PHYSICAL REVIEW B VOLUME 59, NUMBER 2 1 JANUARY 1999-II

Expansion of the vortex cores in $YBa_2Cu_3O_{6.95}$ at low magnetic fields

J. E. Sonier,* R. F. Kiefl, J. H. Brewer, D. A. Bonn, S. R. Dunsiger, W. N. Hardy, R. Liang, and R. I. Miller
TRIUMF, Canadian Institute for Advanced Research and Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1

D. R. Noakes and C. E. Stronach
Department of Physics, Virginia State University, Petersburg, Virginia 23806

(Received 27 October 1998)

Muon-spin-rotation spectroscopy has been used to measure the effective size r_0 of the vortex cores in optimally doped $YBa_2Cu_3O_{6.95}$ as a function of temperature T and magnetic field H deep in the superconducting state. While r_0 at $H=2$ T is close to 20 Å and consistent with that measured by scanning tunneling microscopy at 6 T, we find a striking increase in r_0 at lower magnetic fields, where it approaches an extraordinarily large value of about 100 Å. This suggests that the average value of the superconducting coherence length ξ_{ab} in cuprate superconductors may be much larger than previously thought at low magnetic fields in the vortex state. [S0163-1829(99)50702-9]

The vortex core in a type-II superconductor is a region in which the superconducting order parameter $\psi(\mathbf{r})$ is strongly suppressed. The size of the vortex core is therefore closely related to the coherence length ξ, which is the smallest length over which $\psi(\mathbf{r})$ can change appreciably. Some time ago Caroli *et al.*[1] predicted that a discrete spectrum of quasiparticle excitations exists within a radius ξ of the vortex axis. A scanning tunneling microscopy (STM) experiment on the conventional type-II superconductor $NbSe_2$ by Hess *et al.*[2] confirmed the existence of these localized states in the vortex core. Since then both muon-spin-rotation (μSR) (Ref. 3) and STM (Ref. 4) measurements have shown that the vortex core size r_0 in $NbSe_2$ decreases with increasing magnetic field, in a manner which scales with the increased strength of the vortex-vortex interactions. These same techniques[3,5,6] have also shown that r_0 shrinks with decreasing temperature, as predicted by the so-called "Kramer-Pesch effect."[7]

The electronic structure of the vortex cores in the high-T_c superconductors (HTS's) is less certain. Experiments performed on $YBa_2Cu_3O_{7-\delta}$ (YBCO) (Refs. 8 and 9) and $Nd_{1.85}Ce_{0.15}CuO_{4-\delta}$ (NCCO) (Ref. 10) seem to support the existence of a few bound quasiparticle states in the vortex core. On the other hand, no evidence of such localized states was found in a recent STM study of the vortex core in under- and overdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSSCO).[11] Instead the tunneling spectra in the vortex core resembled the pseudogap which forms at the Fermi surface in the normal state of this material. It should be noted that the vortex lattice studied in Ref. 11 was either melted or consisted of randomly pinned pancake vortices.

It is now widely accepted that the order parameter in the hole-doped HTS's (which excludes NCCO) have a $d_{x^2-y^2}$-wave symmetry. Several authors have pointed out[12,13] that bound quasiparticle states are unlikely to exist in a vortex of a $d_{x^2-y^2}$-wave superconductor because of the nodes which are present in the energy gap function $\Delta_{\hat{k}}=\Delta_0(\hat{k}_x^2-\hat{k}_y^2)$ along the directions $|\hat{k}_x|=|\hat{k}_y|$. One way of explaining experiments on HTS's which support localized states in the vortex core, is to introduce additional components into $\psi(\mathbf{r})$ (e.g., a d_{xy}-wave component).[14] However, there is currently no direct evidence for an order parameter of mixed symmetry in the bulk of HTS's.

