Vortex States and Phase Diagram of Multi-component Ginzburg-Landau Theory with Competing Repulsive and Attractive Vortex Interactions

Shi-Zeng Lin and Xiao Hu

WPI Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba 305-0044, Japan

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We investigate the behavior of vortices of multi-component superconductivity, realized in MgB$_2$ and Fe-based superconductors, within the framework of Ginzburg-Landau (GL) theory in terms of numerical calculations of the time-dependent GL equations and the variational method. It is revealed that close to the critical point of the composite system the inter-component coupling makes the system behave as a single component superconductivity in most cases. However, when the bare mean-field critical points of the two components coincide with each other, and furthermore the inter-band coupling disappears at the same temperature, interesting phenomena occur as follows. Vortices interact attractively at large separation and repulsively at short distance in certain parameter space. Because of the non-monotonic interaction profile, phase separations between vortex clusters of triangular order and the Meissner state take place, which indicates a first-order phase transition associated with the penetration of the magnetic field into a superconductor sample. Phase diagrams of vortex states are then constructed with the associated magnetization curve. It is found that all these behavior interpolates the features of the type I and II superconductors.

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I. INTRODUCTION

A quantized vortex is a topological excitation of superfluidity and superconductivity as the hallmark of a single wave function for the macroscopic quantum state. Revealed first by Abrikosov based on the celebrated Ginzburg-Landau (GL) theory, a vortex in superconductor carries a normal core with size of the order of superconducting coherence length $\xi$, and a quantized magnetic flux distributed over the London penetration depth $\lambda$; in superconductors categorized as type II with $\kappa = \lambda/\xi > 1/\sqrt{2}$, as opposed to type I with $\kappa < 1/\sqrt{2}$, vortices repel each other because of the circular supercurrents and thus form a triangular vortex lattice. In type I superconductors, vortices would attract each other in order to gain the superconducting condensation energy, and thus collapse into a continuum of normal region at equilibrium. The recently discovered multi-band superconductors, such as MgB$_2$[1] and iron pnictide superconductors[2], can exhibit novel phenomena[3–9] (see Ref.[10] for a review), without counterpart in single-band superconductors. It was first proposed theoretically by Babaev and Speight[11][12] that, when the London penetration depth falls in between the two coherence lengths, vortices may attract at large separation and repel at short distance because of the competition of different length scales in different condensates. It was then discussed by Moshchalkov et al. that this situation was realized in their sample of MgB$_2$, as manifested by the unconventional stripe and gossamer-like vortex patterns[13]. They coined the term of type 1.5 superconductor for the class of multi-band superconductors.

While this scenario is intriguing and has attracted considerable interests[14–16], there are several points waiting for further investigation. In the theoretical side, one notices that the original proposal was based on weak inter-component coupling limit, and the discussions were implicitly extended to low-temperature regime. In doing so, one should always keep in mind that GL theory works only close to the critical point of the composite system, at least in principle. Any result appearing only away from the critical point needs a careful and independent check. In the experimental side, the observed inter-vortex separation $\sim 2\mu m$ is much larger than the distance associated with the possible energy minimum estimated by the theory[11], lacking a consistent understanding. The random vortex configurations reported in Refs.[13][17] seem incompatible with common experiences in material science: particles governed by the Lennard-Jones interactions form solids with regular orders, and thus those random patterns are hard to be considered as a property of equilibrium at usual conditions in absence of random pins.

In the present work, we reveal first a case that the bare mean-field critical points of the two components coincide with each other, and furthermore the inter-band coupling disappears at the same temperature. We introduce two vortices into a square superconductor by setting appropriate boundary condition, and find with the approach of time-dependent GL (TDGL) that, for appropriate parameters in the GL free energy functional, the two vortices are separated by a distance associated with an energy minimum, which does not change with the system size for simulations. This verifies the attraction between vortices at large distance and repulsion at short distance. The vortices are found stable against thermal fluctuations. We evaluate the full dependence of interaction potential on vortex separation by the variational method. Distribution of vortices are then simulated based on the Langevin dynamics. Instead of uniform vortex lattice in type II superconductors as well as the lamella structure in type I superconductors, we observe phase separations among clusters of irregularly ordered vortices and Meissner regions, which indicates a first-order phase transition associated with penetration of vortices into the system upon increase of external magnetic field. Based on these observations we construct the phase diagram for superconductors with the novel vortex interaction.

We also investigate the vortex interaction when two components have different bare critical points and a finite inter-band interactions.
coupling. Close to the critical point of the composite system, the superconductivity in different components is strongly correlated and only one divergent length associated with the variation of order parameters at the vortex core exists. Thus vortices are purely repulsive or attractive close to the critical point.

It is noticed that novel vortex attractions were discussed 40 years ago in single-band superconductors, which caused phase separation between Meissner phase and vortex lattice, and discontinuous jumps in magnetization, especially at low temperature (see Ref. [18] for review). These superconductors are characterized by small GL numbers, and the attractive vortex interactions were attributed to correction to the GL approximation from the BCS theory [19] [20], which is different from the system discussed by [11] [12] and addressed in the present work.

The remaining part of the paper is organized as follows. In Sec. II, we present the free energy functional and the structure of a vortex. In Sec. III, we present the results obtained by numerical simulations of TDGL. In Sec. IV, the interaction of a vortex. In Sec. III, we present the results obtained by numerical simulations of TDGL. In Sec. V, the vortex configuration is simulated based on the Langevin dynamics. Sec. VI is devoted discussions, and the paper is concluded by Sec. VII.

II. MODEL

The GL free energy functional with interband scattering is given by

\[ F = \sum_{i=1,2} \left[ \frac{\alpha_i}{|\alpha_i|} |\Psi_i|^2 + \frac{\beta_i}{2m_i} |\Psi_i|^4 + \frac{1}{2m_i} \left( \frac{\hbar^2}{\epsilon^2} \right) \Psi_i^2 \right] + \frac{1}{\xi^2} (\nabla \times A)^2 - \gamma (\Psi_i^\dagger \Psi_2 + \Psi_2^\dagger \Psi_1), \]

with all symbols conventionally defined [21]. Here we focus on the Josephson-like inter-band coupling with strength \( \gamma \), noticing that the main results remain qualitatively the same even including other possible interactions. For MgB\(_2\) \( \gamma > 0 \), while for iron-based superconductors, \( \gamma \) is presumably negative [22]. The temperature dependence of the quadratic terms are \( \alpha_i(T) = \alpha_i(0)(1 - T/T_c) \) with \( \alpha_i(0) < 0 \), and \( \gamma(T) = \gamma(0)(1 - T/T_c) \). We notice that in this case the physics is the same for the whole temperature regime starting from \( T_c \) except a renormalization of length. We leave the discussion on more general cases to Sec. VI.

