Low Temperature Limit of the Vortex Core Radius and the Kramer-Pesch Effect in $NbSe_2$

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Muon spin rotation (μSR) has been used to measure the magnetic field distribution in the vortex state of the type-II superconductor $NbSe_2$ ($T_c = 7.0$ K) below $T = 2$ K. The distribution is consistent with a highly ordered hexagonal vortex lattice with a well resolved high-field cutoff associated with the finite size of the vortex cores. The temperature dependence of the core radius is much weaker than the temperature dependence predicted from the Bogoliubov–de Gennes theory. Furthermore, the vortex radius measured by μSR near the low temperature quantum limit is about an order of magnitude larger than predicted.

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One of the most remarkable aspects of superconductivity is the lattice of magnetic vortices which forms in a type-II superconductor in the presence of an external magnetic field H. The associated inhomogeneous magnetic field peaks at the vortex centers where the screening current density vanishes. Within Ginzburg-Landau (GL) theory, the distribution of internal fields, $n(B)$, depends on the two fundamental length scales for superconductivity: the magnetic penetration depth λ and the coherence length ξ. In the case of an isolated vortex, λ is the characteristic length over which the magnetic field decays exponentially away from the core, whereas ξ is the length scale over which the superconducting order parameter rises from zero at the vortex center to its bulk value outside the core. A vortex core radius r_0 can be defined as the distance from the core center to the point where the supercurrent density $J(\mathbf{r}) = |\nabla \times \mathbf{B}(\mathbf{r})|$ is a maximum. Near T_c, r_0 is of the order of ξ; however, at low temperatures the analytical GL expression for the spatial variation of the order parameter within a vortex, i.e., $\Delta(\mathbf{r}) = \Delta_{\mathrm{BCS}} \tanh(r/\xi)$, becomes invalid. From numerical solutions of the quasiclassical Eilenberger equations, Kramer and Pesch determined Δ_{BCS} within a vortex at low temperature and defined the core size (ξ_{KP}) from the slope of the order parameter (Δ_0) near the vortex center [1],

$$\xi_{\mathrm{KP}} = \Delta_{\mathrm{BCS}} \Big/ \lim_{r\to 0} \frac{\Delta(r)}{r}. \tag{1}$$

In theory, r_0 is of the order of ξ_{KP} but is more closely related to experimental observables such as $n(B)$. In particular, a finite r_0 leads to a high-field cutoff in the magnetic field distribution. In this way the magnetic field distribution is sensitive to the size of the vortex cores and hence ξ_{KP}.

In the simplest picture of a vortex in an s-wave superconductor, r_0 is independent of temperature well below T_c since the finite, isotropic energy gap suppresses quasiparticle excitations. However, real vortices can support bound quasiparticle states with energies below the gap, and these may have a pronounced effect on the vortex core radius even when $T/T_c \ll 1$. Such states were first predicted in 1964 by Caroli *et al.* [2]. Based on calculations with the Bogoliubov–de Gennes equations (BdG) and Eilenberger quasiclassical theory, Kramer and Pesch (KP) predicted that the vortex core size decreases as a linear function of temperature [1],

$$\xi_{\mathrm{KP}} = \xi_{\mathrm{BCS}} T/T_c \qquad (T_c^2/E_F \ll T \ll T_c), \tag{2}$$

where $\xi_{\mathrm{BCS}} \sim 1/\Delta_{\mathrm{BCS}}$ is the BCS coherence length and E_F is the Fermi energy. At temperatures below T_c^2/E_F (the so-called "quantum limit"), the quasiclassical prediction which assumes a continuum of bound quasiparticle states breaks down. To investigate the behavior of r_0 at lower temperatures, Hayashi *et al.* self-consistently solved the BdG equations for a single s-wave vortex [3]. Below the quantum limit where there is no thermal smearing of bound quasiparticle states, the shrinking of the vortex core saturates to $\xi_{\mathrm{KP}} \approx 10$ Å, for parameters appropriate to $NbSe_2$ [4,5]. The temperature at which the shrinking of the core radius saturates is $T_{\mathrm{KP}} \approx T_c/(k_F \xi_{\mathrm{BCS}}) \approx 500$ mK [3].