In a previous study,[15] we determined the size of the vortex cores in the underdoped compound $YBa_2Cu_3O_{6.60}$. The electronic structure of the cores in underdoped YBCO has yet to be investigated with STM, although one may anticipate a local density of states resembling the normal-state pseudogap, as in underdoped BSCCO.[11] In Ref. 15, r_0 was found to change as a function of T and H in a manner similar to that observed in $NbSe_2$, but with a considerably weaker temperature dependence. Hayashi *et al.*[16] recently suggested that this may indicate that the quantum limit is established at a much higher temperature in $YBa_2Cu_3O_{6.60}$ because of the small value of ξ relative to that in $NbSe_2$. Generally speaking, ξ is considered to be "short" in the HTS's (e.g., <20 Å).[17] This is one of the primary features which distinguish them from conventional superconductors. In $YBa_2Cu_3O_{6.60}$, r_0 was found to be as large as 80 Å at low magnetic fields, which suggests that ξ is in excess of 20 Å. However, this is a phase with a T_c of 60 K, so ξ is expected to be somewhat larger than in a higher-T_c sample. Thus, it is of great interest to check the size and field dependence of r_0 in optimally doped $YBa_2Cu_3O_{6.95}$, with the maximum T_c of 93 K. Unlike in underdoped YBCO, the formation of the pseudogap in $YBa_2Cu_3O_{6.95}$ appears to coincide with the superconducting gap at T_c. The STM study of the vortex core by Maggio-Aprile *et al.*[8] in near optimally doped YBCO clearly shows two peaks within a gaplike structure, indicating the presence of bound quasiparticle states.

In this paper we present μSR measurements of the effective vortex core size in $YBa_2Cu_3O_{6.95}$ as a function of temperature and magnetic field applied along the $\hat{\mathbf{c}}$ axis of the crystals. Our measurements of r_0 are shown to be consistent with the STM study of Ref. 8 at $H=6$ T. Surprisingly, we find that at low fields r_0 increases to a comparatively large value of 100 Å. A simple interpretation of this result would be that the length scale over which the order parameter changes in the region of the vortex core (i.e., the definition of the coherence length as pertaining to the vortex state) is considerably larger than the nominal and accepted value of about 20 Å measured in high magnetic fields.

We report here measurements of r_0 in three different samples of $YBa_2Cu_3O_{6.95}$. The magnetic field distributions in two of these samples were previously recorded.[18] The first (TW1) was a mosaic of three crystals whereas the other (TW2) was a single crystal. All of these crystals contained twin boundaries and had transition temperatures of 93.2(0.25) K. We also report here measurements taken in TW2 after removing the twin boundaries. Detwinning was achieved by applying uniaxial stress to the crystal with the sample heated to no more than 250 °C in an oxygen atmosphere. Subsequent to the mechanical detwinning process, the crystal was reannealed to set the oxygen doping level. The μSR experiments were performed on the M15 and M20 surface beamlines at TRIUMF. Our experimental setup is described elsewhere.[19]

Although μSR does not directly probe the electronic structure of the vortex cores, it does sample the distribution of local magnetic fields in the vicinity of the cores. The spin of an implanted muon precesses at a frequency which is directly proportional to the local magnetic field at the muon site. Since the local magnetic field rises to a maximum in the vortex cores where superconductivity is destroyed, r_0 is directly related to the high-field tail in the measured field distribution. The size of the core is not strictly defined, however, because there is no sharp discontinuity in spatial quantities between a normal vortex core and the surrounding superconducting material. Here, as in our previous work,[3,15] we define r_0 to be the radius about the vortex axis at which the supercurrent density $J_s(\mathbf{r})$ reaches its maximum value. This feature allows us to accurately monitor changes in the effective size of the vortex cores. The supercurrent density $J_s(\mathbf{r})$ is obtained from the field profile $\mathbf{B}(\mathbf{r})$ through the Maxwell relation $J_s(\mathbf{r})=|\nabla\times\mathbf{B}(\mathbf{r})|$. In fitting the measured muon spin precession signal, some modeling of $\mathbf{B}(\mathbf{r})$ is required. However, to appreciate the accuracy of the present study it is important to realize that the $J_s(\mathbf{r})$ profile does not depend on the validity of the model assumed, since it is essentially the same for any function $\mathbf{B}(\mathbf{r})$ which fits the data well.