For convenience, we define the following lengths \( \lambda_i = \sqrt{m_i c^2 \beta_i / 8\pi|\alpha_i| \epsilon^2} \) and \( \xi_i = \sqrt{\epsilon^2 / 2m_i|\alpha_i|} \), the penetration depth and coherence lengths in the respective single-band condensates (\( \gamma = 0 \)). For the present interest, we adopt the coefficients in the GL free energy functional Eq. (1) such that at \( T = 0 \), \( \xi_1 = 51\text{nm}, \lambda_1 = 25\text{nm}, \xi_2 = 8\text{nm}, \) and \( \lambda_2 = 30\text{nm} \) at very low temperatures. The inter-band coupling is \( \gamma(0) = -0.4\alpha_1(0) \).

We introduce the dimensionless quantities for convenience,

\[ x = \lambda_1 x', \quad \Psi_i = \Psi_{10} \Psi_i', \quad A = \lambda_1 H_{1c} \sqrt{2} \Psi_i', \quad F = \frac{m_i}{4\pi} F', \]

\[ \gamma = \gamma' |\alpha_1|, \quad B = H_{1c} \sqrt{2} B', \quad J = \frac{2\pi \Psi_{10}^2 \xi_1^2}{m e} J', \]

where \( \Psi_{10}^2 = |\alpha_1|/|\beta_1| \) is the bulk field, \( H_{1c} = \sqrt{4\pi |\alpha_1| \Psi_{10}^2} \) the thermodynamic critical field of the first condensate. \( B \) is the magnetic induction and \( J \) is the supercurrent.

For clarity, we drop the prime in the dimensionless quantities in the following calculations. Then we have the free energy in the dimensionless units

\[ F = \sum_{i=1,2} \left[ \frac{a_i}{|a_i|} |\Psi_i|^2 + \frac{b_i}{2m_i} |\Psi_i|^4 + \frac{1}{m_i} \left( \frac{1}{\xi_i} \nabla - \frac{A}{\xi_i} \right) \Psi_i^2 \right] + (\nabla \times A)^2 - \gamma (\Psi_1^\dagger \Psi_2 + \Psi_2^\dagger \Psi_1), \]

where \( \kappa_1 = \lambda_1/\xi_1 \) is the GL parameter.

Minimizing \( F \) with respect to \( \Psi_i \) and \( A \), we obtain the GL equations

\[ -\Psi_1 + |\Psi_1|^2 \Psi_1 + \left( \frac{1}{i \xi_1} \nabla - \frac{A}{\xi_1} \right) \Psi_1 - \gamma \Psi_2 = 0, \]

\[ -\frac{a_1^2}{a_1} \Psi_2 + \frac{b_2}{\beta_1} |\Psi_2|^2 \Psi_2 + \frac{m_1}{m_2} \left( \frac{1}{i \xi_2} \nabla - \frac{A}{\xi_2} \right) \Psi_2 - \gamma \Psi_1 = 0, \]

\[ \nabla \times \nabla \times A = \frac{1}{\xi_1} (\Psi_1 \nabla \Psi_1 - \Psi_1 \nabla \Psi_1^\dagger) - |\Psi_2|^2 A + \frac{m_i}{m_2} \left( \frac{1}{i \xi_2} \nabla \Psi_2 \nabla \Psi_2 - \Psi_2 \nabla \Psi_2^\dagger - |\Psi_1|^2 A \right) \]

Equation (6) describes the screening of the magnetic field by the superconducting condensates. Using the London approximation, the effective London penetration depth for two-band superconductors is

\[ \lambda = 1/\sqrt{|\Psi_{10}|^2 + |\Psi_{20}|^2}, \]

where \( \Psi_{10} \) is the bulk value of the \( i \)th superconducting condensate. The response of two-band superconductors to magnetic fields is described by a single length scale \( \lambda \), because both condensates couple to the same gauge field. For \( \gamma = 0 \), we have \( \Psi_{10} = 1 \) and \( \Psi_{20} = \sqrt{\alpha_2 \beta_1 / \alpha_1 \beta_2} \). The interband coupling shifts the bulk value and thus modifies the corresponding penetration depth.

Next we construct a vortex solution to Eqs. (3), (5) and (6). It is observed that the two condensates should have the same vorticity and phase around the vortex core to save energy if \( \gamma > 0 \), while for \( \gamma < 0 \) the phase shift should be \( \pi \). For condensates with different winding number, the vortex is fractional quantized and the energy diverges logarithmically with vortex size in bulk [23], and thus thermodynamically unstable. Without loss of generality, we focus on the positive \( \gamma > 0 \) as in the case of MgB\(_2\) [1]. Presuming a straight vortex line, and we look for a vortex with the following structure

\[ \Psi_1 = f_1(r)e^{i\theta}, \quad A = \frac{na(r)}{\kappa_1 r} e^i\theta, \]

where \( a(r) \) is the vortex core profile.
where $r$ is the distance from the vortex core, $e_\theta$ the unit vector in the azimuthal direction and $n$ the vorticity. Substituting the ansatz into Eqs. (4), (5) and (6), we have

$$-f_1(r) + f_1^\prime(r) - \frac{n^2(a - 1)^2}{\kappa^2 f_1} - f_1 - \gamma f_2 = 0,$$

(9)

$$-\frac{n^2 a^2}{\kappa f_1} f_2(r) + \frac{\beta_2}{\beta_1} f_2^3(r) + \frac{m_1}{m_2} \left(\frac{n^2 (\alpha_2 - 1) f_1}{\kappa^2 f_2} - \frac{n^2 a - 1}{\kappa^2 f_2} - \gamma f_1 + \gamma f_2 = 0,ight.
$$

(10)

$$\partial_r^2 a - \frac{1}{r} \partial_r a + \left(\frac{f_1^2}{f_2} + \frac{m_1}{m_2} f_2^2\right)(1 - a) = 0.$$

(11)

