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Effect of delocalized vortex core states on the specific heat of Nb

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The magnetic field (B) dependence of the electronic specific heat for a simple BCS type-II superconductor has been determined from measurements on pure niobium (Nb). Contrary to expectations, the electronic specific heat coefficient $\gamma(T,B)$ is observed to be a sublinear function of B at fields above the lower critical field H_{c1}. This behavior is attributed to the delocalization of quasiparticles bound to the vortex cores. The results underscore the ambiguity of interpretation that arises in specific heat studies of this kind on newly discovered type-II superconductors, and also emphasize the need to do such measurements under field-cooled conditions.

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Specific heat measurements on type-II superconductors in the vortex state are sensitive to low-energy quasiparticle excitations. In fully gapped superconductors the low-lying excitations are traditionally thought of as being confined to the vortex cores.[1] In this case the coefficient of the linear term in the specific heat c as a function of temperature, i.e., the Sommerfeld coefficient γ, is proportional to the density of vortices, and hence a linear function of the internal magnetic field B.[2] The situation is different in superconductors with a highly anisotropic energy gap or gap nodes. In these cases there is a major contribution to the electronic specific heat at low temperatures from delocalized quasiparticles. The flow of superfluid around a vortex lowers the energy of quasiparticles delocalized near the gap minima, resulting in a finite density of states (DOS) at the Fermi energy and a corresponding nonlinear field dependence for $\gamma(B)$.[3] For an anisotropic gap, such behavior is expected only if the energy shift exceeds the gap minimum. Thus, $\gamma(B)$ tells us something about the gap structure.

What has not been considered in the interpretation of many such studies is that even for the case of a simple BCS superconductor characterized by an isotropic energy gap, the quasiparticles are not strictly confined to single vortices. Quasiparticle states bound to the vortex cores become delocalized when their spatially extended wave functions overlap those from nearest-neighbor vortices. The overlap is enhanced at higher magnetic fields where the vortices are closer together, but there is also some overlap as soon as there is more than one vortex in the sample. Likewise, the degree of delocalization increases with increasing temperature due to thermal population of higher-energy core states, characterized by wave functions extending further out from the core center. This is the so-called Kramer-Pesch (KP) effect.[4]

Recently, the field dependence of the vortex electronic excitations has been confirmed by thermal conductivity[5] and muon spin rotation[6] (μSR) experiments on V_3Si. By detecting the change in the vortex core size, μSR measurements on V_3Si have confirmed that the delocalized quasiparticles detected by thermal conductivity originate from the vortex cores. These delocalized core states should have a profound influence on the field dependence of the specific heat, which probes the electronic DOS at the Fermi level, both inside and outside the vortex cores. Recent calculations[7] in the framework of the quasiclassical Eilenberger theory show that for an isotropic energy gap, $\gamma(B) \propto B$ behavior persists only up to a crossover field B^*, above which the overlap of core states results in a sublinear dependence of $\gamma(B)$ on B. Strictly speaking B^* is temperature dependent, reduced by thermal population of the more energetic and spatially extended core states.

To date there has been no clear experimental verification of a crossover field $B^*(T)$ in a fully gapped type-II superconductor. While there have been numerous specific heat studies on BCS type-II superconductors, rarely is $\gamma(B)$ observed to be a linear function of B. One reason is that there are very few "simple" BCS type-II superconductors. For example, specific heat measurements on the widely studied superconductor $2H$-$NbSe_2$ show that $\gamma(B)$ is a nonlinear function of B even at low fields.[8–10] There is now good evidence that $2H$-$NbSe_2$ is a multiband superconductor, with a different size energy gap on two different sheets of the Fermi surface.[5,11] The nonlinearity of $\gamma(B)$ can be attributed to two-band superconductivity,[12] giving rise to a large vortex-core size at low fields.[9,13]