As in Refs. 3 and 15, the local field due to the vortex lattice at any point in the $\hat{a}$-$\hat{b}$ plane was modeled with a theoretical field distribution generated from a Ginzburg-Landau (GL) model[20]

$$B(\mathbf{r})=B_0(1-b^4)\sum_{\mathbf{G}}\frac{e^{-i\mathbf{G}\cdot\mathbf{r}}uK_1(u)}{\lambda_{ab}^2G^2}, \tag{1a}$$

where

$$u^2=2\xi_{ab}^2G^2(1+b^4)[1-2b(1-b)^2], \tag{1b}$$

B_0 is the average magnetic field, $\mathbf{G}$ are the reciprocal lattice vectors, $b=B_0/B_{c_2}$, ξ_{ab} is the GL coherence length and $K_1(u)$ is a modified Bessel function. We do not expect the conventional GL model to be valid deep in the superconducting state. However, this model gives a very good fit to the measured field distribution, which is all that is required to generate the corresponding $J_s(\mathbf{r})$ profile needed to determine r_0. The summation in Eq. (1) is taken over all reciprocal lattice vectors $\mathbf{G}$ of a triangular vortex lattice. This assumption is reasonable, because for field-cooled samples the vortex lattice geometry at low T is governed by the geometry of the lattice at the pinning temperature. We have shown previously[21] that the vortex lattice in our $YBa_2Cu_3O_{6.95}$ crystals is strongly pinned at low T and remains so upon warming up to $T\approx0.7T_c$. The lattice in the detwinned crystal depins at similar high temperatures. In a $d_{x^2-y^2}$-wave superconductor, the vortex lattice is predicted to be nearly triangular at temperatures close to T_c (e.g., see Ref. 22). We note that even if the lattice is not triangular, a good fit still yields the appropriate $J_s(\mathbf{r})$ profile.

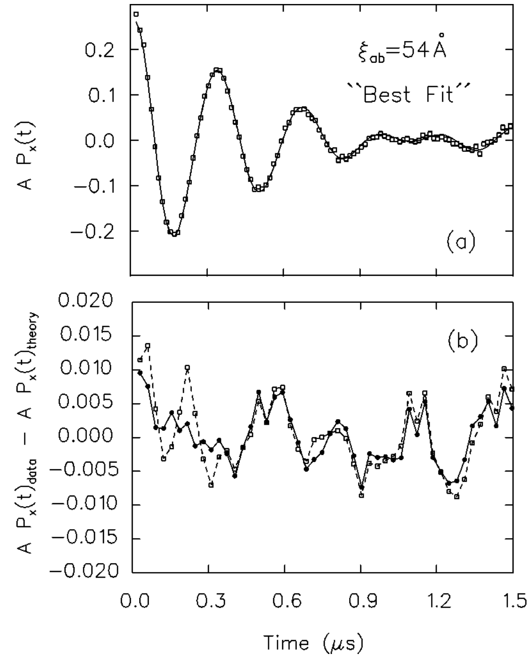

FIG. 1. (a) The muon precession signal in $YBa_2Cu_3O_{6.95}$ after field cooling to $T=5.8$ K in a magnetic field $H=0.498$ T. The solid line is a fit described in the text. (b) Difference between the measured precession signal and the theoretical polarization function [in (a)] assuming $\xi_{ab}=54$ Å (solid circles) and $\xi_{ab}=20$ Å (open squares). For visual clarity, we have doubled the bin size used in (a) and not shown the error bars ($\approx\pm0.003$).