In the limit of $r \to \infty$, the wave functions recover the bulk values $f_{10}$ and $f_{20}$. Defining $f_{20} = \eta f_{10}$ with $\eta > 0$, we have the equations for $f_{10}$ and $\eta$

$$-f_{10}^2 - \frac{n^2 a^2}{\kappa^2} + \eta = 0,$$

$$-\frac{n^2 a^2}{\kappa^2} \eta + \frac{\beta_2}{\beta_1} \eta^3 (1 + \eta) - \gamma = 0.$$

(13)

The radial variation of the wave functions and vector potential in the asymptotic region of $r \to \infty$ can be found and are given by

$$f_1 = \sqrt{1 + \eta} + \xi_0 \exp \left(\frac{1}{\sqrt{2} \xi_0} \right),$$

(14)

$$f_2 = \xi_0 \left(\frac{\alpha_2}{\alpha_1} + \frac{\gamma}{\eta}\right) \exp \left(-\frac{1}{\sqrt{2} \xi_0} \right),$$

(15)

$$a = 1 + \xi_0 \exp \left(-\frac{1}{\sqrt{2} \xi_0} \right).$$

(16)

At large distance, there is only one length scale for the two condensates. The penetration depth can be obtained straightforwardly

$$\lambda_v = \frac{1}{\sqrt{\frac{m_1 \xi_0}{m_2 \xi_0} \left(\frac{\alpha_2}{\alpha_1} + \frac{\gamma}{\eta}\right) + (1 + \eta)} .$$

(17)

To calculate the coherence length, we substitute Eqs. (14) and (15) into Eqs. (9) and (10) and linearize the equations. $\xi_0$ is equivalent to the length scale of the small fluctuations in the bulk, and is given by the largest solution to the equation

$$\left(2 + 3 \eta \gamma - 1 \right) \left(\frac{2}{\sqrt{2} \xi_0^2} \right) + \left(2 \frac{\alpha_2}{\alpha_1} + 3 \frac{\gamma}{\eta} - \frac{m_1}{m_2} \frac{1}{\kappa^2 \xi_0^2}\right) - \gamma^2 = 0.$$  

(18)

It is clear that the interband scattering modifies the coherence length and penetration depth in a nontrivial way.

![FIG. 1: (color online). Left: schematic view of two vortices in a superconducting square disk. Right: numerical discretization scheme. $\Psi^{\mu}(\eta)$ is defined on nodes, $J$, $A$ and $U$ are defined on bonds, and $B_i$ is defined inside the plaquette.

III. TDGL APPROACH

To study the interaction between vortices, the structure of the nonlinear vortex core is important and numerical calculations are necessary. We first calculate the structure of vortex and their interaction by minimizing the free energy in terms of TDGL equations defined in the following way

$$\frac{\hbar^2}{2m_i D_i} \left(\partial_t + \frac{2e}{\hbar} \Phi\right) \Psi_i = -\frac{\delta F}{\delta \Psi_i} + \zeta_i,$$

(19)

$$\frac{\sigma}{c} \left(-\partial_t A + \nabla \Phi\right) = -\frac{\delta F}{\delta A} + \zeta_A,$$

(20)

with $D_i$ the diffusion constant, $\sigma$ the normal conductivity, and $\Phi$ the electric potential. By choosing a proper gauge, we can take $\Phi = 0$. $\zeta_i$ represents thermal noises satisfying $\langle \zeta_i \rangle = 0$ and $\langle \zeta_j(x_1, t_1) \zeta_k(x_2, t_2) \rangle = \Gamma_j \delta(x_1 - x_2) \delta(t_1 - t_2)$, with $j, k = 1, 2$ and $A$. Since we are primarily interested in the equilibrium properties, detailed dynamic relaxation process is irrelevant. Here, time is in units of $t_1 = \xi_0^2 / D_1$, the normal conductivity $\sigma$ in units of $c^2 r_1 / 4 \pi \lambda^2$. 

A. Numerical techniques

In order to integrate the TDGL equations, we generalize the numerical method developed for single component superconductors to two-component superconductors and solve the TDGL equations Eqs. (19) and (20) numerically. For the parameters we are interested, the line tension of vortices is high, therefore we approximate vortices as straight lines. The problem is then simplified into two dimensions. To maintain the gauge invariance after discretization, we use the link variable defined as

$$U_\mu(x, y) = \exp \left\{ i \int_{\mu_0}^\mu A_\mu(\xi_\eta) d\xi_\eta \right\},$$

(21)

where $\mu$ is either $x$ or $y$. Then the TDGL equations can be rewritten as

$$\partial_t \Psi_1 - \frac{1}{\kappa_1} \sum_{\mu=x,y} U_\mu^{\ast} \delta_{\mu}(U_\mu \Psi_1) - \Psi_1 + |\Psi_1|^2 \Psi_1 - \gamma \Psi_2 - \xi_1 = 0,$$

(22)
\[
\frac{m_D}{m_c} \frac{D^2}{2} \nabla^2 \Psi_2 - \frac{m_1}{m_2} \frac{1}{\mu + \varepsilon} \sum_{\mu = i,j} U^*_\mu \partial_\mu (U_\mu \Psi_2)
+ \frac{a^2}{pt_2} \Psi_2 + \frac{b^2}{pt_2} |\Psi_2|^2 \Psi_2 - \gamma \Psi_1 - \zeta_2 = 0,
\]
(23)

\[
\sigma \partial_\alpha A + \nabla \times \nabla \times \mathbf{A} = J + \zeta A,
\]
(24)

\[
J_\mu = \frac{1}{2 \kappa_1} [U^* \psi_\mu \partial_\mu (U_\mu \psi_1) - U_\mu \psi_\mu \partial_\mu (U^*_\mu \psi_1)]
+ \frac{m_1}{m_2} \left( \frac{1}{2 \kappa_1} [U^* \psi_\mu \partial_\mu (U_\mu \psi_2) - U_\mu \psi_\mu \partial_\mu (U^*_\mu \psi_2)] \right).
\]
(25)

