The magnetic field dependence of the vortex core size in the multi-band superconductor NbSe$_2$ has been determined from muon spin rotation measurements. The spatially extended nature of the quasiparticle core states associated with the smaller gap leads to a rapid field-induced shrinkage of the core size at low fields, while the more tightly bound nature of the states associated with the larger gap leads to a field-independent core size for fields greater than 4 kOe. A simple model is proposed for the density of delocalized core states that establishes a direct relationship between the field-induced reduction of the vortex core size and the corresponding enhancement of the electronic thermal conductivity. We show that this model accurately describes both NbSe$_2$ and the single-band superconductor V$_3$Si.

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the muon after an average lifetime of 2.2 $\mu$s, a positron is emitted preferentially along the direction of the muon spin. The time evolution of the muon spin polarization is determined by detecting decay positrons from an ensemble of $\sim 2 \times 10^7$ muons. The exact functional form of the muon spin polarization depends on $n(B)$. Further details of the experimental technique used here can be found in Ref. [25]. The $\mu$SR time spectra were fit assuming a Ginzburg-Landau (GL) model for the spatial field profile given by

$$B(\mathbf{r}) = B_0(1 - b^4) \sum_\mathbf{G} e^{-i\mathbf{G} \cdot \mathbf{r}} \frac{u K_1(u)}{\lambda_{\text{GL}}^2 G^2},$$

(1)

where $b = B/B_c$, $B_0$ is the average internal field, $\mathbf{G}$ are the reciprocal lattice vectors, $K_1(u)$ is a modified Bessel function, $u^2 = 2 \xi_{\text{ab}}^2 G^2 (1 + b^4)(1 - 2b(1 - b)^2)$, $\xi_{\text{ab}}$ is the GL coherence length, and $\lambda_{\text{GL}}$ is the magnetic penetration depth. As explained in Ref. [13], previous $\mu$SR works have demonstrated that the field-dependence of the parameter $\xi_{\text{ab}}$ reflects changes in the vortex core size due to changes in the electronic structure of the vortex cores.

Figure 1 shows fast Fourier transforms (FFTs) of both the muon spin precession signal at $H = 4$ kOe and the fit to Eq. (1). The FFTs closely resemble $n(B)$ for a hexagonal vortex lattice, but are significantly broadened by the apodization used to reduce ringing and noise in the FFT due to the finite time-range and the short muon lifetime, respectively. The lineshape is also broadened by a Gaussian distribution of fields from randomly oriented nuclear dipolar moments. The width of this distribution was determined to be $\approx 0.25$ MHz. In addition, there is a background peak at $\approx 54.1$ MHz originating from muons stopping outside the sample.

Recently, $\mu$SR measurements on powder samples of Mg$_{1-x}$Al$_x$B$_2$ were modeled assuming two distinct energy gaps, and a two-component field distribution for the vortex lattice [19]. Specifically, this model assumes two distinct coherence lengths, which implies that both large and small vortex cores exist simultaneously in the sample. However, for NbSe$_2$ we find that the data are well described by Eq. (1). A visual inspection of Fig. 1 shows that the fit captures all of the main features of the $\mu$SR lineshape. This is consistent with recent theoretical work predicting that the formation of two vortex sublattices is energetically forbidden in a two-gap superconductor [31].

Recent $\mu$SR measurements of the field dependence of the core size in the single-band superconductor V$_3$Si [20] have confirmed theoretical predictions of field-induced core shrinkage due to QP delocalization [30]. In the case of NbSe$_2$, the delocalization of core states is dependent on both energy gaps. At low fields the rapid reduction of $\xi_{\text{ab}}$ and the simultaneous rapid increase of $\kappa_e$ with increasing magnetic field are consistent with this regime being dominated by loosely bound states associated with the smaller energy gap [3, 9]. If the loosely bound core states associated with the smaller gap have completely delocalized by $H \approx 4$ kOe, then we expect the behavior of $\xi_{\text{ab}}$ at larger fields to be dominated by the larger gap. The saturation of $\xi_{\text{ab}}$ above 4 kOe indicates that the QPs are highly localized in the vortex cores at higher fields. This is in line with STM measurements which show that the bound core states at $H = 10$ kOe are more spatially confined than those at $H = 1$ kOe [32]. We note that even though the shrinking of the core size saturates
above 4 kOe, $\kappa_e$ still exhibits a considerable dependence on field. The reason is that although the number of delocalized QPs per vortex is no longer changing, the increasing number of vortices increases the total number of delocalized QPs (i.e., heat carriers) in the sample. Given that the core size at low (high) field is primarily determined by the small (large) gap, one might naively expect that the BCS relationship $\xi \sim v_F / \pi \Delta_0$, where $v_F$ is the Fermi velocity and $\Delta_0$ is the magnitude of the energy gap, could be used to determine the ratio of the high and low field core sizes. However, recent calculations based on GL theory have shown that this relationship is not applicable to a multi-band superconductor and that a simple expression for the ratio of the two core sizes only exists in the limit of zero interband coupling. For finite interband coupling, the ratio must be calculated numerically and is dependent on a number of material parameters.