Experimentally, strong evidence for bound states within the core comes from scanning tunneling microscopy (STM) in $NbSe_2$ [5]. However, the KP effect, or shrinking of the vortex core at low temperature, has not been verified due to difficulties in extracting a core radius in a model independent way. STM is sensitive to the full density of states which is not so easily related to quantities such as ξ or r_0. For example, Volodin *et al.* [6] have shown

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that the effective core radius measured by STM has a strong voltage bias dependence, which is attributed to the increased angular momentum of the bound states at higher energies. Muon spin rotation (μSR) is an excellent way to measure the internal magnetic field distribution $n(B)$ which can be used to characterize magnetic vortices in type-II superconductors. In particular, if the high-field cutoff in $n(B)$ can be resolved in the time domain, then μSR is a direct measure of r_0 deep in the superconducting state [7]. $NbSe_2$ is an ideal superconductor to study with μSR since (1) the vortex lattice is known to be hexagonal with little disorder and (2) λ and r_0 are in a range that can be measured with excellent sensitivity. In the present Letter we report μSR measurements of the temperature dependence of r_0 in single crystals of $NbSe_2$. We observe a KP effect, but it is considerably weaker than theoretical predictions for an isolated vortex. Furthermore, the core size saturates near $r_0 \approx 72$ Å, which is much larger than the predicted limiting low T value of $r_0(T = 0\ \mathrm{K}) = 10$ Å [3].

Muon spin rotation experiments were performed on the M15 surface muon channel at TRIUMF using a top loading dilution refrigerator. As described elsewhere [8], the implanted spin polarized muons stop randomly on the length scale of the vortex lattice and precess at a rate proportional to local magnetic field, thus providing a direct measure of $n(B)$. Special precautions were taken to suppress the background signal associated with muons which did not stop in the sample. In particular, a cup-shaped veto scintillator was installed behind the silver sample holder to reject events from muons which missed the holder. To eliminate the muon precession signal originating from the holder itself, the sample was mounted on a thin wafer of intrinsic GaAs. (GaAs produces no detectable muon precession signal in the frequency region of interest—65 MHz.) In a separate test we established that samples mounted in this way could be cooled to 20 mK. High statistics runs were made with approximately 40×10^6 muon decay events, which is twice the number of counts recorded in our previous study of $NbSe_2$ [7] in a conventional cryostat above $T = 2$ K. A mosaic of three $NbSe_2$ crystals, which were also used in the previous study, was mounted on the GaAs and covered an area of 60 mm^2. Each crystal showed a similar sharp transition at 7.0 K in resistivity and susceptibility measurements.

Figure 1(a) shows a fast Fourier transform (FFT) of the muon spin precession signal measured at 400 mK in an applied field of 0.5 T. The displayed curve is essentially the magnetic field distribution in the sample broadened slightly by the finite time range in the transformation and the disorder in the flux lattice. In Fig. 1(b), the FFT of the theoretical fit to the measured muon spin precession signal is shown. The small shaded area near zero is attributed to a percentage of the incoming muons (5%) which evade the background suppression system. The asymmetric line

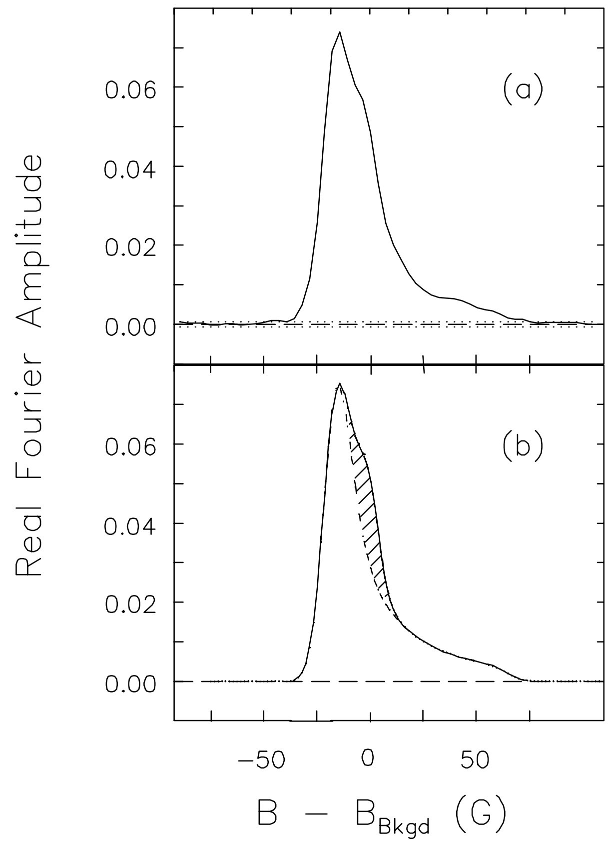

FIG. 1. (a) Fast Fourier transform of the muon spin precession signal at $T = 400$ mK in an applied field of $\mu_0 H = 0.5$ T. (b) Fast Fourier transform of the fitted muon precession signal. The shaded area is the background signal due to muons that miss the sample. Note the close agreement with the measured spectrum and the high-field cutoff due to the finite size of the vortex cores.

shape is characteristic of a well-ordered hexagonal vortex lattice, as suggested by the absence of a shoulder on the low-field side in Fig. 1. Note the greatest spectral weight occurs below the average field which is attributed to the Van Hove singularity produced by the local field at the midpoint between nearest-neighbor vortices. For the purposes of the present study the most important feature in Fig. 1 is the high-field cutoff, since this is a measure of the field distribution in the vicinity of the vortex core and thus the size of the vortex cores. Furthermore, the high-field cutoff seen in the data [Fig. 1(a)] is accurately reproduced by the theoretical FFT [Fig. 1(b)].