The disk is partitioned into square meshes of size \( h \) as schematically shown in Fig. [1]. The magnetic field in the pla-
quette with the index \(( i, j )\) is

\[
B_{z, i, j} = \frac{1 - W_{z, i, j}}{ik_1 h^2}
\]
with \( W_{z, i, j} = U^*_{i, j+1} U_{i, j} U_{i, j} U_{i+1, j} \).
(26)

and the supercurrent

\[
J_{x, i, j} = \frac{1}{2 \kappa_1 h} (U_{i, j} \Psi_1^{(1)} \Psi_1^{(1)} - U_{i, j}^* \Psi_1^{(1)} \Psi_1^{(1)})
+ \frac{m_1}{m_2} (U_{i, j} \Psi_1^{(2)} \Psi_1^{(2)} - U_{i, j}^* \Psi_1^{(2)} \Psi_1^{(2)})
\]
(27)

where \( \Psi^{(k)} \) denotes the \( k \)th condensate. The \( y \) component is obtained similarly. After the discretization, the TDGL equations become

\[
\partial_t \Psi_1^{(1)} = (1 - |\Psi_1^{(1)}|^2) \Psi_1^{(1)} + \gamma \Psi_1^{(2)} + \xi_1^{(1)} + \frac{1}{2k_1^2} \left( \frac{U_{i, j} \Psi_1^{(1)} \Psi_1^{(1)} + U_{i, j+1}^* \Psi_1^{(1)} \Psi_1^{(1)} + 2 \Psi_1^{(1)} \Psi_1^{(1)} - 2 \Psi_1^{(1)} \Psi_1^{(1)}}{h^2} \right),
\]
(28)

\[
\partial_t \Psi_1^{(2)} = (-a_1 \psi_1^{(2)} + b_1 \psi_1^{(2)} - \gamma \psi_1^{(1)} + \xi_1^{(2)} + \frac{1}{2k_1^2} \left( \frac{U_{i, j} \psi_1^{(2)} \psi_1^{(2)} + U_{i, j+1}^* \psi_1^{(2)} \psi_1^{(2)} + 2 \psi_1^{(2)} \psi_1^{(2)} - 2 \psi_1^{(2)} \psi_1^{(2)}}{h^2} \right),
\]
(29)

\[
\partial_t U_{x, i, j} = -\frac{i}{\sigma} U_{x, i, j} \text{Im} \left\{ \frac{W_{x, i, j} - W_{x, i+1, j}}{h^2} + U_{x, i, j} \Psi_1^{(1)} \Psi_1^{(1)} + \frac{m_1 \Psi_i \Psi_{i+1}}{2k_1^2} U_{x, i, j} \Psi_1^{(2)} \Psi_1^{(2)} + \xi_1^{(1)} \right\},
\]
(30)

\[
\partial_t U_{y, i, j} = -\frac{i}{\sigma} U_{y, i, j} \text{Im} \left\{ \frac{W_{y, i, j} - W_{y, i+1, j}}{h^2} + U_{y, i, j} \Psi_1^{(1)} \Psi_1^{(1)} + \frac{m_1 \Psi_i \Psi_{i+1}}{2k_1^2} U_{y, i, j} \Psi_1^{(2)} \Psi_1^{(2)} + \xi_1^{(1)} \right\}.
\]
(31)

Equations (28), (29), (30) and (31) are integrated by the forward Euler method.

Vortices are introduced through the boundary condition

\[
A(r + L) = A(r) + \nabla \chi, \quad \Psi_1^r (r + L) = \Psi_1^r (r) \exp(i 2\pi \chi / \Phi_0),
\]
(32)

with \( l = x, y \) and \( \chi_x = H_a L_y \) and \( \chi_y = 0. \) \( H_a \) is the applied magnetic field and should obey the vortex quantization condition via \( \oint \mathbf{A} \cdot d\mathbf{l} = 2m \Phi_0 \) with an integer \( m \), which yields \( H_a = 2m \Phi_0 / L^2 \). Here \( \Phi_0 = \hbar c / 2e \) is the flux quantum.

### B. Vortex structure

We minimize \( F \) in Eq. (1) by solving the TDGL equations numerically under the boundary conditions (32) specifying the number of vortices in the system. The structure of a single vortex obtained by the TDGL equations for \( m = 1 \) is shown in Fig. [2]a). Three characteristic length scales are evident.

### C. Vortex attraction

We then introduce two vortices into a square disk with size \( 10a_1 \leq L \leq 40a_1 \). The disk is large enough for one to neglect the finite-size effect. We find a solution with two vortices separated by \( r_m = 2.7a_1 \), independent on \( L \), as shown in Fig. [2]b). This indicates unambiguously an attractive interaction at large separation and a repulsive interaction at short distance between vortices. The minimal energy associated with this vortex separation is therefore demonstrated to be an intrinsic property of the superconductor. We also confirm the stability of the above vortex solution against thermal fluctuations in the present TDGL approach.

The size of the magnetic flux lies between the radii of the normal cores associated with the two order parameters. As two vortices approaching each other, they attract first by overlapping their normal cores associated with \( \Psi_1 \) as shown in Fig. [2]a). When the two vortices get closer, strong repulsion caused by the magnetic flux sets in. An equilibrium configuration is reached by compromising the attraction and repulsion, where the normal core associated with \( \Psi_1 \) is overlapping strongly while \( \Psi_2 \) is not as shown in Fig. [2]b). Thus vortices
attract at large separation and repel at short distance. It is the competition between the sizes of the normal cores associated with the two components and the area of magnetic flux accompanying the vortex cores that governs the interaction between vortices.

IV. VARIATIONAL CALCULATIONS

To obtain the full dependence of the interaction energy on the vortex separation, one needs to fix vortices at desirable positions. Since vortex is of structure and not a point object, evaluation of vortex interaction at a given distance beyond the London limit is not straightforward [27]. In order to overcome this difficulty we resort to the variational method developed by Jacobs and Rebbi [28] and generalize it to two-band superconductors. The essence of this approach is to construct "good" trial functions for two vortices at given separation.

A. Vortex structure

To reproduce the asymptotic behavior of a vortex at $r \to \infty$, we use the following trial functions for one vortex

$$f_1(r) = \sqrt{1 + \gamma \eta + \exp \left( - \frac{r}{\sqrt{2} \xi_v} \right) \sum_{l=0}^{n} \left( f_{1l} \rho^l / l! \right)}, \quad (33)$$

$$f_2(r) = \sqrt{\frac{\beta_1 \left( \frac{\alpha_2}{\alpha_1} + \gamma \right)}{\beta_2}} + \exp \left( - \frac{r}{\sqrt{2} \xi_v} \right) \sum_{l=0}^{n} \left( f_{2l} \rho^l / l! \right), \quad (34)$$

$$a(r) = 1 + \exp \left( - \frac{r}{\alpha_v} \right) \sum_{l=0}^{n} \left( a_l \rho^l / l! \right), \quad (35)$$
where $f_{1,r}, f_{2,r}$ and $a_i$ are variational parameters. In the limit of $r \to 0$, $f_1 = 0$ and $a \to r^2$ according to Eqs. (9), (10) and (11).