As can be seen from Eq. (1), the magnetic penetration depth $\lambda_{ab}$ is also a fitting parameter in our analysis, extracted simultaneously with $\xi_{ab}$. Fig. 3 shows that $\lambda_{ab}$ increases strongly with $H$ at low fields and displays a weaker, though significant, dependence at higher fields. The Volovik effect has previously been invoked to explain the field dependence of $\lambda_{ab}$ in $s$-wave type-II superconductors. This effect involves a shift of the quasi-particle energy spectrum by an energy $\sim v_F \cdot \mathbf{V}$, where $\mathbf{V}$ is the supercurrent velocity, and it plays a significant role in superconductors with gap nodes. However, for an isotropic $s$-wave energy gap, a significant dependence of $\lambda_{ab}$ on $H$ is only expected if the thermal energy $k_B T$ is Boltzmann’s constant) is comparable to the magnitude of the energy gap. At $T = 20$ mK, $k_B T \approx 10^{-3}$ meV, whereas the size of the small energy gap in NbSe$_2$ is $\approx 10^{-1}$ meV. Therefore we cannot attribute the observed behaviour of $\lambda(H)$ to the Volovik effect.

Calculations of the electronic structure of a single vortex using the Bogoliubov-deGennes equations have shown that the presence of extended quasiparticle states significantly modifies the current density, and hence $B(r)$, around the vortex core. With increasing magnetic field these modified regions overlap. Since Eq. (1) does not account for this, the effect on $B(r)$ shows up in our measurements as a field dependent $\lambda_{ab}$. In other words $\lambda_{ab}$ in Eq. (1) is an effective magnetic penetration depth. We note that the field dependence of $\lambda_{ab}$ is stronger at low field due to the more rapid delocalization of QPs from the vortex cores.

Next we propose a simple model which directly relates our measurements of the vortex core size to the measurements of the electronic thermal conductivity. In the conventional picture of a type-II superconductor, the density of localized QPs at the Fermi energy $N(E_F)_{\text{loc}}$, proportional to $\pi \xi^2 H$, where $\xi$ is the area of a single vortex core and the density of vortices in the sample is proportional to $H$. If we assume that the field-induced density of delocalized QPs is equal to the reduction in $N(E_F)_{\text{loc}}$, then

$$N(E_F)_{\text{deloc}} \propto (\pi \xi^2_0 - \pi \xi^2) H,$$

where $\xi_0 \approx 97$ Å is the low-field value of the core size. Note that $(\pi \xi^2_0 - \pi \xi^2) H$ is also proportional to the reduction of the total core area in the sample due to the delocalization of QP core states.

In a metal, $\kappa_e = (1/3) C v_F l = (1/9) \pi^2 N(E_F) v_F l k_B^2 T$, where $C$ is the heat capacity per unit volume, $k_B$ is Boltzmann’s constant, $v_F$ is the Fermi velocity, and $l$ is the electron mean free path. Since it is the delocalized QPs that carry heat then $\kappa_e \propto N(E_F)_{\text{deloc}}$, and it follows from Eq. (2) that

$$\kappa_e \propto (\pi \xi^2_0 - \pi \xi^2) H.$$

To show that this relationship is physically valid, in Fig. 4 we plot the measured quantities $\kappa_e$ and $(\pi \xi^2_0 - \pi \xi^2) H$ against $(H_{c2}(0)/H)^{1/2}$, which is proportional to the intervortex spacing. We also plot our earlier measurements on V$_3$Si in this way. It can be seen that at large intervortex spacing (low $H$) neither quantity changes significantly. However, as the field is increased and the vortices are brought closer together, both quantities exhibit the same field dependence within experimental uncertainty. This lends further support to the conclusion that in both single-band V$_3$Si and multi-band NbSe$_2$ the field dependences of $\xi_{ab}$ and $\kappa_e$ have a common underlying cause, namely the delocalization of bound QPs.

In summary, we have measured the field dependence of the vortex core size in the multi-band superconductor NbSe$_2$ at $T = 20$ mK. The observed field dependence is explained by the effects of two superconducting energy gaps on the bound core states. In addition, we have experimentally established a direct correlation between

\[ \text{FIG. 3: Field dependence of the magnetic penetration depth in NbSe}_2 \text{ at } T = 20 \text{ mK.} \]
the field-induced reduction of the vortex core area and
the electronic thermal conductivity in both single-band
and multi-band superconductors.

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FIG. 4: Total reduction in core area (left axis, solid squares)
and electronic thermal conductivity $\kappa_e$ (right axis, open tri-
angles) plotted against $(H_c^2/H)^{1/2}$ (which is proportional
to the intervortex spacing) for V$_3$Si and NbSe$_2$. Both quantities
are normalised to their values at $H \sim 70$ kOe for V$_3$Si and
$H \sim 10$ kOe for NbSe$_2$. The dashed lines connect the $\kappa_e$ data
points. (The V$_3$Si data are shifted upwards by 0.5 on the
vertical scale for clarity.)

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