Even the cubic A15 compound V_3Si is not so simple. For a magnetic field applied along the $\langle 001 \rangle$ direction, there is a substantial range of fields over which the hexagonal vortex lattice either gradually distorts into a square lattice[6,14] or coexists with a square lattice.[15] This vortex lattice transition is accompanied by delocalization of quasiparticle core states,[5,6] and occurs at very low fields. Consequently, the specific heat is a linear function of B only over a very narrow field range far below the upper critical field H_{c2}.[16]

In view of these complications, here we investigate the field dependence of $\gamma(B)$ in the elemental type-II superconductor niobium (Nb). A $\langle 001 \rangle$-oriented, 99.99%-purity Nb single crystal was obtained from Goodfellow Corporation. The sample was in the shape of a short cylinder, $\sim$1.8 mm long with a diameter of $\sim$2 mm. Magnetization measurements were made with a superconducting quantum interference device magnetometer and specific heat measurements were made using a Quantum Design physical properties measurement system that utilizes a thermal relaxation calorimeter. The calorimeter is composed of a sapphire sample holder and the addendum heat capacity is essentially field independent for the fields employed in this work. The external field H was directed along [111], which under field-cooled (FC) conditions produces a well-ordered hexagonal vortex lattice in Nb for all fields $H_{c1}<H<H_{c2}$.[17] FC and zero-field-cooled (ZFC) swept-field measurements of the sample magnetization $M(T,H)$ and the specific heat $c(T,H)$ were found to be greatly hampered by flux jumps. Consequently, the FC measurements reported here were done by field cooling the sample from above T_c to the desired temperature for each value of H. On the other hand, the ZFC measurements were done by first cooling the sample in zero field and then increasing H. From ZFC measurements of $M(T)$ at 5 Oe, the Nb crystal was determined to have a sharp superconducting transition temperature of T_c=9.2 K. The zero-temperature extrapolated value of the upper critical field was determined to be $H_{c2}(0)\approx 4.5$ kOe, from which the superconducting coherence length is calculated to be ξ=270 Å. Just above T_c the resistivity of the sample saturates with a value of 0.32 $\mu\Omega$ cm, from which we calculate the electron mean free path to be l=2300 Å. Thus, our sample is well within the clean limit.

Measurements of the sample magnetization $M(H)$ were done to determine the internal magnetic field

$$B=H-4\pi M(1-N), \tag{1}$$

where N=0.379 is the demagnetization factor of our Nb crystal. This value of N was determined by ZFC measurements of $M(H)$ at several temperatures in the Meissner phase, assuming full shielding (B=0). Under FC conditions the quantity $4\pi M$ was found to be very small (with a maximum value of 31 G at H=750 Oe and T=2.25 K), indicating that very little flux is expelled. Since $B\approx H$, it is safe to interpret our measurements of $\gamma(T,H)$ as $\gamma(T,B)$. We note that this equivalence is often assumed in specific heat studies without justification.

The normal-state specific heat of Nb is described by the relation

$$c_{\mathrm{n}}(T)=\gamma_{\mathrm{n}}T+\beta T^3, \tag{2}$$

where γ_{n} is the Sommerfeld constant in the normal state, and $\gamma_{\mathrm{n}}T$ and βT^3 are the electronic and phonon contributions, respectively. FC measurements of the temperature dependence of the specific heat of Nb are plotted in Fig. 1 as $c(T,H)/T$ against T^2. The solid line in the main panel is a fit of the H=5 kOe data below 10 K to Eq. (2), yielding γ_{n}=7.60±0.02 mJ/mol K^2 and β=0.14±0.01 mJ/mol K^4.

