Vortex structure for a $d+is$-wave superconductor

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The uniform phase, the single vortex structure, and the vortex lattice structure of a $d+is$-wave superconductor are studied numerically by simulating the Ginzburg-Landau equations with the finite-element method. In the uniform phase, for superconductors with attractive interactions in both the s- and the d-wave channels, there exists a certain range of the relative strength of interactions (or temperatures) such that a $d+is$ state is stable while at other regions only a d-wave state is stable. More strikingly, the s- and d-wave components of a single vortex in the $d+is$ state exhibit twofold symmetry. The relative phase between these two components is roughly $\pi/2$ for the $d+is$-wave state. In the d-dominant phase, as the magnetic field increases, the impact of the s-wave component on the energy gap can be more significant. The vortex structure changes from a square to an oblique, and finally to a triangular lattice with decreasing s-wave channel interaction (or increasing temperature). [S0163-1829(99)01701-4]

I. INTRODUCTION

There has been considerable experimental and theoretical interest in the determination of the pairing symmetry of high-temperature superconductors, which appears to be a crucial step in the identification of the pairing mechanism and in the subsequent development of a microscopic theory for the high-temperature superconductivity. It is widely accepted that the high-temperature cuprates may attain an unconventional pairing state different from the isotropic s-wave pairing state described by the Bardeen-Cooper-Shrieffer (BCS) theory for low-temperature superconductors. A large number of experiments have been interpreted as the indication of a state with d-wave symmetry, namely, the $d_{x^2-y^2}$ pairing state with lines of nodes in the energy gap. Many experiments on YBCO that directly probed the pairing symmetry by using phase-sensitive devices, such as Josephson junctions or superconducting quantum interference devices (SQUID), provided strong support to the d-wave pairing symmetry.[1–5] Nevertheless, we notice that the possibility of a mixed phase consisting of s- and d-wave components in certain conditions may not be ruled out.[6–8]

The $s+d$-wave symmetry was first discussed by Ruckenstein *et al.*[9] and $d+is$-wave symmetry by Kotliar.[10] In Ref. 10, it was pointed out that the resonating-valence-bond mechanism of high-T_c superconductivity can lead to s-wave-like and d-wave-like superconducting order parameters. At low temperatures, a mixture of s and d waves with a well-defined relative phase close to $\theta=\pi/2$ is energetically favored. The relative phase is of great importance, since only if $\theta=0$ and π can the energy gap have nodes, while a nodeless energy gap and time-reversal symmetry breaking (T breaking) would be developed otherwise. The experiment on fractional vortices observed by Kirtley *et al.*[11] has been considered as the evidence of T breaking in high-T_c superconductors.[12] Recently, the thermal conductivity measurements on $Bi_2Sr_2CaCu_2O_8$ were also invoked in connection with the T-breaking state.[13] Various theories and mechanisms leading to a T-breaking superconducting state have been proposed. For example, a two-dimensional isotropic Fermi liquid with attractive interactions in both s- and d-wave channels was used to examine the possibility of a mixed-phase superconducting state.[14–16] It was shown that in both the weak- and strong-coupling limits a mixed $d+is$ symmetry can be realized in a certain range of the relative interaction strengths in the s and d channels, but there should be no stable mixed $s+d$ state in tetragonal systems. In fact, if the interaction between electrons is assumed to be attractive in the d-wave channel and repulsive in the s-wave channel, the uniform phase is always a pure d-wave pairing state.[17] But an s-wave component can be induced near the inhomogeneous regions, such as the defects and the magnetic vortices.