Although such characteristic features in $n(B)$ are most easily identified in the frequency domain, the data analysis was performed in the time domain where the data are collected and the μSR spectrum is unmodified. Figure 2 shows an example of the measured muon spin precession signal in $NbSe_2$, displayed in a reference frame rotating at the frequency of the background signal. The decay of the signal amplitude is due to the broad distribution of internal magnetic fields. Excellent fits were obtained using a

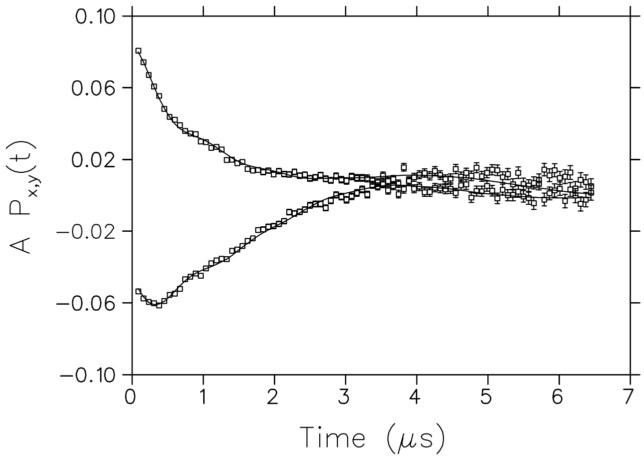

FIG. 2. The real and imaginary components of the muon spin polarization signal from $NbSe_2$ at $T = 400$ mK and $\mu_0 H = 0.5$ T viewed in a reference frame which is rotating at the average Larmor frequency of the muon. The solid curve is the best fit in which the core radius is found to be 72 Å.

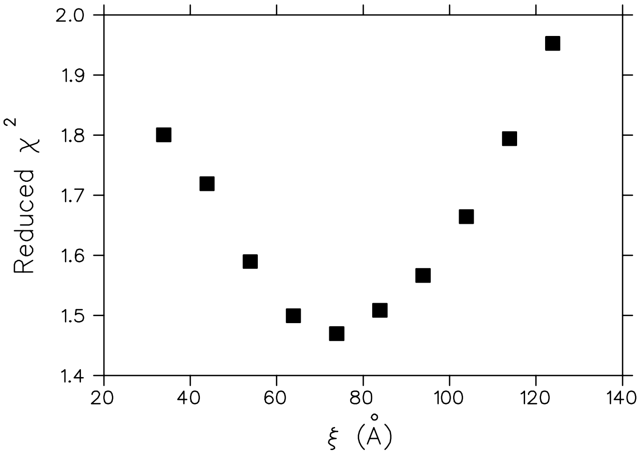

FIG. 3. Reduced χ^2 plotted as a function ξ_{ab} with all other parameters free, for $T = 400$ mK and $\mu_0 H = 0.5$ T.

theoretical muon polarization function (solid curve), which was generated using a magnetic field profile derived from Ginzburg-Landau theory by Yaouanc *et al.* [9]:

$$B(r) = \frac{\Phi_0}{S}(1 - b^4) \sum_G e^{-i\vec{G}\cdot\vec{r}} \frac{uK_1(u)}{\lambda_{ab}^2 G^2}, \tag{3}$$

where $u^2 = 2\xi_{ab}^2 G^2(1 + b^4)[1 - 2b(1 - b)^2]$, Φ_0 is the flux quantum, $K_1(u)$ is a modified Bessel function, G is a reciprocal lattice vector of the vortex lattice, b is the reduced field ($b = B/B_{c2}$), and S is the area of the unit cell for a hexagonal lattice. Values for the model parameters λ_{ab} and ξ_{ab} were extracted, as well as a parameter to take into account a slight broadening of the ideal field distribution due to flux lattice disorder and nuclear dipoles [10]. We then calculate the supercurrent density $J(r)$ from the fitted $B(r)$ using Maxwell's equation $J(\mathbf{r}) = |\nabla \times \mathbf{B}(\mathbf{r})|$ and extract r_0 [the radius from the core center at which $J(r)$ is maximum]. It has been shown previously that the core radius obtained in this way, along with its dependence on field and temperature, is only weakly dependent on the precise model for $B(r)$ provided that the corresponding muon polarization function fits the measured μSR time spectrum well [8]. The sensitivity to the fitted value of ξ_{ab} is demonstrated from Fig. 3, where χ^2 is plotted as a function of ξ_{ab} with all other parameters free to vary. The high quality of the fits is visually apparent in Figs. 1 and 2.

