PHYSICAL REVIEW B VOLUME 53, NUMBER 6 1 FEBRUARY 1996-II

Structures of single vortex and vortex lattice in a *d*-wave superconductor

Ji-Hai Xu, Yong Ren, and Chin-Sen Ting
Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77204
(Received 10 November 1995)

The structures of a single vortex and vortex lattice in a superconductor with $d_{x^2-y^2}$ symmetry are studied self-consistently employing a recently developed Ginzburg-Landau theory. Near a single vortex, we found that an s-wave component of the order parameter is always induced, and it causes the local magnetic-field distribution and the d-wave order parameter to have a fourfold anisotropy. It is shown that there is a strong correlation between the structure of a single vortex and the shape of the vortex lattice. Our numerical calculation indicates that the structure of the vortex lattice is always oblique except for temperatures very close to T_c where it becomes triangular. The possible connection of the result with experiment is also discussed.

The symmetry of the order parameter in high-temperature superconductors is of current interest. Recently, a class of experiments designed to directly probe this quantity have provided strong evidence for a sign change of the order parameter on the Fermi surface,[1–3] consistent with $d_{x^2-y^2}$ symmetry. Thus it is necessary to consider new physics which might arise in a d-wave superconductor.

It is well known that the Ginzburg-Landau (GL) theory is the most useful method to study the basic phenomenology of conventional s-wave superconductivity. Recently, we have derived the microscopic GL equations of a $d_{x^2-y^2}$ superconductor,[4] on the basis of Gor'kov's approach.[5] In our derivation, the interaction between electrons is assumed to be attractive in the d-wave channel and repulsive in the s-wave channel, so that the uniform superconductor always has a purely d-wave pairing state. We showed that the GL free energy for a $d_{x^2-y^2}$ superconductor can be expressed in terms of two order parameters, $\psi_s(\mathbf{r})$ and $\psi_d(\mathbf{r})$:

$$f=\tilde{\alpha}_s(T)|\psi_s|^2-|\psi_d|^2+\tfrac{4}{3}|\psi_s|^4+\tfrac{1}{2}|\psi_d|^4+\tfrac{8}{3}|\psi_s|^2|\psi_d|^2 +\tfrac{2}{3}(\psi_s^{*2}\psi_d^2+\psi_d^{*2}\psi_s^2)+2|\tilde{\Pi}\psi_s|^2+|\tilde{\Pi}\psi_d|^2+(\tilde{\Pi}_x\psi_s\tilde{\Pi}_x^*\psi_d^* -\tilde{\Pi}_y\psi_s\tilde{\Pi}_y^*\psi_d^*+\text{H.c.})+\kappa^2(\boldsymbol{\nabla}\times\mathbf{A})^2. \tag{1}$$

Here we have put the free energy into the dimensionless form with $\tilde{\Pi}=i\boldsymbol{\nabla}-\mathbf{A}$, κ being the GL parameter, and

$$\tilde{\alpha}_s(T)=\alpha_s/(1-T/T_c), \tag{2}$$

where $\alpha_s=4(1+2V_s/V_d)/N(0)V_d$ is a positive constant, with $V_s>0$ $(-V_d<0)$ being the effective interaction strength in s- (d-) wave channel, and $N(0)$ the density of states at the Fermi level. It can be seen that the superconducting state described by Eq. (1) is purely d wave in the bulk with a single transition temperature T_c. This is very different from the earlier work on mixed s and d state, where the interaction was assumed to be attractive in both s- and d channels.[6] Consequently, such a mixed $s+d$ state could persist even in a uniform system, and of course led to two transition temperatures.[6]

In the present work, we will use Eq. (1) to study the structure of vortices in a d-wave superconductor. We should mention that the d-wave vortex was considered by Volovik[7] based on the symmetry consideration. Recently the numerical calculations of single vortex within the framework of the Bogoliubov–de Gennes equations,[8] and of the vortex lattice using phenomenological GL equations[9] have been reported. Here we present a self-consistent calculation for the structures of the single vortex and the vortex lattice on the basis of our microscopic GL theory for a d-wave superconductor.