We have $f_{1,0} = -\sqrt{1 + \gamma n}$, $f_{2,0} = -\sqrt{\frac{2}{\gamma \eta}} \left( \frac{a_1}{a_1} + \frac{a_2}{a_2} \right)$, $a_0 = -1$ and $a_1 = a_0/\lambda$. For a giant vortex with vorticity equal to 2, we have $f_{1,1} = f_{1,0}/(\sqrt{2} \xi_0)$ and $f_{2,1} = f_{2,0}/(\sqrt{2} \xi_0)$ in addition. Other coefficients are variational parameters to be determined numerically.

Denote the whole set of variation parameters $f_{1,r}, f_{2,r}, a_i$ and so on by $\mathbf{v}$. The GL free energy is of fourth order in $V_i$ and has the form of

$$
\mathcal{F} = \mathcal{F}_0 + \sum_i f_{1,i}^0 V_i + \sum_{i \neq j} f_{1,i}^2 V_i V_j + \sum_{i \neq j \neq k} f_{1,ijk}^3 V_i V_j V_k + \sum_{i \neq j \neq k \neq l} f_{1,ijkl}^4 V_i V_j V_k V_l.
$$

We use the Newton method of optimization$^{[29]}$ with the iteration procedure

$$
V_i^{(m+1)} = V_i^{(m)} - \sum_j \left[ H^{-1} \right]_{ij} D_j^{(m)},
$$

where the superscript $(m)$ represents the value at the $m$th step. $D_i = \partial \mathcal{F} / \partial V_i |_{V_i = V_i^{(m)}}$, and the Hessian matrix $H_{ij} = \partial^2 \mathcal{F} / \partial V_i \partial V_j |_{V_i = V_i^{(m)}}, V_j = V_j^{(m)}$. The stationary solution to Eq. (37) corresponds to the (local) minimum of the free energy.

Following the procedure of Eq. (37), we obtain the variational coefficients, from which we can construct the vortex solution. We truncate the higher-order corrections to the trial functions at $n = 6$ and find the solution of a single vortex with vorticity 1. The results reproduce well those obtained by the direct minimization of the GL free energy functional as shown in Fig. 3.

### B. Vortex interaction

We proceed to consider the interaction between two vortices. For convenience, we introduce complex representation of the 2D coordinates $z = x + iy$, and then the winding phase part in Eq. (8) becomes $\exp(i\theta) = \sqrt{z}/z'$. To construct trial functions for two-vortex solution, we follow Ref. $^{[28]}$ and use the conformal transformation of the complex plane

$$
z = (z')^2 - (d/2)^2.
$$

It is straightforward to see that the origin in $z$ have two images in the $z'$ plane at $\pm d/2$, and that when $z'$ varies by $2\pi$, $z$ varies by $4\pi$. This means that we may map a one-vortex solution in $z'$ to a two-vortex solution in the $z$ plane. The phase factor of the two-vortex solution with vortices cores at $z = \pm d/2$ can be constructed by this transform. We seek the wave functions of the form

$$
\Psi(z, z') = \left\{ \left| z - \left( \frac{d}{2} \right)^2 \right| / \left| z'^2 - \left( \frac{d}{2} \right)^2 \right| \right\} \frac{1}{\sqrt{2}} f_1(z, z'),
$$

with $i = 1, 2$. The trial function for $f_i$ can be constructed by the following consideration. For $d \to \infty$, two vortices behave independently, while at $d \sim 0$ two vortices merge and form one giant vortex with vorticity 2. In addition, we need also a term to describe the interaction between two vortices. The trial function therefore can be constructed

$$
f_i(z, z') = \omega f_{1,i}^0 \left( \frac{z - d/2}{2} \right) f_{1,i}^1 \left( \frac{z + d}{2} \right) + (1 - \omega) f_{1,i}^2 \left( \frac{z}{2} \right) + \delta f_i(z, z'),
$$

where $f_{1,i}^1$ and $f_{1,i}^2$ are single-vortex solution with vorticity 1 and 2 respectively obtained by the variational calculations in the previous section, and $\delta f_i$ accounts for the interaction. $\omega$ interpolates two independent vortices solution and one giant vortex solution. The factor in the second term at the right-hand-side of Eq. (40) is to ensure that the wave function vanishes at the vortex cores $z = \pm d/2$. The interaction contribution may be constructed as follows

$$
\delta f_i(z, z') = \left| z^2 - \left( \frac{d}{2} \right)^2 \right| \cos(\sqrt{2}\xi_0 |z|) \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} f_{1,ij} \frac{|z|^i}{2} \left( \frac{z'}{z} \right)^j + \left( \frac{z'}{z} \right)^j.
$$

The first factor is again to make sure that wave function vanishes at the vortex cores, and the second factor accounts for the fact that the interaction vanishes when $z \to \infty$.

Using the similar reasoning parallel to the construction of the trial functions of $\Psi_i$, we can obtain the trial function for $A$

$$
A = \omega \left[ \frac{1}{2} s_i \left( \frac{d}{2} \right)^2 a_{1,i} \left( \frac{z - d}{2} \right) + \frac{1}{2} s_i \left( \frac{d}{2} \right)^2 a_{1,i} \left( \frac{z + d}{2} \right) \right] + \frac{1}{2} s_i \left( \frac{d}{2} \right)^2 a_{2,i} \left( \frac{z}{2} \right) + \delta a(z, z'),
$$

where $a_{1,i}^0$ and $a_{2,i}^0$ are for single-vortex solutions with vorticity 1 and 2. The interaction contribution has the form

$$
\delta a(z, z') = \frac{1}{\cosh(|z|)} \left[ za_1(z, z') + z' a_2(z, z') \right],
$$

with

$$
a_k(z, z') = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} a_{k,ij} \frac{|z|^i}{2} \left( \frac{z'}{z} \right)^j + \left( \frac{z'}{z} \right)^j.
$$

Once the trial functions are constructed, we can do the optimization according to Eq. (37). We put two vortices at $(-d/2, 0)$ and $(d/2, 0)$, and then calculate the distribution of the wave functions, magnetic field and supercurrent. As displayed in Fig. 4 when two vortices approach from $d = 8\lambda$, the condensate in the first band overlaps first, which causes attraction between vortices, see Figs. 4(a) and (b). As $d$ is reduced further, the magnetic fields start to overlap and strong repulsion sets in as shown in Fig. 4(c). Finally, two vortices coalesce into a giant vortex with vorticity 2, see Fig. 4(d).

