Shrinking Magnetic Vortices in V_3Si due to Delocalized Quasiparticle Core States: Confirmation of the Microscopic Theory for Interacting Vortices

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We report muon-spin rotation measurements on the conventional type-II superconductor V_3Si that provide clear evidence for changes to the inner structure of a vortex due to the delocalization of bound quasiparticle core states. The experimental findings described here confirm a key prediction of recent microscopic theories describing interacting vortices. The effects of vortex-vortex interactions on the magnetic and electronic structure of the vortex state are of crucial importance to the interpretation of experiments on both conventional and exotic superconductors in an applied magnetic field.

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In 1964, a breakthrough paper by Caroli, de Gennes, and Matricon [1] showed that in the framework of the microscopic theory, quasiparticles (QPs) bound to an *isolated* vortex of a conventional s-wave type-II superconductor occupy discrete energy levels. Twenty-five years later, localized vortex core states were observed for the first time in $NbSe_2$ by scanning tunneling microscopy (STM) [2]. Our understanding of the vortex state in type-II superconductors has accordingly progressed from Abrikosov's initial prediction [3] based on the macroscopic Ginzburg-Landau (GL) theory [4] to current theories describing the electronic structure of magnetic vortices on a microscopic level. However, it is only in recent years that predictions have emerged from the microscopic theory on the effects of *vortex-vortex interactions*. In analogy with bringing atoms close together to form a conducting solid, increasing the vortex density by applying a stronger magnetic field H enhances the overlap of bound state wave functions of neighboring vortices, resulting in the formation of energy bands that allow the intervortex transfer of QPs [5–8]. This is expected to strongly influence experiments on conventional superconductors that are sensitive to quasiparticle excitations, such as specific heat and thermal transport, and to have profound effects on the magnetic structure of the vortex state. Identifying the potential interplay between vortices and quasiparticles is also of crucial importance in the study of high-temperature superconductors. In these and other exotic superconductors, comparatively little is known about the structure of the vortex state and its effect on experiments in large magnetic fields. It is therefore essential to have a solid understanding of the behavior of interacting vortices in conventional superconductors and to establish the connections with quasiparticle properties.

The effect of delocalized QP core states on the spatial variation of the pair potential $\Delta(r)$ at a vortex site has been considered in the framework of the quasiclassical Eilenberger theory [7–9]. These calculations show that the effect of the intervortex transfer of QPs on $\Delta(r)$ leads to a reduction of the size of the vortex cores with increasing H. Such shrinking of the vortex cores has, in fact, been observed by muon-spin rotation (μSR) [10–16] and STM [17] and has been proposed as a possible explanation for the anomalous low-field behavior observed of the specific heat in conventional superconductors [18,19]. However, experimentally there has been inadequate evidence in support of a causal relationship between the size of the vortex cores and the delocalization of bound QP core states.

An important finding has come by way of recent low-temperature thermal conductivity measurements, which are sensitive only to extended or delocalized electronic excitations. These studies have revealed the existence of highly delocalized QPs down to low magnetic fields in the vortex state of $LuNi_2B_2C$ [20], $YBa_2Cu_3O_{6.9}$ [21], $NbSe_2$ [22], and MgB_2 [23]. In the extreme gap anisotropy superconductors $LuNi_2B_2C$ and $YBa_2Cu_3O_{6.9}$, the dominant contribution to the thermal conductivity is believed to be a field-induced Doppler shift of the QP spectrum outside the vortex cores [24]. Most surprising are the results for $NbSe_2$, long believed to be representative of a simple conventional s-wave superconductor. The high degree of QP delocalization in $NbSe_2$ appears to arise from two-gap superconductivity [22], as is the case for MgB_2 [23]. In these superconductors, the heat at low fields is carried by the QP excitations associated with the smaller of the two energy gaps. This smaller gap is a possible source of the very large low-field value of the core size observed in $NbSe_2$ by μSR [10] and in MgB_2 by STM [25]. On the other hand, the large core size observed at low fields in borocarbide superconductors [15,16] and $YBa_2Cu_3O_{7-\delta}$ [11–13] is not completely understood.