The variation of f with respect to the order parameters ψ_s, ψ_d, and the vector potential $\mathbf{A}$ leads to the differential GL equations, as given in Ref. 4. It is interesting to note that the only parameter in Eq. (1) which depends explicitly on temperature is $\tilde{\alpha}_s(T)$, as given in Eq. (2). The parameter α_s or $\tilde{\alpha}_s(T)$ at $T=0$ could be determined by the material properties of the system. Nevertheless, we note that $\tilde{\alpha}_s(T)$ in Eq. (2) is almost constant in a wide temperature range below $0.9T_c$, and increases dramatically as $T\rightarrow T_c$. We will show that such temperature dependence of $\tilde{\alpha}_s(T)$ has a strong effect on the vortex structures.

In the following, we perform a numerical study of the discretized GL free energy (1) using numerical relaxation approach.[10,11] In order to describe a superconductor in the magnetic field, we use the constraint of fixing the average magnetic induction $\mathbf{B}$ by specifying the total flux Φ in the unit cell, and impose the periodic boundary conditions. If a special gauge is chosen such that A_x is independent of x, we obtain very simple boundary conditions: $A_x(0)=A_x(L_y)$ and $A_y(L_x,y)-A_y(0,y)=\Phi/L_y$. The other boundary conditions need only to obey the gauge invariance and can be taken as[11,12] $A_y(x,L_y)=A_y(x,0)$, $\psi_s(x,L_y)=\psi_s(x,0)\exp(i\Phi/2)$, $\psi_s(L_x,y)=\psi_s(0,y)\exp(iy\Phi/L_y)$, $\psi_d(x,L_y)=\psi_d(x,0)\exp(i\Phi/2)$, and $\psi_d(L_x,y)=\psi_d(0,y)\exp(iy\Phi/L_y)$. With Eq. (1) and the above boundary conditions, we can now realize the relaxation procedure: choosing ψ_s, ψ_s^*, ψ_d, ψ_d^*, A_x, and A_y as independent variables, we can write down the relaxation iteration equations

$$\psi_s^{(n+1)}=\psi_s^{(n)}-\epsilon_1\frac{\partial f}{\partial\psi_s^*}\bigg|^{(n)}, \tag{3}$$

$$\psi_d^{(n+1)}=\psi_d^{(n)}-\epsilon_2\frac{\partial f}{\partial\psi_d^*}\bigg|^{(n)}, \tag{4}$$