The resultant separation dependence of interaction between two vortices is displayed in Fig. 5. The agreement between the estimates on the position of minimal energy derived by the variational technique and by the TDGL equations (Fig. 2(b)) serves a successful check of the validity of the variational calculations. At large separation $r$, the attraction decreases exponentially and the saturated energy corresponds to the self
energies of two isolated vortices. For $r < r_m$, the repulsion increases sharply and the energy at $r = 0$ corresponds to a giant vortex with vorticity 2.

C. Comparison on numerical approaches

To calculate interaction between vortices poses a challenge to theory since vortices are extended objects. In the London limit, the interaction of vortices has been calculated analytically\[21\]. For general cases, one has to introduce constraints to fix two vortices at a desired separation. A legitimate procedure is to fix vortices through the boundary condition Eq. (32). Vortices in a disk of type II superconductor tend to keep away from one another, but they cannot leave the disk as imposed by the boundary condition. By minimizing the free energy, we obtain the interaction energy and the equilibrium vortex separation for a given system size $L$. Gradually increasing $L$, we obtain the interaction energy versus the vortices separation. However, for vortices with attraction at large distance and repulsion at short distance, this approach cannot give the dependence of the interaction energy on vortex separation since the distance between two vortices is always fixed, corresponding to the minimum of the interaction energy. We notice that this approach is still the most legitimate way to prove the existence of attraction at large distance and repulsion at short distance.

In numerical calculations of the GL free energy, one might alternatively introduce pinning to vortices by fixing the amplitude and/or phase of superconductivity order parameter in a certain region near the vortex cores \[30\]. However, this method may introduce artifacts when two vortices are close to each other since the order parameters change dramatically near the vortex core. Furthermore, the local constraints are sometime insufficient to pin vortices when the interaction becomes strong when vortices are close. In contrast, in the variational approach shown above the global structure (such as core
of the vortices and asymptotic behavior far from the core) of
the vortices is maintained, and one only adjusts the detailed
structure through the variational calculations. If the trial func-
tions are appropriately chosen, the variational approach gives
superior results.

V. PHASE TRANSITION AND PHASE DIAGRAM OF
VORTEX STATES

A. Vortex configuration

The novel interaction profile shown in Fig. 5 is expected
to dominate the vortex state of a macroscopic system, and thus
the phase diagram. In order to elucidate the situation, we per-
form numerical simulations using the overdamped Langevin
dynamics [31]

\[ \eta \mathbf{r}/dt = -\partial E/\partial \mathbf{r} + \mathbf{F}^{(n)}, \]

where \( E \) is the pair potential in Fig. 5 and \( \mathbf{F}^{(n)} \) is the white
noise force with \( \langle F^{(n)}(t)F^{(n)}(t') \rangle = 2T\eta \delta(t - t') \) with \( T \)
being the temperature and \( \eta \) the viscosity.

Initially vortices are randomly distributed corresponding to
a high temperature and the system is annealed to \( T = 0 \) by
gradually decreasing \( T \), which yields the ground state. Equation
(45) is solved by the 2nd order Runge-Kutta method and
the simulation box is divided into cells with a cutoff radius \( r_c \)
to accelerate the simulation. We fix the number of vortices \( N_v \)
and set the simulation box with aspect ratio 2 : \( \sqrt{3} \) to accom-
modate the triangular lattice. The magnetic induction is given
by \( B = 2N_v \Phi_0/\sqrt{3}L^2 \) with \( L \) being the length of the simu-
lation box. Periodic boundary condition are used and \( dt = 0.02 \),
\( r_c = 7.8 \) and \( N_v = 400 \). The results are checked successfully
by using finer \( dt \), larger cutoff and more vortices.

A typical ground-state vortex configuration for small aver-
age magnetic induction is presented in Fig. 4(a). A circular
droplet of vortices with internal triangular order is obtained.
This vortex configuration is clearly determined by the vortex
interaction. In the presence of attraction, vortices prefer to
stay together to form a cluster. For a vortex at the cluster sur-
f ace, the number of neighbors is smaller than that inside the
cluster, and thus it bares a higher energy. This results in a
positive surface tension for the vortex cluster, similar to type
I superconductors. The circular cluster minimizes the surface
energy. On the other hand, the repulsion force at short dis-
tance prevents the vortices from collapsing. Due to the repul-
sive force, vortices inside the cluster are triangularly ordered,
same as type II superconductors. The circular cluster of the
closest packing triangular lattice minimizes the total free en-
ergy. The lattice constant \( r_0 \) is slightly smaller than \( r_m \) (see
Fig. 5) due to the contributions from vortices at large separa-
tions where interaction is attractive.

Besides the circular droplet of vortices, vortex stripe and
vortex void are also observed at intermediate densities which
minimize the free energy for the system with given (finite)
size and number of vortices. At a small vortex density, the
droplet phase [Fig. 6(a)] with triangular order is stable. Upon
increasing the magnetic field, the vortex droplet expands, and
at a threshold field a vortex stripe phase [Fig. 6(b)] is pre-
ferred. The stripe then evolves into vortex void configuration
[Fig. 6(c)] when \( B \) is increased further. When \( B \) becomes
even larger, the void structure disappears and a perfect trian-
gular lattice [Fig. 6(d)] emerges and remain stable until the
superconductivity is broken completely at \( H_{c2} \).