All of the data were fit in the time domain with a theoretical muon polarization function constructed from the field profile of Eq. (1). This was multiplied by a Gaussian relaxation function $e^{-\sigma^2t^2/2}$ to account for any residual disorder in the vortex lattice and the contribution of the nuclear dipolar moments to the internal field distribution. The residual background signal was fit assuming a Gaussian broadened distribution of fields. The Fourier transform (FT) of the muon precession signal approximates the internal field distribution and resembles the predicted asymmetric line shape for an ordered lattice of vortices. However, the FT suffers from noise and broadening effects associated with the finite number of events and limited time range, so that the data must be analyzed in the time domain.

Figure 1(a) shows the first 1.5 μs of a typical muon precession signal in $YBa_2Cu_3O_{6.95}$ displayed in a reference

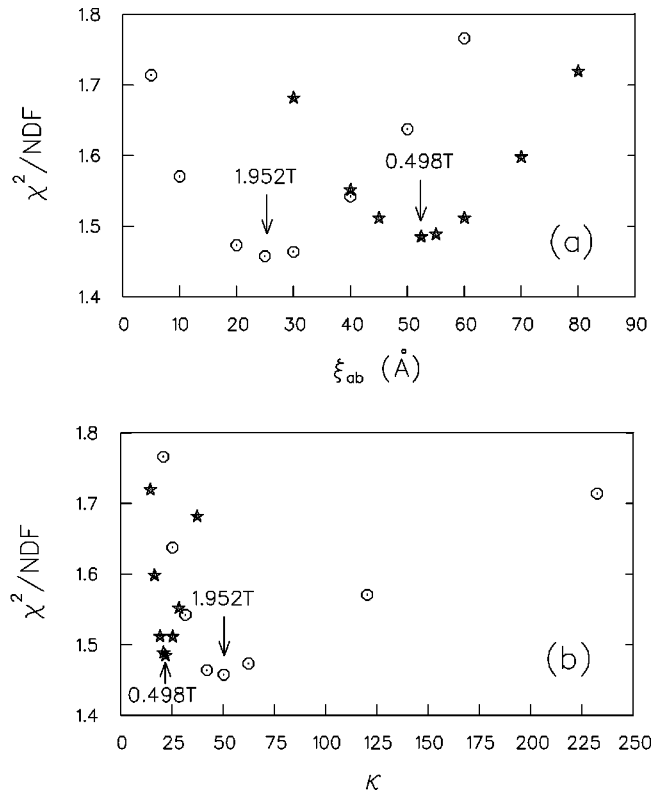

FIG. 2. (a) The ratio χ^2/NDF as a function of (a) ξ_{ab} and (b) κ (from the same fits) for $H=0.498$ T (stars, NDF=1148) and $H=1.952$ T (circles, NDF=1196) at $T=5.8$ K.