The vortex structure and the vortex-lattice structure of a d-wave superconductor have been studied numerically in detail by several methods,[18–22] but there has been no report about these structures of a $d+is$-wave superconductor, which appear to be interesting at least academically. In the present work, we are concerned with the vortex properties of a $d+is$-wave superconductor, and especially the relative phase between the s and d components. The results are obtained by solving the phenomenological Ginzburg-Landau (GL) equations with the finite-element method developed previously.[22] For attractive interactions in both s and d channels, there exists a critical relative strength of the interactions, above (below) which a $d+is$ (pure d-wave) state is stable. There appears to be neither stable s-wave states nor $s+d$-wave states. The order-parameter profiles of the s and d components for a single vortex are studied in detail at different relative interaction strengths. Rather interestingly, the s-wave component in the $d+is$-wave state exhibits a twofold symmetry, in contrast to the fourfold one of the induced s-wave component of a d-wave superconductor. In the mean time, the d-wave component of the $d+is$ state is also twofold symmetric. With decreasing interaction strength in the s-wave channel (or with increasing temperature) the s-wave component decreases gradually and its symmetry changes to be fourfold, while the d component increases and becomes almost rotationally symmetric near the vortex core. Only at very low temperatures is the magnitude of the s-wave amplitude comparable to that of the d-wave component. The relative phase between the s- and d-wave components in the vortex state is discussed in detail at various temperatures. It is also found that the vortex lattice structure changes from a square to an oblique and finally to a triangular lattice with increasing temperature.

II. THE GINZBURG-LAUDAU EQUATIONS

We consider a model of an isotropic two-dimensional Fermi liquid with attractive interactions in both s and d channels. Obviously, when only one of the two interactions is attractive, the ground state is pure with the appropriate pairing symmetry. When both channels are attractive, the competition will lead to either a pure or a mixed pairing symmetry. The GL theory for a superconductor with two attractive channels has been presented by Ren, Xu, and Ting[14] based on Gor'kov equations. The GL equations can be expressed as follows:

$$\left[-\alpha_s+\frac{4}{3}(|S|^2+|D|^2)+\mathbf{\Pi}^2\right]S+\frac{2}{3}D^2S^*+\frac{1}{2}(\mathbf{\Pi}_x^2-\mathbf{\Pi}_y^2)D=0, \tag{1}$$

$$\left[-1+\frac{8}{3}|S|^2+|D|^2+\mathbf{\Pi}^2\right]D+\frac{4}{3}S^2D^*+(\mathbf{\Pi}_x^2-\mathbf{\Pi}_y^2)S=0, \tag{2}$$

$$\nabla\times\nabla\times\mathbf{A}-\nabla\times\mathbf{H_e}+\left\{S^*\mathbf{\Pi}S+\frac{1}{2}D^*\mathbf{\Pi}D+\frac{1}{2}[S^*(\mathbf{\Pi}_x-\mathbf{\Pi}_y)D+D^*(\mathbf{\Pi}_x-\mathbf{\Pi}_y)S]+\text{H.c.}\right\}=0. \tag{3}$$

In these equations, the two order parameters S and D are normalized by $\Delta_0=\sqrt{4/3\alpha\ \ln(T_d/T)}$ with $\alpha\approx 7\zeta(3)/8(\pi T_c)^2$, the space by the magnetic penetration depth λ, and the vector potential $\mathbf{A}$ by $\Phi_0/2\pi\xi$ with $\Phi_0=h/2e$ and ξ being the flux quantum and the coherence length, respectively. In Eq. (1), α_s may be expressed as a function of temperature T:[14,23] $\alpha_s=\ln(T_s/T)/\ln(T_d/T)$, where T_s and T_d may be viewed as the apparent superconducting transition temperatures for the s wave and the d wave, respectively, with $T_s\propto e^{-1/N(0)V_s}$ and $T_d\propto e^{-1/2N(0)V_d}$. Here $N(0)$ is the density of states at the Fermi surface, V_s and V_d are the effective attractive interaction strengths in the s- and d-wave channels, respectively. Finally, $\mathbf{\Pi}=i\nabla/\kappa+\mathbf{A}$ with κ being the GL parameter.