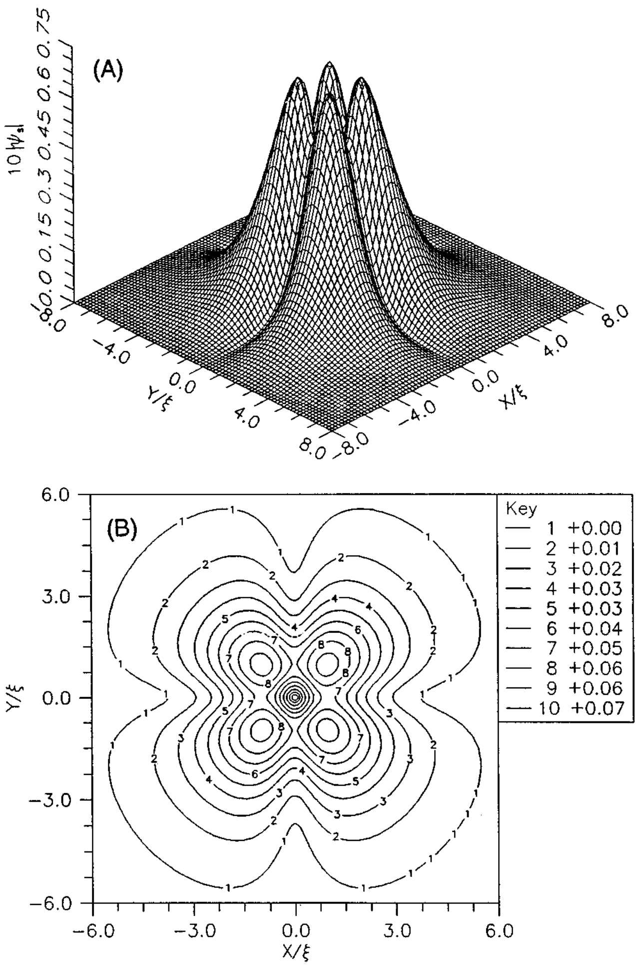

FIG. 1. Distribution of $|\psi_s|$ around a single vortex for $T/T_c = 0.5$, $\alpha_s = 1$, and $\kappa = 2$: (A) surface plot and (B) contour plot.

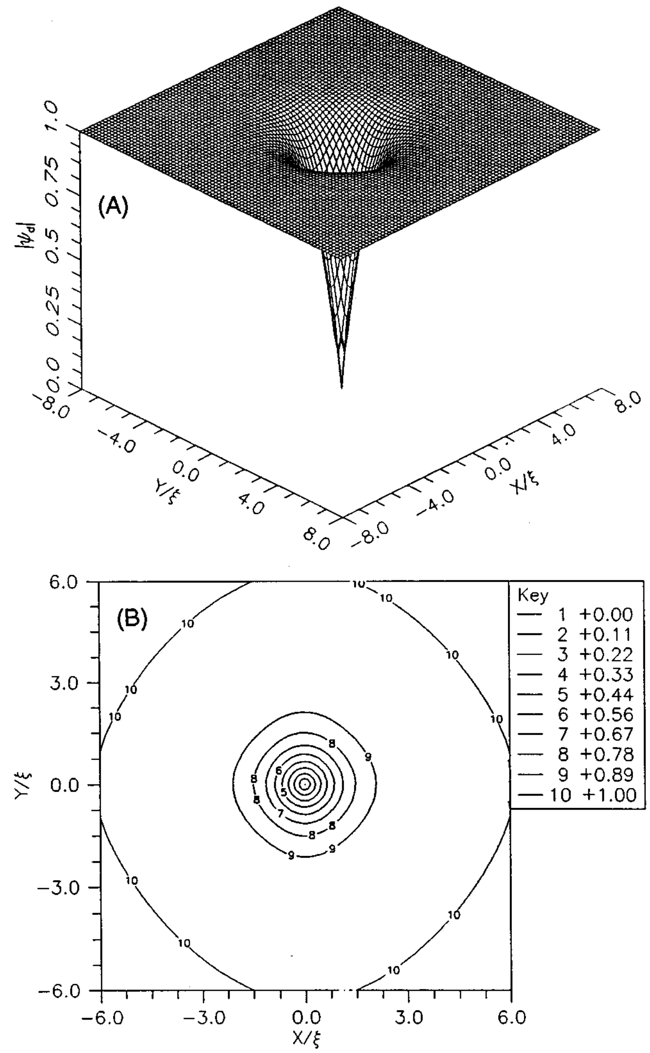

FIG. 2. Same as Fig. 1 but for $|\psi_d|$.

$$A_x^{(n+1)} = A_x^{(n)} - \epsilon_3 \frac{\partial f}{\partial A_x}\bigg|^{(n)}, \tag{5}$$

$$A_y^{(n+1)} = A_y^{(n)} - \epsilon_4 \frac{\partial f}{\partial A_y}\bigg|^{(n)}, \tag{6}$$

where ϵ's are all positive numbers to be adjusted to optimize the convergence rate and n is an integer labeling the generations of iteration. It has been shown that f will monotonically decrease to its optimum state as n increases as long as we choose a proper initial state.[10]