The conventional superconductors V_3Si and Nb provide a unique opportunity to experimentally observe the effects of intervortex QP transfer on the inner structure of a vortex. In contrast to the above-mentioned superconductors, thermal conductivity measurements [22,26] reveal no appreciable delocalization of QP states at low H—as expected when the vortices are nearly isolated. V_3Si is particularly suitable, since it has a simple cubic crystal structure, a relatively high superconducting transition temperature ($T_c = 17$ K), and a large upper critical field ($H_{c2} \approx 185$ kOe). To determine the size of the vortex cores we measured the internal magnetic field distribution in V_3Si by μSR at the Tri-University Meson Facility, Vancouver, Canada. The experiment was performed by implanting spin-polarized muons, which stop randomly in the sample on the length scale ($\sim 10^2$–10^3 Å) of the vortex lattice (VL). The magnetic moment of the muon precesses about the local magnetic field B with a Larmor frequency given by $\nu = \gamma_\mu B$, where $\gamma_\mu = 0.0852\ \mu s^{-1}\,G^{-1}$ is the gyromagnetic ratio of the muon. The spatial distribution of B is determined by measuring the time evolution of the muon-spin polarization via the anisotropic distribution of decay positrons [27].

Small-angle neutron scattering [28] and recent STM [29] images of V_3Si show that for a field applied along the fourfold [001] axis, the VL undergoes a transition from hexagonal to square symmetry. Kogan *et al.* [30] have developed a phenomenological London model that attributes this transition to nonlocality of the relation between the supercurrent density $\mathbf{j}(\mathbf{r})$ and the vector potential $\mathbf{A}$ in a region around the vortex core. This establishes a connection between the vortex structure and the anisotropy of the Fermi surface, which in V_3Si produces fourfold symmetry near the vortex cores. We note that a more general model has recently been developed for fourfold symmetric superconductors, which incorporates the effects of both Fermi surface and gap anisotropy on the vortex structure [31]. At fields below 7.5 kOe where the intervortex spacing is large, the isotropic magnetic repulsion of vortices yields a hexagonal lattice. With increasing field there is an increased overlap of the fourfold symmetric regions of the individual vortices, and the VL evolves into a square at 40 kOe.

The Kogan model uses an arbitrary cutoff factor to overcome the logarithmic divergence of the internal magnetic field $B(r)$ at the vortex sites. We find that the μSR data are fit much better using a GL analog of the Kogan model, which properly accounts for the finite size of the vortex cores [32]. The spatial profile of the periodic local magnetic field in the GL formalism is given by

$$B(r) = B_0(1 - b^4)\sum_{\mathbf{G}} \frac{e^{-i\mathbf{G}\cdot\mathbf{r}} u K_1(u)}{\lambda^2 G^2 + \lambda^4(n_{xxyy}G^4 + dG_x^2 G_y^2)}. \tag{1}$$

Here $b = B/B_{c2}$ is the reduced field, B_0 is the average internal field, $\mathbf{G}$ are the reciprocal lattice vectors, $K_1(u)$ is a modified Bessel function, $u^2 = 2\xi^2 G^2(1 + b^4)[1 - 2b(1 - b)^2]$, ξ is the GL coherence length, and n_{xxyy} and d are dimensionless parameters arising from the nonlocal corrections. The quartic n_{xxyy} term is an isotropic correction, whereas the biquadratic d term controls the fourfold anisotropy.

Figure 1 shows Fourier transforms of both the measured muon-spin precession signal and the fit to the data in the time domain at 50 kOe applied parallel to [001]. In agreement with the imaging experiments, we obtained excellent fits to a square VL above 40 kOe, a hexagonal VL below 7.5 kOe, and to a rhombic unit cell with an apex angle $\beta \approx 60°$–$90°$ at intermediate fields. These fits and those to Kogan's model also yielded the following results: (i) For all H, $n_{xxyy} \approx 0$. This is consistent with an analogous model developed by Affleck, Franz, and Amin [33], who found that the quartic correction makes a negligible contribution. (ii) Below 7.5 kOe, excellent fits were obtained with $d = 0$. This indicates that the VL is not strongly tied to the underlying crystal lattice, as was

