ the local density of states at the Fermi surface. Then, we can write the Laplace
 450 transformation of the kernel difference at $p \rightarrow 0$

$$H_{ii'}(p=0) = \int H_{ii'}(s) ds = \frac{\lambda_{ii'} \bar{\Delta}_{i'0}}{\lambda_{\max}} \int \frac{\bar{\Delta}_{i'}(s)}{\bar{\Delta}_{i'0}} \left[1 - \frac{N_{i'}(s)}{N_{i'}} \right] ds. \quad (\text{A.33})$$

451 Now we suppose $\bar{\Delta}_{i'}(s)/\bar{\Delta}_{i'0}$ approaches zero in the insulating region and is of the order of 1
 452 in the metallic region. $N_{i'}(s)/N_{i'}$ also passes from $0 \rightarrow 1$ in a few interatomic distances from
 453 the boundary. Therefore, the integrand in Eq. (A.33) is nonvanishing only in a width of order
 454 of the lattice constant a . We can then estimate $H_{ii'}(p=0)$ as

$$H_{ii'}(p=0) = \frac{\lambda_{ii'} a}{\lambda_{\max} \xi_1} \bar{\Delta}_{i'0}. \quad (\text{A.34})$$

455 Comparing Eq. (A.31) with Eq. (A.34), we can finally obtain

$$\frac{1}{b_{ii}} = \frac{N_i a}{\gamma_i \lambda_{\max}} \quad \text{and} \quad \frac{1}{b_{12}} = \frac{1}{b_{21}} = 0. \quad (\text{A.35})$$

456 At this stage, we would like to point out that $1/b_{ii'} = 0$ ($i \neq i'$) is only an approxima-
 457 tion and will become nonzero in the higher-order calculation. Even for a contact between
 458 a superconductor and an insulator, the Cooper pairs can still diffuse into the insulating re-
 459 gion with some probability. Algebraically, this means that the gap function $\bar{\Delta}_{i'}(s)$ will al-
 460 so extend into the $s < 0$ region, and we can roughly estimate $\bar{\Delta}_{i'}(s) \sim \sum_{i''} T_{i'i''} \bar{\Delta}_{i''0} e^{\xi_1 s/a}$
 461 ($s < 0$) with $T_{i'i''}$ the element of the transmission matrix at the boundary. Including the $s < 0$
 462 part in the integration of Eq. (A.33) and noting $N_{i'}(s)/N_{i'} \approx 0$ in this region, we can get
 463 $H_{ii'}(p=0) = (\lambda_{ii'} a / \lambda_{\max} \xi_1) (\bar{\Delta}_{i'0} + \sum_{i''} T_{i'i''} \bar{\Delta}_{i''0})$. Plugging into Eq. (A.31), the coefficients
 464 of boundary terms are given by

$$\frac{1}{b_{ii}} = \frac{N_i a}{\gamma_i \lambda_{\max}} (1 + T_{ii}), \quad \frac{1}{b_{12}} = \frac{N_1 a}{\gamma_1 \lambda_{\max}} T_{12} \quad \text{and} \quad \frac{1}{b_{21}} = \frac{N_2 a}{\gamma_2 \lambda_{\max}} T_{21}. \quad (\text{A.36})$$

465 With the transmission coefficient from the superconductor to the insulator $T_{ii'} \ll 1$, we can
 466 obviously see that Eq. (A.35) is a good approximation.