When temperature is not too close to T_c, the most interesting feature of a single vortex is that the s-wave component with an amplitude of about 0.1 is induced around the core, as shown in Figs. 1(A) (surface plot) and 1(B) (contour plot) where we have taken $\alpha_s = 1$, $T/T_c = 0.5$, and $\kappa = 2$. One can clearly see that the distribution of $|\psi_s|$ exhibits the profile in the shape of a four-leafed clover, which is in perfect agreement with our analytical result.[4] We find that the presence of this fourfold symmetric s-wave component causes redistribution of the d-wave order parameter $|\psi_d|$ (Fig. 2) and the local magnetic field h (Fig. 3) around the vortex. Namely, both $|\psi_d|$ and h show fourfold anisotropy far away from the core, even though they are isotropic close to the vortex center. By increasing κ, we find that the qualitative feature of the single vortex does not change, but the fourfold anisotropic structure of h moves far away from the vortex center.

Figures 4(A) and 4(B) show the phases of the d-wave and s-wave order parameter respectively. Far away from the core, the slight asymmetry in the x and y directions is due to the special gauge choice used in our calculation. We all know that the phase itself, like the vector potential $\mathbf{A}$, is not a physical observable and allows to have an arbitrary gauge choice. The quantity we are interested in is the phase difference between s- and d-wave order parameters, which is gauge-choice independent. We clearly see from Fig. 4 that near the vortex core, the induced s-wave component has an opposite winding relative to the d-wave order parameter. Our calculation also shows that the qualitative behavior of the single vortex structure remains unchanged in a wide temperature range below T_c, because $\tilde{\alpha}_s$ is of the same order of magnitude as long as the temperature is not too close to T_c.

As $T \to T_c$, $\tilde{\alpha}_s$ may become very large [see Eq. (2)]. In this case, we find that although the fourfold symmetric s-wave component is still induced around the vortex, its magnitude decreases as $1/\tilde{\alpha}_s$ and may become very small. Such a small s-wave component ($\sim 10^{-3}$ for $T/T_c = 0.95$)

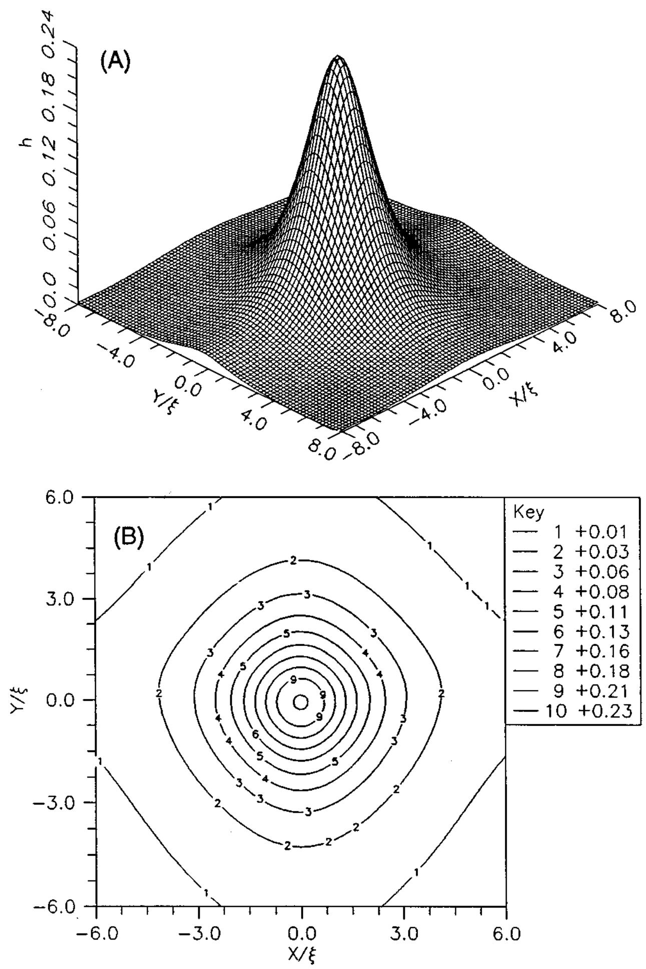

FIG. 3. Same as Fig. 1 but for h.