III. BULK HOMOGENEOUS PHASE

Let us first consider the bulk homogeneous phase of a superconductor in the absence of an applied magnetic field in some detail, in complement to a previous simple analytic discussion.[14] In the mixed-phase state, we simply set D to be real and positive by some gauge transformation. Now let the relative phase angle of S be ϕ, and the ratio between the moduli of S and D be β, which are variation parameters to be optimized. With these ingredients, the free-energy density functional of the uniform phase pertinent to the above GL equations can be expressed solely in terms of D as

$$f=-(2\alpha_s\beta^2+1)D^2+\left(\frac{4}{3}\beta^4+\frac{1}{2}+\frac{8}{3}\beta^2+\frac{4}{3}\beta^2\cos 2\phi\right)D^4, \tag{4}$$

which can be minimized with respect to D to give

$$f_{min}=-\frac{1}{2}\frac{(2\alpha_s\beta^2+1)^2}{\frac{8}{3}\beta^4+\frac{16}{3}\beta^2+\frac{8}{3}\beta^2\cos 2\phi+1}. \tag{5}$$

At this stage it is evident that for any α_s and β, the energy is minimized by $\phi=\pm\pi/2$, i.e., $(S,D)\propto(\pm i\beta,1)$ always minimizes the free energy. Of course, if $\beta=0$ the relative phase makes no sense at all. With $\phi=\pm\pi/2$, we are ready to perform the final optimization with respect to β to find, after some basic algebraic manipulations,

$$\left[\frac{\alpha_s}{2\alpha_s\beta^2+1}-\frac{4\beta^2+2}{8\beta^4+8\beta^2+3}\right]\beta=0, \tag{6}$$

which determines the optimum ratio β as a function of α_s. $\beta=0$ is a trivial solution. For $\beta\neq 0$ but near a critical point so that $\beta\to 0$, the above equation can be solved rigorously up to second order in β:

$$\beta^2=\frac{3\alpha_s-2}{4-4\alpha_s}\quad \text{as}\quad \beta\to 0. \tag{7}$$

So self-consistency determines the critical value of α_s as $\alpha_s^*=2/3$. If $1>\alpha_s>2/3$, we have $\beta^2>0$, while if $\alpha_s<2/3$, the only possible solution is the trivial solution $\beta=0$.

To conclude, for the specific form of the GL theory we are using (and $\alpha_s<1$), the uniform phase is either a mixed-phase state $d\pm is$ or a pure d-wave state, and can be nothing else. The transition value of $\alpha_s^*=\frac{2}{3}$ implies that there exists a temperature $T^*=T_s^3/T_d^2$ at which a second-order transition would take place, as obtained previously in Ref. 14.

To see clearly the relevant parameter regions where the different pairing states lie, we plot α_s as a function of T_s and T in Fig. 1. T and T_s are in units of T_d, while T_s and T_d are related to the strengths of the attractive interactions in the s and d channels as mentioned above. Note that T_s is chosen to be smaller than T_d because it was pointed out that in both the weak-coupling and very strong coupling limits the d-wave phase always has a higher apparent T_c.[10] In most actual cases, T_s seems to be very small compared to T_d. Therefore, from Fig. 1, we can see that the uniform $d+is$ wave may only be stabilized at extremely low temperatures.

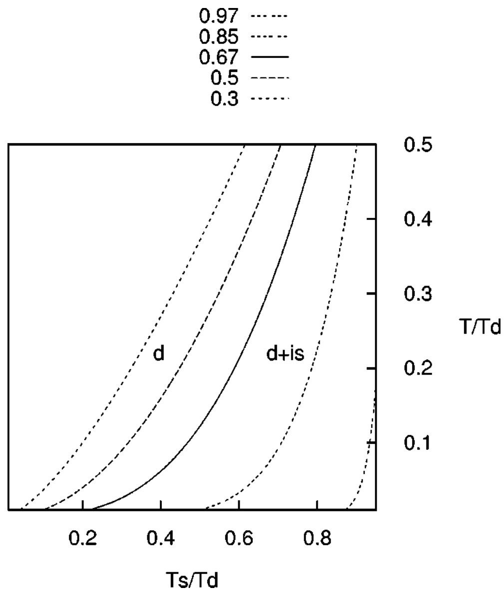

FIG. 1. Contour plots of α_s vs temperature T and apparent transition temperature of s-wave T_s, compared with the apparent transition temperature of d-wave T_d.