At $T\ll T_c$ the specific heat is described by

$$c(T,H)=\gamma(T,H)T+\beta T^3+c_{\mathrm{es}}(T,0) \tag{3}$$

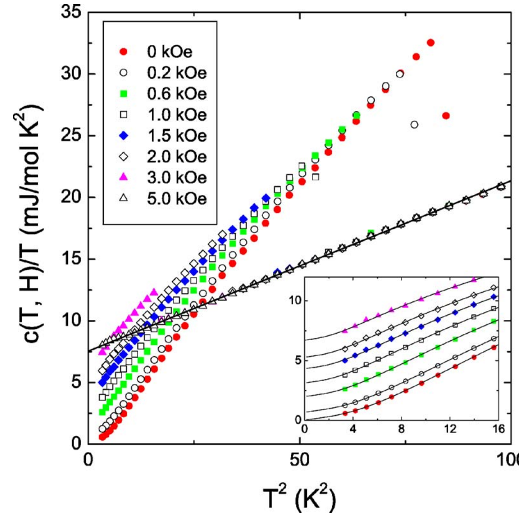

FIG. 1. (Color online) Temperature dependence of the specific heat at several different applied magnetic fields, plotted as $c(T,H)/T$ vs T^2. The measurements were taken under FC conditions. The solid line through the normal-state data at H=5 kOe is a fit described in the main text. Inset: Extrapolation of the low-temperature data to 0 K.

$$=\gamma(T,H)T+c(T,0), \tag{4}$$

where $c_{\mathrm{es}}(T,0)$ is the electronic specific heat in the superconducting medium surrounding the vortex cores. To determine the Sommerfeld coefficient $\gamma(H)\equiv\lim_{T\to 0}c(T,H)/T$, the low-$T$ data shown in the inset of Fig. 1 were extrapolated to $T\to 0$ K assuming

$$\frac{c(T,H)}{T}=\gamma(T,H)+\beta T^2+\frac{ae^{-bT_c/T}}{T}. \tag{5}$$

The last term is the limiting low-temperature BCS expression for $c_{\mathrm{es}}(T,0)$ divided by T. At H=0 kOe, the fit to Eq. (5) yields $c_{\mathrm{es}}(T,0)/\gamma_n T_c$=10.19 exp($-1.64T_c/T$). As shown in Fig. 2, $\gamma(B)$ is a linear function of B only up to $H\approx 0.22H_{c2}$.

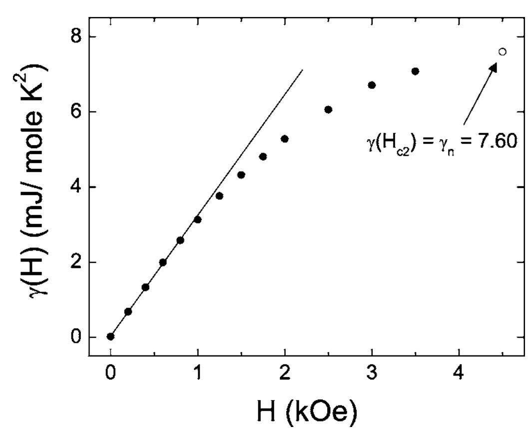

FIG. 2. Magnetic field dependence of the Sommerfeld coefficient. The open circle indicates γ at H_{c2}.