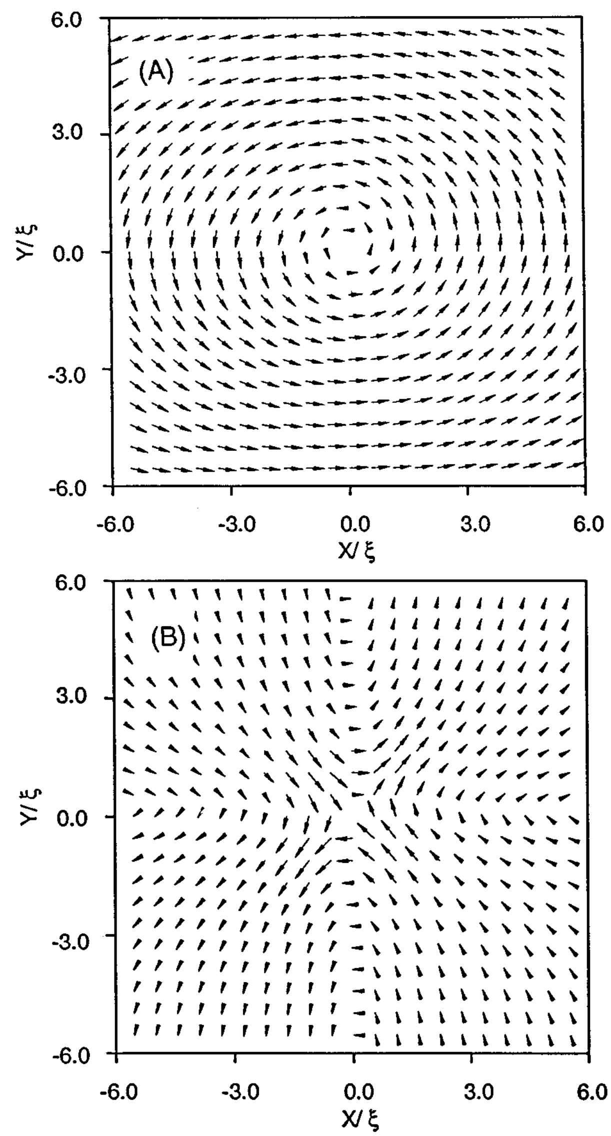

FIG. 4. Phases of ψ_d (A) and ψ_s (B).

has a little effect on the distribution of ψ_d and h. So, the vortex structure in this case is basically isotropic, similar to that in a conventional s-wave superconductor.

The structure change of a single vortex from fourfold anisotropic to isotropic with temperature will affect the vortex lattice structure. To check this, we have studied the vortex lattice described by Eq. (1) using numerical relaxation method in a rectangular unit cell with two vortices. The periodic boundary condition is also used. The ratio of $R = a_y / a_x$ (where a_x and a_y are our discretized lattice parameters in x and y directions, respectively) controls the shape of the vortex lattice.[12] For example, $R=1$ corresponds to the square, while $R=\sqrt{3}$ corresponds to the triangular lattice. We have calculated the dependence of the free energy on R for various temperatures at fixed external magnetic field $H=0.8$ and $\kappa=2$ (variations of H and κ only change results slightly, with the qualitative physics remaining unchanged; precisely, with the increase of H and κ the minimum of the free energy tends to shift toward a slightly smaller R). We find that when $T/T_c=0.5$, the free energy is minimized by $R=1.35$, signaling that an oblique vortex lattice is stable. Figure 5(A) shows the oblique lattice formed by the local magnetic field. The oblique lattice is expected to be preferred in a wide temperature range, because $\tilde{\alpha}_s$ is almost constant. However, as $T \rightarrow T_c$, the minimum of the free energy moves very rapidly toward $R=\sqrt{3}$, i.e., the triangular lattice is stabilized, as shown in Fig. 5(B) where we have taken $T/T_c=0.95$.