At the end of this section, we would like to remark that there are two degenerate bulk phases, i.e., the $d+is$ phase and the $d-is$ phase. With a nonzero s component, they are T-breaking states because one can never transform one of them into another by simple U(1) gauge transformations.

IV. VORTEX STRUCTURE

The vortex structure of pure d-wave superconductors has been studied numerically with the finite element method.[22] In a magnetic field the s wave is induced near the core of the vortex. The induced s-wave component decays as $1/r^2$ and its amplitude profile exhibits a fourfold symmetry. In our case, the GL equations have the same form as that used in a d-wave superconductor except the sign before α_s is changed from positive to negative.[22] So we perform numerical simulations for the $d+is$-wave superconductor with the same finite-element method.

The finite-element method with biquadratic polynomial functions and triangular element cells is used to solve the GL equations and the periodic boundary condition is used to mimic the bulk properties.[24] We study the vortex structure from strong attractive strength in the s-wave channel (or from very low temperature) to repulsive interaction in the s-wave channel (or high temperature). The calculations performed for α_s ranged from 0.97 to -1. We find that the symmetry and structure of the vortex change with variation in α_s. Figures 2 and 3 give the comparison of the amplitudes of the s- and d-wave components at four typical values of α_s. Here we fix the parameter $\kappa=3$, and use a square unit cell of grid size 19×19 with an area of $158\xi^2$ threaded by one vortex. It can be seen clearly that when α_s is smaller than but close to 1, the s-wave component is of twofold symmetry. With the decrease of α_s, an additional s-wave component is induced. For example, at $\alpha_s=0.7$, the four-leafed clover shows up but the overall symmetry is still twofold. When α_s is smaller than the critical value $\alpha_s^*=\frac{2}{3}$, as

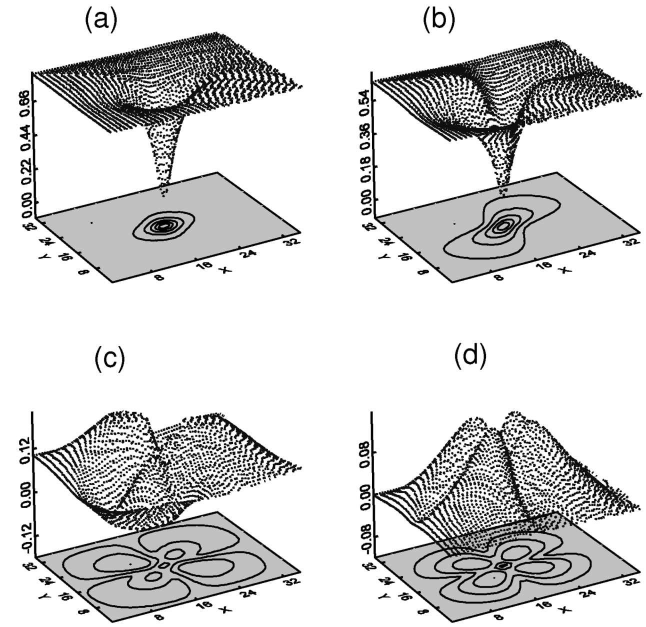

FIG. 2. Surface-contour plots of the amplitude of s-wave component of a single vortex. The parameter κ is set to 3, and one vortex was threaded in a cell of 19×19 grid size with an area of $158\xi^2$, and (a) $\alpha_s=0.97$, (b) $\alpha_s=0.85$, (c) $\alpha_s=0.7$, (d) $\alpha_s=0.5$.

shown in Fig. 2(d), where $\alpha_s=0.5$, the s wave exhibits the fourfold symmetry just as that for a d-wave superconductor with one repulsive channel and one attractive channel,[18–20,22] which can be thought to stem from the fact that at this stage the homogeneous bulk phase is a pure d-wave state (i.e., the s channel appears to be effectively repulsive). Also, the magnitude of s-wave component decreases gradually as α_s decreases, and the s-wave component changes from dominant to subdominant. On the other hand, it can be seen that when the s wave is comparably large [as in Fig. 2(a)], the d-wave component has two leaves protruding and two leaves con-