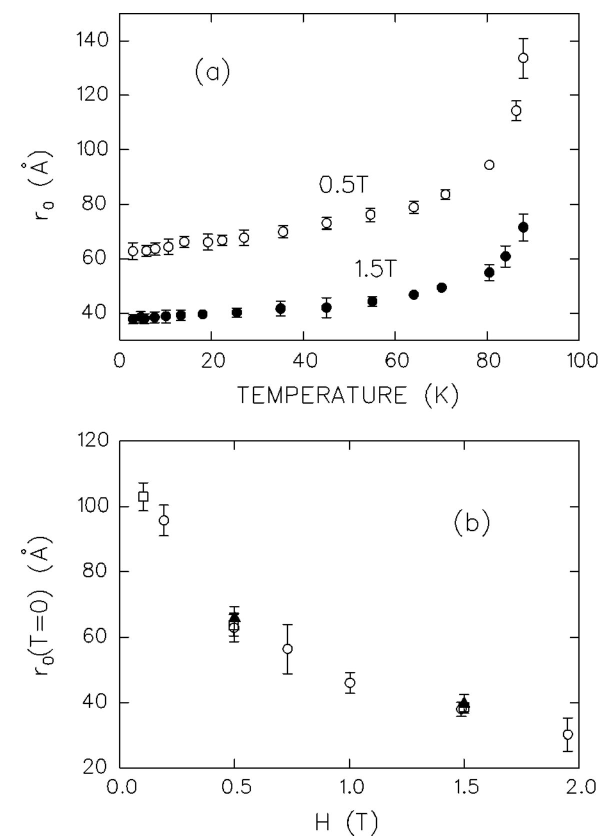

FIG. 3. (a) The temperature dependence of r_0 at 0.5 T (open circles) and 1.5 T (solid circles) in twinned $YBa_2Cu_3O_{6.95}$ (TW1). (b) The magnetic-field dependence of r_0 extrapolated to $T=0$. The twinned crystals TW1 and TW2 are shown as open circles and squares, respectively, whereas the detwinned crystal is denoted by solid triangles.

frame rotating at 3.3 MHz below the Larmor precession frequency of a free muon. The solid curve is a fit (actually performed over the first 6 μs) to the theoretical polarization function assuming $\xi_{ab}=54$ Å, with all other fitting parameters unconstrained. The difference between this fit and the measured spectrum is shown in Fig. 1(b), compared to the same assuming $\xi_{ab}=20$ Å. Note that the quality of the fit is most affected by a change in ξ_{ab} at early time, where the amplitude of the signal originating from the vortex lattice is largest. The ratio of χ^2 to the number of degrees of freedom (NDF) for fits assuming different values of ξ_{ab} is shown in Fig. 2(a) for two different magnetic fields. Due to the high statistics of the measured field distribution (i.e., typically 2×10^7 muon decay events), χ^2/NDF is greater than 1. Figure 2(b) shows that $\kappa=\lambda_{ab}/\xi_{ab}$ obtained from the same fits also depends on H.

Figure 3(a) shows the temperature dependence of r_0 at $H=0.5$ T and 1.5 T in sample TW1. The error bars represent the statistical uncertainty in the fitted values of ξ_{ab}. Both sets of data show a slight decrease in r_0 with decreasing temperature which is essentially linear below 50 K. The strength of the term linear in T is comparable to that previously reported in $YBa_2Cu_3O_{6.60}$,[15] which indicates that thermal vibrations are an unlikely source of the observed behavior. On the other hand, this linear term is considerably weaker than in $NbSe_2$,[3,6] a result consistent with the prediction of Ref. 16 that a vortex core containing only a few discrete bound states will stop shrinking below a relatively high saturation temperature. It should be noted that the core size is also predicted to shrink dramatically with decreasing T in a pure $d_{x^2-y^2}$-wave superconductor,[13] which does not agree with the weak temperature dependence observed here in YBCO.

Figure 3(b) shows the magnetic-field dependence of r_0 extrapolated to $T=0$. Included in this figure are data from all three samples. Note that there is excellent agreement between the twinned and detwinned crystals. In Ref. 15 it was shown that detwinning a $YBa_2Cu_3O_{6.60}$ single crystal had virtually no effect on the deduced values of r_0, even though there was evidence for distortions in the vortex lattice caused by twin boundary pinning. We find that the fitted parameter ξ_{ab} changes as a function of T and H in a manner similar to that of r_0, with $\xi_{ab}\approx[0.828(23)r_0+0.72(1.24)]$ Å. Thus at large H where r_0 is small, we have $\xi_{ab}\approx r_0$. It is important to note, however, that unlike r_0, the precise behavior of ξ_{ab} does depend on the theoretical model used for $B(\mathbf{r})$. Although the GL model is invalid here, our measurements in both $NbSe_2$ and $YBa_2Cu_3O_{7-\delta}$ qualitatively resemble the T and H dependence of the core size predicted from a quasiclassical treatment of a vortex in both an s-wave and a $d_{x^2-y^2}$-wave superconductor.[16,23]

Some of the data in Fig. 3(b) are replotted in Fig. 4, along with the measurements of $r_0(H)$ in $YBa_2Cu_3O_{6.60}$ (from Ref. 15). As was the case in $NbSe_2$, both λ_{ab} and the ratio λ_{ab}/r_0 ($\sim\kappa$) at $T=0$ are well described by relations linear in H, so that