Since the stable vortex configuration presumes the minimal
surface area, the transition fields between two configurations
can be evaluated by comparing the surface areas associated
with the configurations. For a vortex droplet, the surface
energy is \( 2\pi R_0 r_c \) with the radius of the cluster \( R = \sqrt{3N/2\pi} \)
and the surface tension \( \sigma_s \). For a stripe configuration, the
surface energy is \( 2L\sigma_s \). The energy consideration gives the transi-
tion field at \( B_{c1} = \Phi_0/\pi r_0^2 \). Similar argument gives the fields
of other structure transitions: transition from vortex stripe to
vortex void at \( B_{c1} = (2\pi \sqrt{3} - 3)\Phi_0/(3\pi r_0^2) \), and transition
from vortex void to vortex lattice at \( B_{c2} = 2\Phi_0/\sqrt{3}r_0^2 \). The nu-
merical results are consistent with these analytical estimates.
It is noted that these transition fields depend on the shape of
the simulation box. In the thermodynamic limit, the circular
vortices droplet is the only ground state at low magnetic field.

B. Phase transition and phase diagram

The phase transition between the Meissner region and a
vortex cluster indicates unambiguously a first-order phase
transition, at which clusters of vortices penetrate into the sys-

tem upon increasing the external magnetic field [11]. The transi-
tion magnetic field \( H_{c1} \) is given by \( H_{c1} = 4\pi(\epsilon - n_1\Delta)/\Phi_0 \), with \( n_1 \approx 3, \epsilon \) and \( \Delta \) defined in Fig. 4 for the energy
of a single vortex line and the energy drop associated with the
vortex attraction per unit length. The contribution from the
attraction component is small since \( \epsilon \gg \Delta \) (see Fig. 5), and
therefore \( H_{c1} \) is close to that of a type II superconductor with
flux-line energy per unit length \( \epsilon \). For large magnetic fields a
uniform vortex lattice of triangle (Fig. 6(d)) has been observed
same as type II superconductors.

Now we can construct a mean-field phase diagram of vor-
xite states in the two-component superconductors. The \( H - T \)
phase diagram is depicted in Fig. 7(a), where the upper critical
field \( H_{c2} \) is the same of a type II superconductor determined
solely by the condensate with the smaller coherence length. The \( B - T \) phase diagram is given in Fig. 7(b), with the bound-
ary between the phase separation and the uniform triangular
vortex lattice given by \( B_{c1} = n_2\Phi_0/r_n^2 \) with \( n_2 \approx 2/\sqrt{3} \).

It is illuminating to compare the response to applied magneti-

c field in the present system with those in conventional
type I or type II superconductors. For type II supercon-
ductors, an extremely dilute vortex lattice penetrates into a su-
perconducting sample at \( H_{c1} \) and the magnetization curve is
continuous at the penetration. For type I superconductors, the
magnetic field penetrates into the sample and breaks the su-
perconductivity at \( H_c \) associated with a jump in the magneti-

cation curve. For superconductors with competing repulsive
and attractive inter-vortex interaction, clusters of vortex lat-
tice with given lattice constant \( r_0 \) penetrate into the sample associated with a discontinuous jump in magnetic induction from zero to \( B_{c1} \). It then increases gradually with the external magnetic field until \( H_{c2} \) at which the superconductivity is destroyed (see inset of Fig. 7). Therefore, the magnetic behavior of these superconductors interpolates those of the type I and type II superconductors.

### C. Effect of thermal fluctuations

It has been revealed that thermal fluctuations should be weak in MgB\(_2\). \[23\]. In the present case, the competition between long-range attraction and short-range repulsion may enhance thermal fluctuations, and warrants additional treatment. Phase diagrams of particles with a hard-core repulsion plus an attractive tail have been investigated intensively. It is known that the first-order gas-lattice phase boundary starts from \( T = 0 \) and \( \rho = 0 \), and that all other transitions, such as gas-liquid, liquid-lattice and possible lattice-lattice transformations, take place at temperature \( k_B T / E_0 \sim O(1) \), where \( E_0 \) is the strength of attractive potential (see for example \[22\]). In the present flux-line system, the typical flux segment relevant to distortion of vortex lattice is estimated as \( L_{\Phi} \approx \sqrt{\epsilon a^2 / \Delta} \) with \( \Delta \approx r_0 \), which minimizes the energy associated with the tilt modulus and vortex interaction (see for example \[33\]). This gives an effective attraction potential \( \epsilon_{\text{eff}} = L_{\Phi} \Delta = \sqrt{\epsilon a^2 \Delta^3} \). To estimate \( \epsilon \) and \( \Delta \), we neglect the inter-band coupling (\( \gamma = 0 \)) for simplicity. The attraction is caused by the overlap of the condensate \( \Psi_1 \), and thus has an order of the energy of normal core \( \Delta \approx \left( \frac{\phi_0}{2 \pi} \right)^2 \frac{1}{\lambda^2} \). The energy per unit length of a single vortex is contributed from the normal cores of two condensates and the magnetic energy, and is given by \( \epsilon \approx \left( \frac{\phi_0}{2 \pi} \right)^2 \frac{1}{\lambda^2} + \left( \frac{\phi_0}{2 \pi} \right)^2 \ln \left( \frac{1}{\epsilon} \right) \). Assembling these results and taking into account the mean-field temperature dependence for the lengths, the condition \( k_B T \approx \epsilon_{\text{eff}} \) for various phase transitions to occur \[32\] spells as \((1 - T / T_c) \approx fG_1\), where \( f \sim 100 \) for a system with coherence length and penetration depth of the same order, \( G_1 \equiv \frac{1}{2} \left( \frac{k_B T_c}{E_0} \right)^2 \) is the Ginzburg index for the first component with \( \xi_1(0) \) the coherence length at zero temperature and \( H_{1c} \equiv 4\pi \alpha_1^2 / \beta_1 \). Since \( G_1 \sim 10^{-6} \) as shown in Ref. \[23\], the thermal fluctuations are weak except the very small regime close to \( T_c \), i.e. \( 1 - T / T_c \sim 10^{-4} \), where gas-liquid, liquid-lattice and lattice-lattice transformations may be possible.