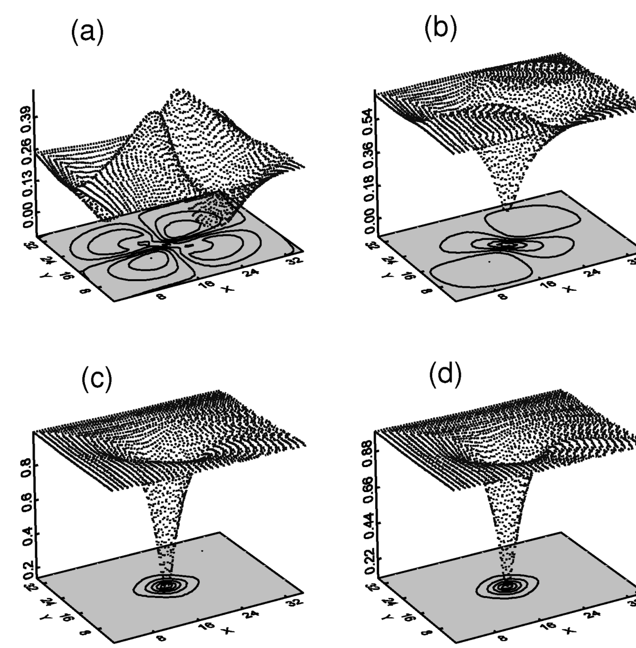

FIG. 3. Same as Fig. 2 but for d-wave components.

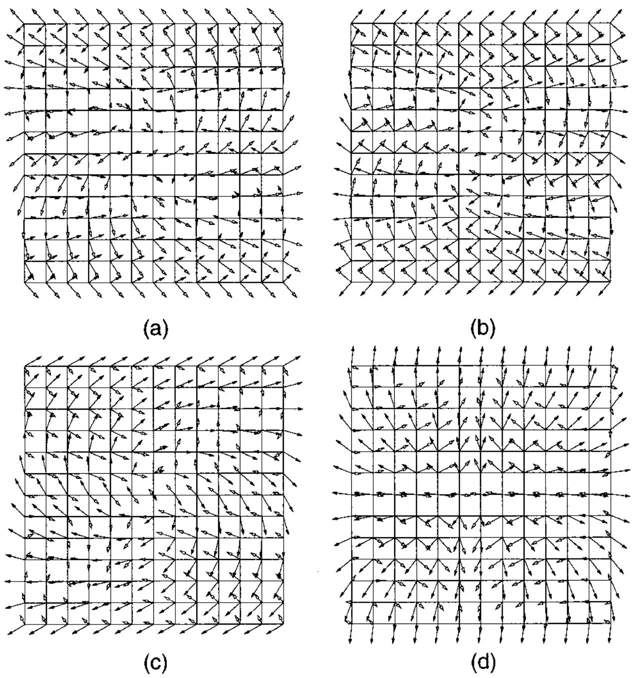

FIG. 4. The relative phase between s-wave and d-wave components corresponding to the vortex as in Figs. 2 and 3, but here in (d) $\alpha_s=-1$. The s-wave component order parameter is represented with a white arrow and the d-wave component with a black one. The angle between the two vectors is the relative phase. The length of the vectors represents the amplitude of s-wave and d-wave component, normalized by the maximum of themselves separately.