It is interesting to note the correlation between the single vortex structure and the vortex lattice. In a wide range below T_c, the d-wave order parameter and the local magnetic-field distribution exhibit fourfold anisotropy around the vortex, caused by the presence of a sizable s-wave component. These anisotropic single vortices tend to form an oblique vortex lattice. On the other hand, when $T \rightarrow T_c$ and $\tilde{\alpha}_s$ becomes large, the induced s-wave component is strongly suppressed. Although it still shows fourfold symmetry, its magnitude is too small to affect the single vortex structure. Consequently, both ψ_d and h have isotropic distribution around the vortex core, similar to the s-wave vortex. These isotropic isolated vortices prefer to have a triangular vortex lattice, identical to the vortex lattice in an s-wave superconductor,[13] as expected.

In the above calculation, the orientation of the vortex lattice has been assumed to be along the [100] axis. We also

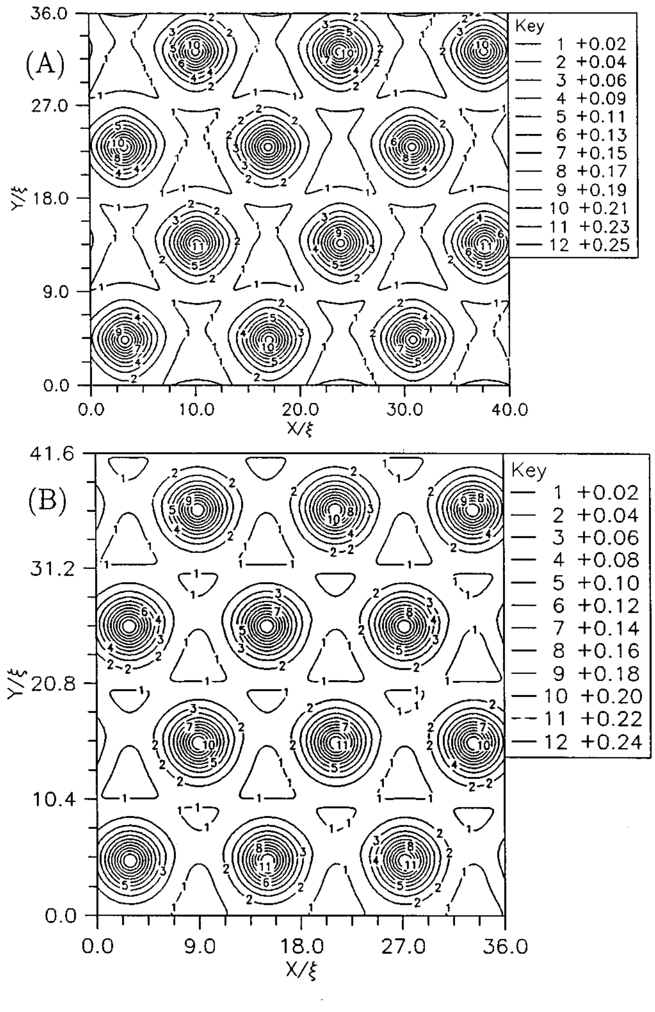

FIG. 5. Contour plots of the local magnetic field h for (A) $T/T_c = 0.5$ and $R = 1.35$, corresponding to an oblique lattice; (B) $T/T_c = 0.95$ and $R = \sqrt{3}$, corresponding to a triangular lattice. The solution in the rectangular unit cell with two vortices has been replicated three times in the x direction and two times in the y direction.