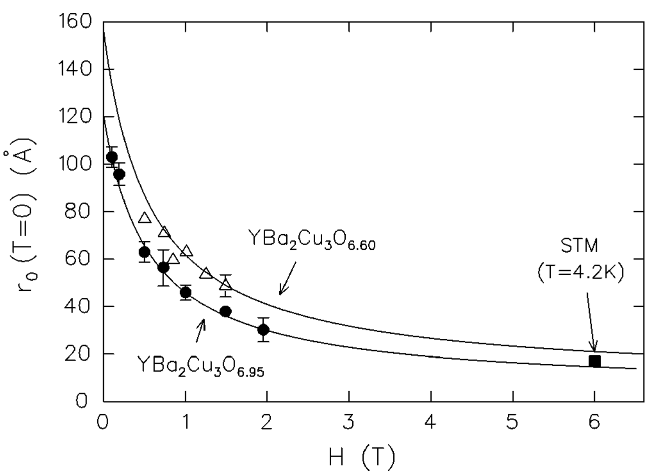

FIG. 4. The magnetic-field dependence of r_0 in $YBa_2Cu_3O_{6.95}$ (solid circles) and $YBa_2Cu_3O_{6.60}$ (open triangles) extrapolated to $T=0$. The solid square at $H=6$ T is the value of $\xi_{ab}\approx r_0$ deduced from the STM experiment (Ref. 8) on twinned $YBa_2Cu_3O_{7-\delta}$ at $T=4.2$ K. The solid curves are explained in the text.

$$r_0(H)=\frac{\lambda_{ab}(H)}{\lambda_{ab}(H)/r_0(H)}=r_0(0)\frac{[1+\beta H]}{[1+\gamma H]}. \qquad (2)$$

Recently the field dependence of λ_{ab} has been attributed to nonlinear and nonlocal effects[24] and a field-induced Doppler shift of the extended quasiparticle states associated with a $d_{x^2-y^2}$-wave vortex.[25] In sample TW1 which constitutes the most complete data set for $YBa_2Cu_3O_{6.95}$, $r_0(0)=120.7$ Å, $\beta=0.075$ T^{-1}, and $\gamma=1.82$ T^{-1}. On the other hand, in the twinned $YBa_2Cu_3O_{6.60}$ sample of Ref. 15 we find that $r_0(0)=156.3$ Å, $\beta=0.094$ T^{-1}, and $\gamma=1.77$ T^{-1}. The solid curves in Fig. 4 represent Eq. (2) with the corresponding values of $r_0(0)$, β, and γ. These extrapolations suggest that the shrinking of the vortex cores saturates at large H. Note that Eq. (2) can be written strictly in terms of the intervortex spacing L (since $L\propto\sqrt{H}$).

Maggio-Aprile *et al.*[8] attributed the two peaks observed in the spectrum for tunneling into a vortex core of YBCO at $T=4.2$ K and $H=6$ T, to the lowest bound quasiparticle energy level $E_{1/2}=5.5$ meV. Using the formula $E_{1/2}=2\mu\Delta_0^2/E_F$ from Ref. 1 and taking ξ_{ab} at low T to be equivalent to the BCS coherence length $\xi_0=\hbar v_f/\pi\Delta_0$, gives $\xi_{ab}=(2\hbar^2/m_e\pi^2E_{1/2})^{1/2}\approx 17$ Å. This result ($\approx r_0$) is plotted in Fig. 4. The agreement with the extrapolated curve from our μSR measurements[26] is striking and raises the possibility that the vortex cores in $YBa_2Cu_3O_{6.95}$ are conventional-like (i.e., they contain localized quasiparticle states). Several theoretical studies (e.g., see Ref. 14) have suggested that bound states may arise from a second component in the order parameter, induced by spatial variations in the $d_{x^2-y^2}$-wave component in the vicinity of a vortex core. If this is the case, the core expansion will be accompanied by the formation of numerous bound states, which should be detectable by STM. Thus far, STM has not been used to probe the vortex structure at low magnetic fields in the HTS's.