As shown in Fig. 4, there is a weak temperature dependence to the core radius. Calculations by Hayashi *et al.* [3], which take into account the bound states within the core, predict a much stronger temperature dependence of the core radius (see inset of Fig. 4). The disagreement with the theory of Ref. [3] is striking. In particular, the core radius as measured by μSR does not show the predicted strong KP effect and seems to saturate at a value much larger than the predicted low T limit of 10 Å.

It is important to understand why detailed calculations of the KP effect in $NbSe_2$ do not agree with the μSR measurements of the core radius. Some authors [1] have predicted a finite current density and cusp in the magnetic field at the center of the vortex core at low temperatures, although this is not true for the most recent calculations of Ref. [3]. Since Eq. (3) does not allow for such a cusp, one might imagine there is some systematic offset between the fitted r_0 and where the peak in $J(r)$ actually occurs. However, Eq. (3) does describe the cutoff quite well as may be seen in Fig. 1. Furthermore, it seems unlikely such an effect could mask a large temperature dependence. A more plausible explanation for the disagreement is that the KP effect is diminished by the vortex-vortex interactions and/or zero point motion of vortices.

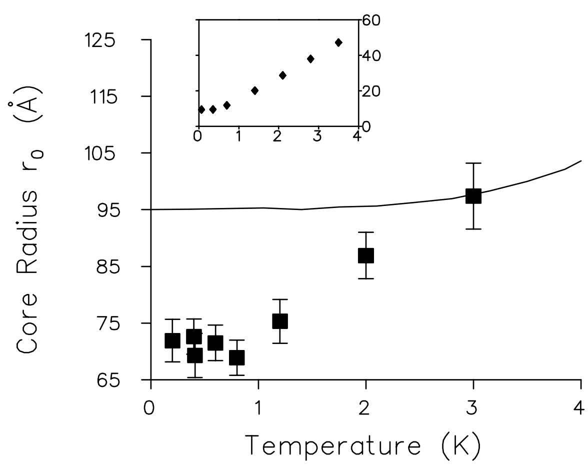

FIG. 4. The temperature dependence of the vortex core radius in $NbSe_2$ at $\mu_0 H = 0.5$ T. The solid curve is the BCS prediction for the temperature dependence of the BCS coherence length, $\xi_{\rm BCS}$, scaled such that $\xi_{\rm BCS}(T = 3\text{ K}) = r_0$. Inset: The prediction from Ref. [3] of the temperature dependence of $\xi_{\rm KP}$, assuming $\xi_{\rm BCS}(T = 0\text{ K}) = 84$ Å and $k_F \xi_{\rm BCS} = 16$.

The calculations to date of the temperature dependence of the coherence length and core radius in the Bogoliubov–de Gennes and Eilenberger formalisms are all done for a stationary isolated vortex. We note that μSR [7], STM [11], and heat capacity measurements [12] have indicated that the core radius expands in low magnetic fields, presumably due to vortex-vortex interactions. The observed field dependence of r_0 is qualitatively consistent with solutions of the Eilenberger equations (i.e., above the quantum limit) obtained recently by Ichioka *et al.* for the vortex lattice in an s-wave superconductor [13].

Related effects may also play a role in the observed temperature dependence. For example, the core radius measured by μSR is averaged over zero point motion. This would increase the low temperature value of r_0 and thereby hide the KP effect one would see for fixed vortices. So far there is no detailed theory of zero point motion. We note that thermal fluctuations of the vortices cannot explain the large core radius at low T, since the amplitude of the fluctuations vanishes as $T \rightarrow 0$ K. Furthermore, thermal fluctuations would actually strengthen the temperature dependence measured by the μSR technique.

In conclusion, μSR measurements of the core radius in $NbSe_2$ show a surprisingly weak temperature dependence down to temperatures as low as 200 mK. This does not agree with recent detailed calculations of an isolated vortex in $NbSe_2$. It appears that vortex-vortex interactions and zero point motion have a pronounced effect on the vortex radius and its temperature dependence. There remains a significant gap between the current theory of noninteracting vortices and measurements of real vortices in a finite magnetic field. It is remarkable that physics of vortex cores in conventional type-II superconductors is still not well understood. Clearly there is need for improved measurements at lower magnetic fields and a theory which takes into account the finite magnetic field and resulting vortex interactions.

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