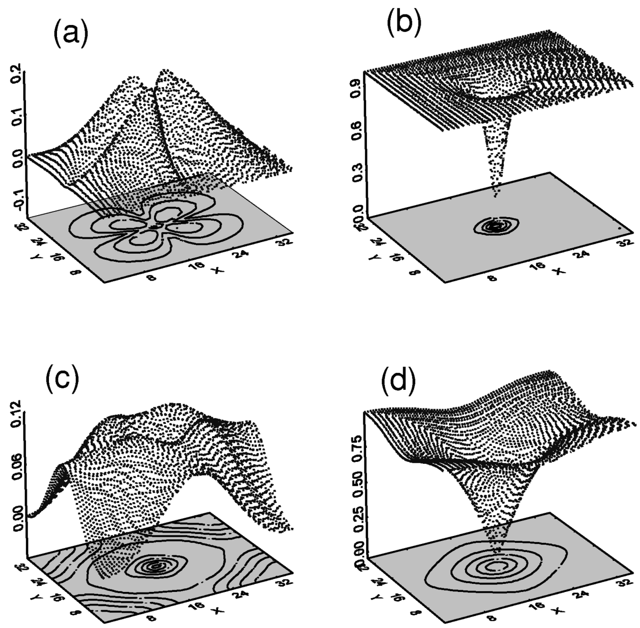

FIG. 5. Surface-contour plots of the amplitude of s-wave component and d-wave component at different magnetic fields: (a) for s component and (b) for d component of a superconductor with one flux threaded in a cell of 19×19 grid size with an area of $323\xi^2$, which gives a magnetic induction of $B_1\approx 0.02B_{c2}$; (c) for s component and (d) for d component of a superconductor with one flux threaded in a cell of 19×19 grid size with an area of $30\xi^2$, which gives a magnetic induction of $B_2\approx 0.2B_{c2}$. The parameter κ is set to 3, and $\alpha_s=0.65$.

cave with a twofold symmetry [as in Fig. 3(a)]. With decreasing α_s, the two protruding parts decrease and two concave parts move toward the center of the vortex, as shown in Figs. 3(b)–3(d). For $\alpha_s\leqslant\alpha_s^*$, the d-wave profile bears the same fourfold symmetry as that for the case of $\alpha_s\leqslant 0$.[22] The newly found twofold symmetry of the s-wave and d-wave components of a $d+is$ superconductor is quite interesting. Such a symmetry lowering is inherent in the fact that the two T-breaking phases respond differently to the magnetic field.

The interesting changes in symmetry and magnitude of the s- and d-wave components as α_s decreases from above to below $\frac{2}{3}$ are also accompanied by the changes in the relative phase between the s- and d-wave components around the vortex. Figure 4 represents the comparison of the relative phase at various values of α_s. For α_s close to 1 [Figs. 4(a) and 4(b)], the s- and d-wave components have almost the same magnitude and winding symmetry, so a relative phase of roughly $\pi/2$ is maintained almost everywhere except near the center of the vortex. Interestingly, for α_s close to α_s^* [Fig. 4(c)] and $\alpha_s\leqslant 0$ [Fig. 4(d)], the windings of the s- and d-wave components are very different, with one of them being negative and the other being positive, so that there appear regions of rapid variation of the relative phase. Domain walls with relative phases of almost 0 or π are directed along the X and Y axes separating the whole unit cell into four domains. In most parts of these domains the relative phase is close to 2θ with θ as the cylindrical angle.

We have also examined the effects of changing magnetic field on the vortex structure. Figure 5 gives the comparison of the s- and d-wave components at different magnetic fields with $\alpha_s=0.65$. With increasing magnetic fields, the s-wave component changes more significantly than the d-wave component does. Notice that, although the uniform bulk phase is a d wave at this value of α_s, the higher-field-induced s component may have significant impact on the transport

TABLE I. The dimensionless free-energy density f as a function of R and α_s. See the text for other parameters.

$R\backslash f\backslash\alpha_s$	0.97	0.85	0.7	0.5	-1.0
1.889	3.813460	3.409653	3.423665	3.410546	3.393548
1.732	3.783806	3.419661	3.409780	3.407971	3.392622
1.545	3.726939	3.446315	3.401404	3.397067	3.394437
1.3636	3.677390	3.508033	3.408743	3.572941	3.398383
1.1818	3.864845	3.568033	3.420000	3.412556	3.404588
1.0	3.652432	3.58466	3.4475	3.414125	3.412521

since its maximum amplitude is about 12% of the maximum d-wave amplitude in a relatively large region.[25] We believe that, although the relative phase between s- and d-wave components is nonzero for most cases in the presence of a magnetic field, only when the field-induced s component is not negligible with respect to that of the d-wave component in a relatively large region would the energy gap of the mixed waves play an important role in the thermomagnetic transport: the development of a non-negligible energy gap leads to the heat transport by quasiparticles vanishing at very low temperatures, which can result in a flat plateau in the thermal conductivity as a function of field.[13]