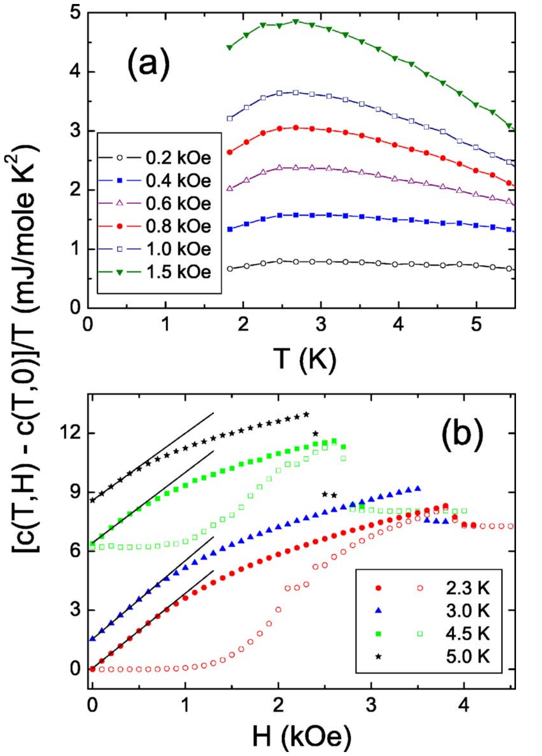

FIG. 3. (Color online) (a) Temperature dependence of $[c(T,H)-c(T,0)]/T$ at several fields measured under FC conditions. (b) Field dependence of $[c(T,H)-c(T,0)]/T$ at several temperatures below T_c. The open and solid symbols correspond to ZFC and FC measurements, respectively. The downturn at high fields for each data set indicates $H_{c2}(T)$. For visual clarity the data at $T=3.0$, 4.5, and 5.0 K are vertically offset.

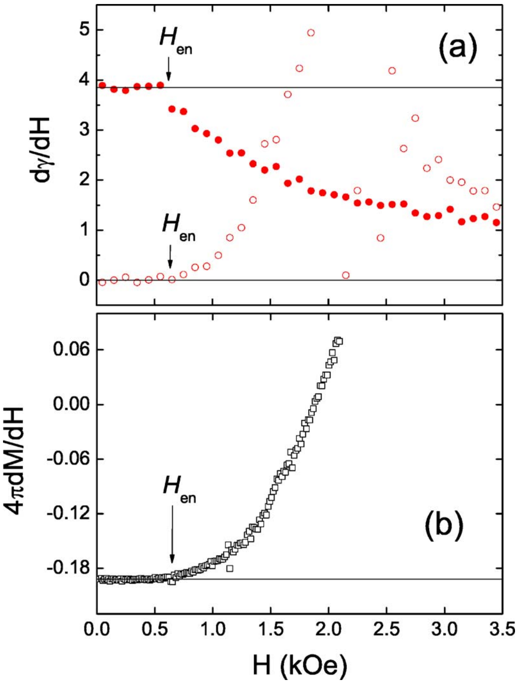

FIG. 4. (Color online) Magnetization and specific heat data at $T=2.3$ K. (a) FC (solid circles) and ZFC (open circles) measurements of $d\gamma/dH$, and (b) ZFC measurements of dM/dH. The ZFC measurements were done by first cooling the sample in zero field to $T=2.3$ K and then increasing H.

The temperature and magnetic field dependences of the difference $[c(T,H)-c(T,0)]/T$ are plotted in Fig. 3. At low temperatures this quantity reflects $\gamma(T,H)$, as inferred from Eq. (4). In Fig. 3(a) we see that below 2.5 K, $[c(T,H)-c(T,0)]/T$ decreases with decreasing T. We attribute this behavior to shrinking of the vortex cores (i.e., the KP effect), which reduces the contribution of the zero-energy DOS per vortex to the specific heat. The effect is more pronounced at higher H, due to the increased density of vortices. Above 2.5 K, $[c(T,H)-c(T,0)]/T$ decreases with increasing T due to the subtraction of the $H=0$ specific heat jump at T_c, and hence does not reflect the temperature dependence of γ. From the field dependence of $[c(T,H)-c(T,0)]/T$ measured under FC conditions [see Fig. 3(b)], we conclude that $\gamma(B)\propto B$ up to a temperature-dependent crossover field.