Effects of thermal fluctuations have also been investigated by Langevin dynamics. In order to avoid possible artifacts due to insufficient annealing, we heat the system from the ground state with vortex configurations such as that shown in Fig. 3(a). At finite temperatures the perimeter of the cluster wiggles while both the cluster itself and the inner triangular order remain stable. Only at temperatures close \( T_c \), single vortices are evaporated from the cluster surface. These simulation results are consistent with the above estimate on thermal fluctuations in the present system. Through all the simulations, we cannot find any random vortex patterns, such as gossamer- or stripe-like ones \[13\].
VI. DISCUSSIONS

Here we discuss a more general case that each condensate has individual mean-field critical point $T_{ci}$ in absence of coupling and a finite inter-band coupling. The inter-band scattering couples two bands and enhances the critical temperature to $T_c > T_{ci}$. (24)

For $T < T_{ci}$ and weak inter-band coupling $\gamma \ll 1$, the superconductivity is realized independently, and the physics is qualitatively the same as that of two decoupled bands $\gamma = 0$. (11)

For $T_{ci} < T < T_{c2}$, the superconductivity in the band 1 is induced by the the band 2 through the Josephson coupling. It is the regime discussed in Ref. [12]. When $T_{ci} < T < T_c$, the superconductivity is purely induced by the inter-band coupling. The physics can be quite different in different temperature regimes. We notice that in principle the GL theory is valid only close to $T_c$, and thus in the highest temperature region.

From Eq. (1), $T_c$ is given by the condition $\alpha_1(T)\alpha_2(T) - \gamma^2 = 0$, where $\alpha_i(T)$ depends on the temperature and can be derived from the BCS theory [35]. Close to $T_c$, $\tau \equiv \frac{\tau^2 - \alpha_1\alpha_2}{\alpha_1\alpha_2} = (T - T_c)/T_c \ll 1$, the order parameters up to the leading order can be derived from Eqs. (4) and (5) for a uniform superconductor [14]

$$\Psi_{10}^2 = \frac{\alpha_1^2}{\alpha_1^2/\beta_1 + \alpha_2^2/\beta_2},$$  
(46)

$$\Psi_{20}^2 = \frac{\alpha_2^2}{\alpha_1^2/\beta_1 + \alpha_2^2/\beta_2}. $$

(47)

We then consider some deviations from the bulk values $\Psi_i = \Psi_{i0} + \phi_i$. From Eqs. (4) and (5), the deviations are governed by

$$\alpha_1\phi_1 + 3\beta_1\Psi_{10}^2\phi_1 - \frac{\hbar^2}{2m_1} \nabla^2\phi_1 - \gamma\phi_2 = 0,$$

(48)

Taking the solution of form $\phi_i \sim \exp[-\kappa/(\sqrt{2}\xi_v)]$, we can derive the coherence length which is divergent at $\tau \rightarrow 0$, $\xi_v = \sqrt{(\frac{\alpha_2}{4m_1} + \frac{\alpha_1}{4m_2})\hbar^2 \frac{1}{\gamma^2}}$. We emphasize that there is only one coherence length for the two order parameters when $\tau \rightarrow 0$. The London penetration depth is still given by Eq. (7) with the order parameters given in Eqs. (46) and (47). Calculations of the order parameters near $H_{c2}$ and of the spatial correlation of $\langle \Psi_i(r)\Psi_i(0) \rangle$ when thermal fluctuations are present yield only one divergent coherence length consistently. Therefore, the superconductors are either type I or type II.

Since it was discussed that vortex attraction originates from the overlapping of normal vortex cores, [11] let us check the temperature dependence of the structure of a single vortex ranging from 0 to $T_c$. For simplicity, we take $\alpha_i(0) = \alpha_i(0)(1 - T/T_{ci})$ and assume $\beta_i$ and $\gamma$ are $T$-independent. The parameters at $T = 0$ are the same as those in the previous sections. The vortex structure is shown in Fig. 8 for several typical temperatures. It becomes clear that the sizes of vortex cores for $\Psi_1$ and $\Psi_2$ get closer to each other as $\tau$ approaches 0. Analytical calculations on the structure of the nonlinear vortex core also reveal an identical size for the vortex cores associated with the two components close to $T_c$. Therefore, the interaction between vortices is purely repulsive in the present case.

This result is understandable since the inter-band coupling is dominant at $\tau \ll 1$, and thus the superconductivity in the two bands is strongly correlated and described by a unique coherence length. Nevertheless, if the inter-band coupling $\gamma(T)$ and $\alpha_i(T)$ all vanish at a single temperature $T_c$ as discussed in the previous sections, there will be two divergent lengths and thus different core sizes for the two components. This permits vortices to exhibit the peculiar interaction profile shown in Fig. 8. Therefore, we find that the non-monotonic inter-vortex interaction, and thus the peculiar phenomena discussed above, only appear when the inter-band coupling and $\alpha_i(T)$ all vanish at $T_c$ within the framework of the GL theory.

VII. CONCLUSION

We have investigated the interaction between vortices in two-band superconductors. When the size of the magnetic flux of a vortex lies between the sizes of the two normal cores associated with the two condensates, the interaction between vortices is attractive at large separation and repulsive at small separation. This was demonstrated clearly by the time-dependent Ginzburg-Landau calculations on two vortices in a superconducting disk. The equilibrium distance between two vortices is independent of the size of the disk for simulations, which clearly shows the existence of energy minimum in the interaction potential. The full dependence of interaction energy on the vortex separation is obtained by the variational calculations. The two methods give the same estimate on the vortex separation with minimal free energy.
We have studied stable vortex configurations for a large number of vortices by Langevin dynamics adopting the novel distance dependence of vortex interaction. Circular vortex clusters coexisting with Meissner phase are observed for small and intermediate vortex densities. The transition from Meissner state into vortex states is therefore of first order associated with a sharp increase of magnetization. The superconductivity associated with the triangular vortex lattice is suppressed by a strong magnetic field in the same way of a type II superconductor. Therefore, the magnetic behavior of these superconductors as summarized in the mean-field phase diagrams interpolates those of the type I and type II superconductors. In most temperature regions except very close to the critical point, thermal fluctuations are weak for small Ginzburg number, the same as single-band superconductors.

The above interesting phenomena take place provided, first, the bare mean-field critical points of the two bands coincide with each other and the inter-band coupling vanishes at the same temperature, which permit two divergent core sizes associated with the two condensates even close to the critical point; second, the parameters in the Ginzburg-Landau free energy are appropriate to achieve the relations among the two coherence lengths and the penetration depth.

When two condensates have different bare transition temperatures and the inter-band coupling is finite, the superconductivity is induced by the inter-band scattering when temperature is sufficiently close to the critical point of the composite system. In this case, superconductivity in the two bands couples strongly, and only one divergent coherence length exists, and thus the superconductors are either type I or type II.

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