In conclusion, we have observed a large increase in the size of the vortex cores in $YBa_2Cu_3O_{6.95}$ at low magnetic fields, similar to the behavior reported in the conventional superconductor $NbSe_2$. The expansion of the cores appears to be a general property of superconductors in the vortex state. The agreement with STM measurements based on a conventional treatment of the vortex core in $YBa_2Cu_3O_{6.95}$, supports the existence of localized states in the core.

We thank K. Machida for helpful discussions. This work was supported by NSERC and US AFOSR Grant No. F49620-97-1-0297.

*Present address: Los Alamos National Laboratory, Los Alamos, New Mexico 87545.

[1] C. Caroli, P. G. de Gennes, and J. Matricon, Phys. Lett. **9**, 307 (1964).
[2] H. F. Hess *et al.*, Phys. Rev. Lett. **62**, 214 (1989).
[3] J. E. Sonier *et al.*, Phys. Rev. Lett. **79**, 1742 (1997).
[4] U. Hartmann, T. Drechsler, and C. Heiden, Proc. SPIE **1855**, 140 (1993).
[5] A. P. Volodin, A. A. Golubov, and J. Aarts, Z. Phys. B **102**, 317 (1997).
[6] R. I. Miller *et al.* (private communication).
[7] L. Kramer and W. Pesch, Z. Phys. **269**, 59 (1974).
[8] I. Maggio-Aprile *et al.*, Phys. Rev. Lett. **75**, 2754 (1995).
[9] K. Karrai *et al.*, Phys. Rev. Lett. **69**, 152 (1992).
[10] X. Jiang *et al.*, Physica C **254**, 175 (1995).
[11] Ch. Renner *et al.*, Phys. Rev. Lett. **80**, 3606 (1998).
[12] Y. Wang and A. H. MacDonald, Phys. Rev. B **52**, 3876 (1995).
[13] M. Ichioka *et al.*, Phys. Rev. B **53**, 15 316 (1996).
[14] M. Franz and Z. Tešanović, Phys. Rev. Lett. **80**, 4763 (1998).
[15] J. E. Sonier *et al.*, Phys. Rev. Lett. **79**, 2875 (1997).
[16] N. Hayashi *et al.*, Phys. Rev. Lett. **80**, 2921 (1998).
[17] Note that most estimates of ξ in YBCO are inaccurately obtained from measurements of the upper critical field H_{c2} near T_c, where the vortex lattice is dominated by thermal fluctuations; e.g., see K. K. Nanda, Physica C **265**, 26 (1996).
[18] J. E. Sonier *et al.*, Phys. Rev. B **55**, 11 789 (1997).
[19] R. F. Kiefl *et al.*, Hyperfine Interact. **86**, 467 (1994).
[20] A. Yaouanc, P. Dalmas de Réotier, and E. H. Brandt, Phys. Rev. B **55**, 11 107 (1997).
[21] J. E. Sonier *et al.*, Phys. Rev. Lett. **72**, 744 (1994).
[22] M. Franz, I. Affleck, and M. H. S. Amin, Phys. Rev. Lett. **79**, 1555 (1997).
[23] M. Ichioka, A. Hasegawa, and K. Machida, Phys. Rev. B (to be published).
[24] M. H. Amin, I. Affleck, and M. Franz, Phys. Rev. B **58**, 5848 (1998).
[25] I. Vekhter, J. P. Carbotte, and E. J. Nicol, Phys. Rev. B **59**, 1417 (1998).
[26] Note that our measurements are consistent with accepted values of H_{c2} in $YBa_2Cu_3O_{6.95}$ (>100 T). In Fig. 4, the coherence length which is related to H_{c2} is that at high magnetic field near the superconducting-to-normal phase boundary, not the value at low field.