467 For a typical two-band superconductor, we can estimate $\gamma_i \lambda_{\max} / N_i \sim \xi_1^2$ with $\xi_1 \sim 10^{-4}$ cm
 468 and the lattice constant $a \sim 10^{-8}$ cm, which will give $b_{ii} \sim 1$ cm. Therefore for a bound-
 469 ary separating a two-band superconductor from an insulator we can set $\xi_1 / b_{ii'} \approx 0$. This
 470 leads to the boundary condition $d\bar{\Delta}_i/ds = 0$ from Eq. (A.21). For an arbitrary supercon-
 471 ducting domain and in the presence of the magnetic field, we can generalize this result to
 472 $(\nabla - i\mathbf{A}) \Delta_i \cdot \mathbf{n} = 0$ according to Eq. (A.18). With the phenomenological superconducting or-
 473 der parameter $\Psi_i \propto \Delta_i$, we can finally write down the boundary condition $(\nabla - i\mathbf{A}) \Psi_i \cdot \mathbf{n} = 0$
 474 for the interface of two-band superconductor and insulator.

475 B Discussion on convergence and relaxation time in numerical 476 simulations

477 In this Appendix, we would like to justify the choice of the snapshot time at $t = 10^4 t_0$
 478 in our numerical simulations from two perspectives. On one hand, we take the time step
 479 $\Delta t = 0.5 t_0$ in our numerical calculations and treat a simulation as converged when the rel-
 480 ative variation of the order parameter $|\Psi_1|$ between two sequential steps is smaller than
 481 10^{-8} . Our computational results indicate that for the $15\xi_1 \times 15\xi_1$ superconducting system-
 482 s with different defect configurations, the system will consistently reach the convergence
 483 before the snapshot time $10^4 t_0$. On the other hand, we can define an average velocity
 484 $\bar{v} = \sum_{\delta=1}^W |\mathbf{r}_\delta(t + \Delta t) - \mathbf{r}_\delta(t)| / (W \Delta t)$ for the vortices in the system, where $\mathbf{r}_\delta = (x_\delta, y_\delta)$
 485 with $\delta = 1, 2, \dots, W$ stands for the instantaneous position of each vortex core. As an exam-
 486 ple, we discuss the $15\xi_1 \times 15\xi_1$ mesoscopic sample in the presence of an isotropic impurity
 487 with the disorder strength $g = -0.5$ here. In the procedure of simulations, we notice that

488 the vortex number in the sample will no longer change beyond $t \approx 10^3 t_0$. We then plot the
 489 variations of \bar{v} with t for the vortex cluster state and the vortex lattice phase in Fig. 14. It
 490 can be seen from Fig. 14 that the \bar{v} evolves with t and eventually stabilizes at $t < 10^4 t_0$.
 491 Therefore, it is justified for us to take the snapshots at $t = 10^4 t_0$ to present the stable vortex
 492 dynamics.

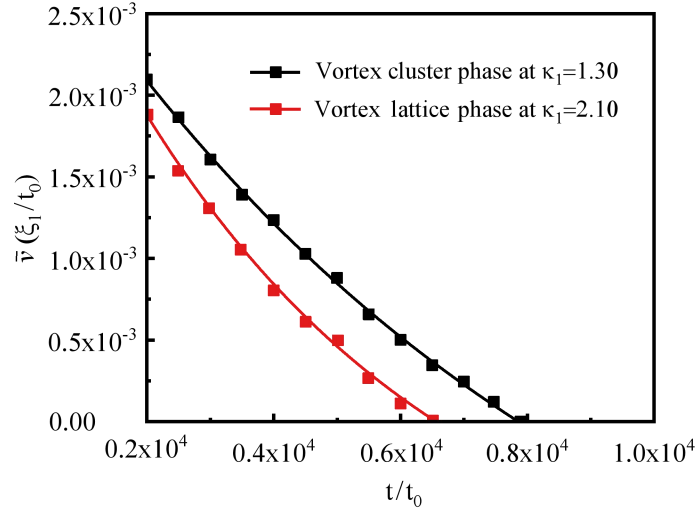


Figure 14: Variations of the average velocity \bar{v} with time t at the presence of an isotropic defect with the radius $0.5\xi_1$ in the $15\xi_1 \times 15\xi_1$ type-1.5 superconductor. We set the external magnetic field $H = 0.8H_0$ in the numerical simulations.

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