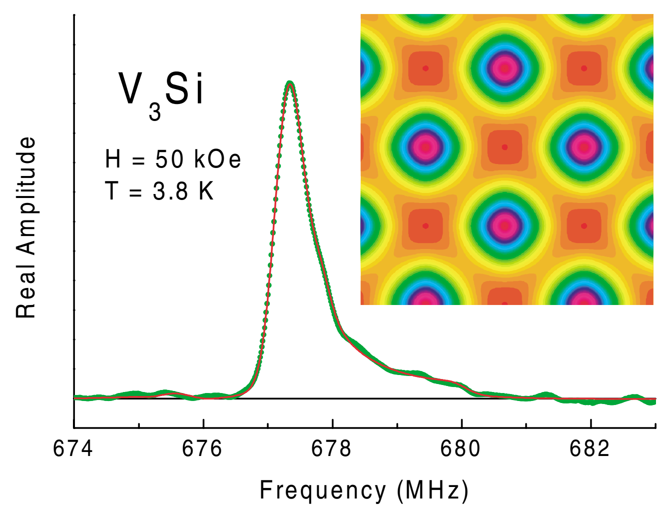

FIG. 1 (color). Fourier transform (FT) of the muon spin precession signal (green circles) in V_3Si at $T = 3.8$ K and $H = 50$ kOe. The FT provides an approximate illustration of the internal magnetic field distribution but is broadened by the apodization procedure used to smooth out the ringing effects of the finite-time window (0–3 μs) and the noise from reduced counts at later times. Additional broadening due to VL disorder and nuclear magnetic dipoles is accounted for by a Gaussian broadening width of $\sigma \approx 1.0\ \mu s^{-1}$. The solid red curve is the FT of the fit in the time domain, assuming the field profile $B(r)$ given by Eq. (1). The inset is a contour plot of the function $B(r)$ obtained from the fit.

determined by STM. (iii) Above 7.5 kOe, the orientation of the vortex cores determined by our analysis (see the Fig. 1 inset) is that which is expected for close packing of square vortices.

The field dependence of λ, ξ, d, and β are shown in Fig. 2. At low fields where the lattice is hexagonal, $\lambda \approx 1060$ Å and $\xi \approx 42$ Å, which are consistent with previously determined values of these parameters. Above 7.5 kOe there is a slight nonphysical increase in the fitted values of λ and ξ, reflecting the beginning of the gradual transition to a square VL. At higher fields ξ decreases and continues to do so when the VL completes its transition to a square at 40 kOe.

Gygi and Schlüter [34] have shown that the pair potential $\Delta(r)$, which in general is a numerical function, varies on two length scales, ξ_1 and ξ_2. The first is defined from the slope of $\Delta(r)$ near the center of the vortex core

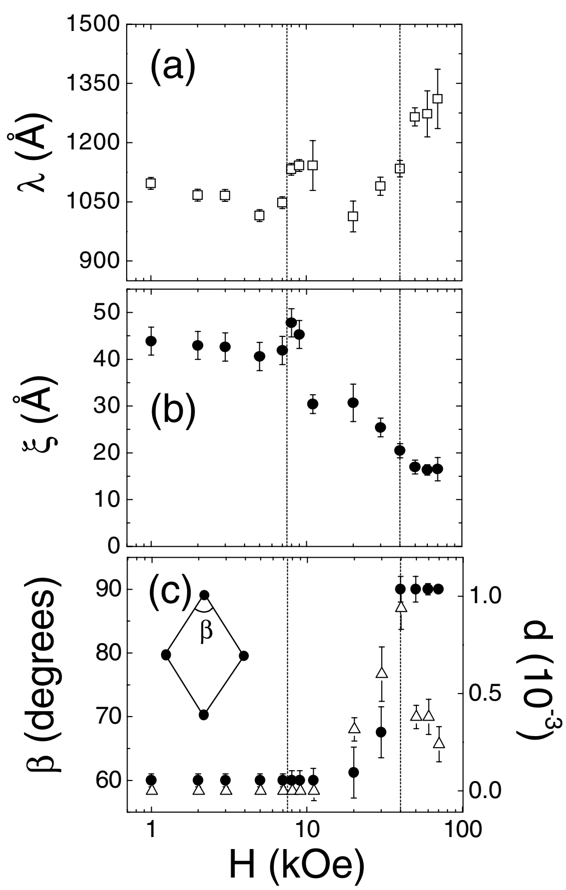

FIG. 2. The magnetic field dependence of the fit parameters at $T = 3.8$ K. (a) The magnetic penetration depth λ. (b) The coherence length ξ. (c) The apex angle β (solid circles) and the anisotropy parameter d (open triangles). The dashed vertical lines indicate the field range over which the VL continuously evolves from hexagonal to square symmetry. Immediately above 7.5 kOe, d and β are poorly determined, because the VL is only slightly distorted from hexagonal symmetry.