To clearly see the field range over which γ is a linear function of B, in Fig. 4(a) we show the derivative $d\gamma/dH$ of the $\gamma\approx[c(T,H)-c(T,0)]/T$ data at $T=2.3$ K. For both FC and ZFC measurements, $d\gamma/dH$ is constant only at low fields. In this same low-field range, $\gamma(T,H)$ is determined to be zero from the ZFC measurements. Thus, the nonzero value of $d\gamma/dH$ in the FC data at low fields must result from trapped vortices below the lower critical field H_{c1}. To see that this is indeed the case, we determined the field of first vortex entry $H_{\mathrm{en}}(T)$ from ZFC measurements of $M(H)$ for increasing H. As shown in Fig. 4(b), the increase of dM/dH at H_{en} agrees with the decrease (increase) of $d\gamma/dH$ in the FC (ZFC) measurements of the specific heat. This was also determined to be the case at the other temperatures. We note that $H_{c1}(T)$ is somewhat lower than $H_{\mathrm{en}}(T)$, if one assumes there is a Bean-Livingston barrier[18] that both impedes the entry of flux when the field is increased above $H_{c1}(T)$, and traps flux below $H_{c1}(T)$ in the FC measurements.

The observation of the simple relation $\gamma(B)\propto B$ only in FC measurements below $H_{\mathrm{en}}(T)$, indicates that the trapped vortices form a highly disordered lattice, in which they behave as isolated vortices. The disorder apparently disrupts the connection between the local DOS of nearest-neighbor vortices that is found in a well-ordered lattice.[19] At fields immediately above $H_{\mathrm{en}}(T)$, $\gamma(B)$ exhibits a sublinear dependence on B. As explained in Ref. 19, the sublinear dependence of $\gamma(B)$ on B is due to the shrinkage of the vortex cores that occurs as a result of the delocalization of the higher-energy core states. While this may seem at odds with electronic thermal conductivity measurements of Nb that indicate only a small degree of quasiparticle delocalization just above H_{c1},[20] the details of the experimental method must be considered. In Ref. 20 the thermal conductivity $\kappa(H)$ was measured in both monotonically increasing and decreasing field. In Fig. 3 the increasing field ZFC measurements of $c_{\mathrm{e}}(T,H)$ exhibit an upward curvature above H_{en}. This indicates that the flux has some difficulty entering the sample even above H_{en}. We note that the measurements of Ref. 20 are often cited in the literature as the most archetypal example of $\kappa(H)$ for a clean conventional type-II superconductor. However, here we see that the intervortex transfer of quasiparticles at low fields in Nb is greatly enhanced for a highly ordered vortex lattice generated under FC conditions.

The crossover field for an isotropic-gapped superconductor was determined in Ref. 7 to be $B^*(0.1T_c) \approx 0.33H_{c2}$. Here we find for Nb that $B^*(0.1T_c) \leqslant H_{\mathrm{en}}(0.1T_c) \approx 0.21H_{c2}$. The ratio of the minimum to maximum superconducting energy gaps on different Fermi sheets in Nb is estimated to be ~ 0.8.[21] According to Ref. 7, gap anisotropy of this size reduces the crossover field to $B^*(0.1T_c) \approx 0.25H_{c2}$. Thus, the small difference in gap values may be sufficient to explain the complete absence of a crossover field above H_{en}.

In summary, the T-linear coefficient of the electronic specific heat $\gamma(T,B)$ has been determined for pure Nb in the vortex state. Contrary to popular belief, $\gamma(T,B)$ is not a linear function of B at fields immediately above H_{c1}. Our results support theoretical calculations showing that even in a simple BCS type-II superconductor, $\gamma(T,B)$ is a sublinear function of B over a wide region of the vortex phase. This calls into question specific heat studies on type-II superconductors that have reported $\gamma(B) \propto B$ behavior persisting up to fields close to H_{c2}. We suspect inaccuracies in the $T \rightarrow 0$ K extrapolation procedure are partially responsible, but also stress the importance of small field increments in specific heat measurements of this kind. Last, the effect of delocalized quasiparticle core states on the field dependence of the specific heat should be considered when attempting to identify the pairing symmetry of a newly discovered superconductor by this method. In other words, the absence of $\gamma(B) \propto B$ behavior is not necessarily an indication of unconventional superconductivity.

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