consider the possibility of along the [110] direction. In this case, we can still use the same boundary conditions as we did for the [100] direction, but the coordinates in Eq. (1) must be rotated by 45°. Under this transformation, the free energy becomes

$$
\begin{aligned}
f = {} & \tilde{\alpha}_s(T)|\psi_s|^2 - |\psi_d|^2 + \tfrac{4}{3}|\psi_s|^4 + \tfrac{1}{2}|\psi_d|^4 + \tfrac{8}{3}|\psi_s|^2|\psi_d|^2 \\
& + \tfrac{2}{3}(\psi_s^{*2}\psi_d^2 + \psi_d^{*2}\psi_s^2) + 2|\tilde{\Pi}\psi_s|^2 + |\tilde{\Pi}\psi_d|^2 + (\tilde{\Pi}_x\psi_s\tilde{\Pi}_y^*\psi_d^* \\
& - \tilde{\Pi}_y\psi_s\tilde{\Pi}_x^*\psi_d^* + \mathrm{H.c.}) + \kappa^2(\boldsymbol{\nabla}\times\mathbf{A})^2. \qquad (7)
\end{aligned}
$$

We have repeated the numerical relaxation calculation using the above equation for the orientation of the vortex lattice along the [110] direction. We still find that the oblique lattice is stable in a wide temperature region, similar to that in the [100] direction. Furthermore, we note that the free energy for both cases is almost the same, and is still slightly higher along the [110] direction.

Our results indicate that for a single vortex in a superconductor with $d_{x^2-y^2}$ symmetry, one expects to have a fourfold symmetric vortex structure in a wide temperature range. We believe that this fourfold anisotropy of the single vortex, in principle, could be realized by directly measuring the distribution of the local magnetic field around the vortex using the scanning superconducting quantum interference devices.[2] Correspondingly, one would also expect to observe an oblique vortex lattice in a wide temperature region. In fact, such an oblique lattice structure has been recently observed by small angle neutron scattering on $YBa_2Cu_3O_7$ samples.[14] Only when temperature is very close to T_c, the isotropic single vortex and a triangular vortex lattice structures may become possible.

We thank Dr. Z. D. Wang for a useful discussion on the numerical relaxation method. This research was supported by the State of Texas through the Texas Center for Superconductivity at the University of Houston, the Texas Advanced Research Program, and by the Robert A. Welch Foundation.

[1] D. A. Wollman, D. J. Van Harlingen, W. C. Lee, D. M. Ginsberg, and A. J. Leggett, Phys. Rev. Lett. **71**, 2134 (1993).
[2] C. C. Tsuei *et al.*, Phys. Rev. Lett. **73**, 593 (1994).
[3] J. H. Miller, Jr. *et al.*, Phys. Rev. Lett. **74**, 2347 (1995).
[4] Y. Ren, J. H. Xu, and C. S. Ting, Phys. Rev. Lett. **74**, 3680 (1995).
[5] L. P. Gor'kov, Zh. Éksp. Teor. Fiz. **36**, 1918 (1959) [Sov. Phys. JETP **9**, 1364 (1960)].
[6] R. Joynt, Phys. Rev. B **41**, 4271 (1990).
[7] G. E. Volovik, JETP Lett. **58**, 469 (1993).
[8] P. I. Soininen, C. Kallin, and J. A. Berlinsky, Phys. Rev. B **50**, 13 883 (1994).
[9] A. J. Berlinsky, A. L. Fetter, M. Franz, C. Kallin, and P. I. Soininen, Phys. Rev. Lett. **75**, 2200 (1995).
[10] S. L. Alder and T. Piran, Rev. Mod. Phys. **56**, 1 (1984).
[11] Z. D. Wang and C. R. Hu, Phys. Rev. B **44**, 918 (1991).
[12] M. M. Doria, J. E. Gubernatis, and D. Rainer, Phys. Rev. B **41**, 6335 (1990).
[13] W. H. Kleiner, L. M. Roth, and S. H. Autler, Phys. Rev. **133**, A1266 (1964).
[14] B. Keimer *et al.*, J. Appl. Phys. **76**, 6778 (1994).