$$\xi_1 = \Delta_0 / \lim_{r\to 0} \frac{\Delta(r)}{r} \tag{2}$$

(Δ_0 is the BCS superconducting energy gap), whereas ξ_2 is the length scale over which $\Delta(r)$ rises to its asymptotic value Δ_0. In Ref. [34] these two length scales were shown to coincide at temperatures larger than $T_c/2$, while at very low temperatures $\xi_1 \ll \xi_2$, due to thermal depopulation of the higher-energy bound core states. From μSR measurements of the temperature dependence of the vortex core size [27,35], we have previously established that variations of ξ reflect changes in ξ_1. This is because μSR is most sensitive to the rapid variation of $B(r)$ in the spatial region governed by ξ_1, rather than the small variation of $B(r)$ between ξ_1 and ξ_2. Therefore we attribute the reduction of ξ above 7.5 kOe to a decrease in ξ_1. Solutions of the microscopic theory show that the rapid increase of $\Delta(r)$ near $r = 0$ is accompanied by a similar rise of the supercurrent density $j(r)$ in the same region [7,8,34], such that ξ_1 and the location of the maximum in $j(r)$ exhibit similar behavior as a function of H and T. Consequently, we can define an effective vortex core size r_0 as the distance from the core center ($r = 0$) to the location where $j(r)$ reaches its maximum value, measured along the line connecting nearest-neighbor vortices. The parameter r_0 can be obtained in a nearly model-independent way using the Maxwell relation, $j(r) = |\nabla \times \mathbf{B}(\mathbf{r})|$, where $B(r)$ is obtained from fitting the μSR time spectrum. Because r_0 is not a fit parameter, the details of the theoretical model for $B(r)$ are not very important in this procedure. What is essential is that the model for $B(r)$ yields excellent fits, as was the case using Eq. (1).

In Fig. 3(a) we compare the field dependence of r_0 in V_3Si to the electronic thermal conductivity κ_e measured previously [22]. For the first time we see the expected field dependence of the core size in a single-gap conventional s-wave superconductor. In contrast to $NbSe_2$ [10] and MgB_2 [25], the low-field value of r_0 is consistent with the coherence length calculated from H_{c2}. At low fields, where only a modest overlap of the QP core states of neighboring vortices is expected, both r_0 and κ_e exhibit a weak dependence on H. The change in r_0 over this range of H is primarily due to the superposition of the $j(r)$ profiles of nearest-neighbor vortices. This is indicated by the open circles in Fig. 3. Above 7.5 kOe there is an additional contribution to the shrinking core size, which is accompanied by a simultaneous increase in the electronic thermal conductivity. Together these observations signify a change in the slope of $\Delta(r)$ at the vortex center, due to an increased overlap of the bound state wave functions of adjacent vortices. As shown in Fig. 3(a), the transformation to a square VL begins at the field where the delocalization of QPs becomes significant. Thus, the increased strength of the vortex-vortex interactions apparently drives the symmetry change of the

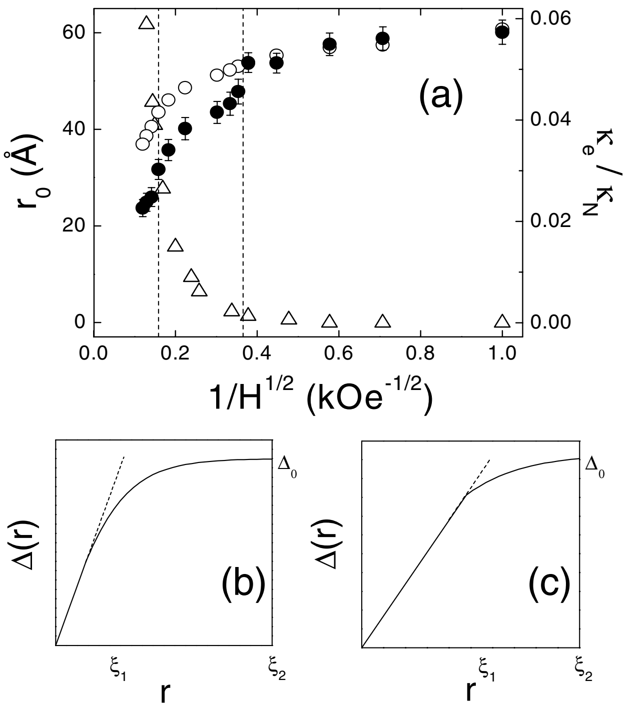

FIG. 3. (a) The magnetic field dependence of the vortex core size r_0 measured by μSR (solid circles) at $T = 3.8$ K, and the electronic thermal conductivity κ_e/T (open triangles) from Ref. [22] extrapolated to $T \rightarrow 0$ (and normalized to the value κ_N/T at H_{c2}). The open circles indicate the reduction of r_0 due to the superposition of $j(r)$ profiles from individual vortices, calculated assuming the low-field value of ξ. The data are plotted as a function of $1/H^{1/2}$, which is proportional to the intervortex spacing $L = (\Phi_0/H \sin\beta)^{1/2}$, where Φ_0 is the magnetic flux quantum. The dashed vertical lines indicate the field range over which the VL undergoes a continuous hexagonal-square transition. A schematic of the pair potential $\Delta(r)$ as a function of distance from the vortex core center at high (b) and low (c) magnetic field.

lattice to reflect the fourfold symmetry of the individual vortices.

The experimental results presented here for V_3Si confirm one of the key predictions of theoretical works that advocate the importance of intervortex QP transfer to the detailed structure of the VL. This important detail should be a consideration in the interpretation of any experiment on a type-II superconductor in an applied magnetic field.

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