V. VORTEX LATTICE STRUCTURE

As we know, it is quite difficult to observe experimentally the detailed structure of a single vortex; therefore the influence of the single vortex structure on the arrangement of many vortices, which can be detected experimentally, is particularly interesting and important. We can study the vortex lattice structure using the finite-element method by threading two vortices in a rectangular unit cell. The vortex lattice shape is controlled by choosing the ratio R of the side lengths of the cell, and the steady-state solutions are obtained for various values of R in a unit cell with a fixed area (thus with a fixed magnetic induction). By comparing the free energies for various R at each α_s, we can find the equilibrium vortex lattice structure with the optimal value of R that minimizes the free energy. Table I presents the free-energy density f versus R and α_s. Note that $R=1$ corresponds to the square lattice, $R=\sqrt{3}$ corresponds to the triangular lattice, and intermediate values $1<R<\sqrt{3}$ correspond to oblique vortex lattices. It can be observed that the equilibrium lattice structure changes from a square to an oblique, and finally to a triangular lattice with decreasing α_s (from 0.97 to -1). The vortex lattice structure is affected by the structure and symmetry of a single vortex. In the previous section we have concluded that the structure and symmetry of the s- and d-wave components change with variation in α_s. The field distribution is affected by these changes as we now show. Figures 6(a) and 6(b) give the field distributions of $\alpha_s=0.97$ and $\alpha_s=-1$, with the same parameters as in Fig. 2. It is interesting to notice that the field distribution is anisotropic

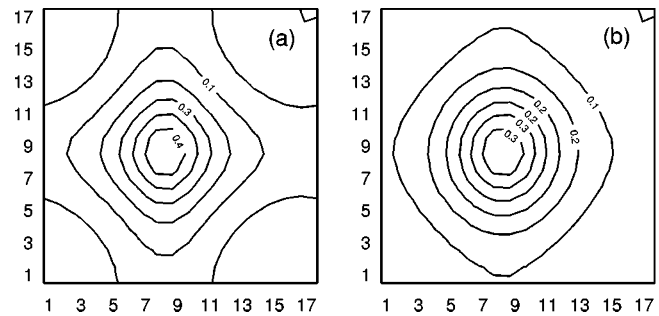

FIG. 6. The contour plots of local magnetic-field distribution for (a) $\alpha_s=0.97$, (b) $\alpha_s=-1$ with the same parameter as in Fig. 2.

and has a square profile in the middle region of the vortex at $\alpha_s=0.97$, while it has an oblique square profile at $\alpha_s=0.85$, and $\alpha_s=0.7$ (not plotted here). On the other hand, the field distribution is almost concentric around the vortex core at $\alpha_s=-1$. So the symmetry of the vortex lattice is strongly correlated with the local structure of a single vortex.

VI. SUMMARY

Numerical discussions have addressed the single vortex and vortex lattice structure of superconductors with attractive interactions in both the s- and d-wave channels. The $d+is$ state is stable when the relative strength α_s is higher than a critical value α_s^*. Simulation results of the single vortex have shown that its structure and symmetry also change across α_s^*. The relative phase between the s- and d-wave components for a $d+is$-wave state is different from that for a pure d-wave state. At low temperatures, the impact of the s-wave component in the d-dominant phase on the energy gap can be more significant as the magnetic field increases. The vortex lattice structure is also affected by the symmetry of the single vortex. It changes from a square to an oblique, and finally to a triangular lattice with the decrease of α_s.

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[23] The physical properties as a function of temperature discussed later are only qualitative, as the present T dependence of α_s is not quantitatively rigorous in the whole temperature range.

[24] Actually, we study the equilibrium state of a $d+is$ superconductor at various α_s by simulating the time-dependent GL equations with the finite element method described in Ref. 22.

[25] For a typical pure d-wave superconductor ($\alpha_s = -1.0$), the maximum amplitude of the field-induced s-wave component is only about 5% of the maximum d-wave amplitude and the s wave is distributed in a very small region under the same magnetic field (not shown here).