

## Effect of the vortex core on the magnetic field in hard superconductors

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Using approximate analytical and numerical solutions of the conventional Ginzburg-Landau equations we calculate the small-angle neutron-scattering cross section and the variance of the field distribution as measured by muon-spin rotation for superconductors with large Ginzburg-Landau parameter  $\kappa$ . Our results prove that a proper account of the finite size of the vortex core is important, even at relatively low fields. This finding provides a natural explanation for the recently observed field dependence of the CeRu<sub>2</sub> form factor and of the YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.95</sub> penetration depth. [S0163-1829(97)04418-4]

The study of the vortex state in high temperature and heavy fermion superconductors is presently a subject of intense investigation. Numerous publications are devoted to the measurement of the magnetic penetration length  $\lambda$  since this is one way to probe the nature of the low-energy excitations and the symmetry of the pairing state. Among the possible experimental techniques available to investigate the vortex lattice, small-angle neutron-scattering (SANS) and muon-spin rotation ( $\mu$ SR) experiments are unique since they directly probe the bulk of the material and allow us to determine not only the field and temperature dependence of  $\lambda$  but also its value at low temperature; see the recent Refs. 1–6. To extract quantitative information from SANS and  $\mu$ SR measurements, a detailed theory of the magnetic field inside the superconductor is needed, going beyond the London model which treats the vortex cores as mathematical singularities. The finite core size was considered in Refs. 7–9.

In this paper we compute the Fourier components of the magnetic field in a type-II superconductor containing an ideal vortex lattice. We disregard pinning<sup>10</sup> and vortex “phases” such as the glassy or liquid states.<sup>11,12</sup> When accounting for the finite size of the vortex cores within the Ginzburg-Landau (GL) theory we find an unexpected large reduction of all Fourier components down to very low inductions  $B$ . Although our results are based on the conventional GL theory, they still are of relevance for the analysis of unconventional superconductors such as high- $T_c$  superconductors and heavy fermion superconductors. For example, in recent reports<sup>13,14</sup> the effect of the finite size of the vortex core is described as if these compounds were conventional superconductors.

We define an orthogonal reference frame  $(x, y, z)$ , with the external magnetic field  $\mathbf{B}_{\text{ext}}$  applied along the  $z$  axis chosen along one of the three main axes  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$  of the penetration-length tensor such that the vortices are also along  $z$ . For superconductors with large GL parameter  $\kappa = \lambda/\xi \gg 1$  ( $\xi$  is the coherence length) at not too large fields  $B_{\text{ext}} \ll B_{c2}$  ( $B_{c2}$  is the upper critical field) we may approximate the vortex fields by the London model. The London field  $\mathbf{B}(\mathbf{r})$  caused by straight vortices located at sites  $\mathbf{r}_v$  satisfies<sup>15,16</sup>

$$\mathbf{B}(\mathbf{r}) + \text{curl}[\Lambda \text{ curl } \mathbf{B}(\mathbf{r})] = \Phi_0 \sum_v \delta(\mathbf{r} - \mathbf{r}_v) \hat{\mathbf{z}}. \quad (1)$$

Here  $\Phi_0 = 2.07 \times 10^{-15} \text{ Tm}^2$  is the quantum of flux, the sum is over the vortices,  $\delta(\mathbf{r})$  is the two-dimensional  $\delta$  function, and  $\hat{\mathbf{z}}$  is the unit vector along the vortex cores. The eigenvalues of the tensor  $\Lambda$  are expressed in terms of penetration lengths  $\Lambda_a = \lambda_a^2$ ,  $\Lambda_b = \lambda_b^2$ , and  $\Lambda_c = \lambda_c^2$ . Here  $\lambda_a$ ,  $\lambda_b$ , and  $\lambda_c$  are the penetration lengths for currents flowing along the  $a$ ,  $b$ , and  $c$  axes, respectively.

When the vortices form a regular lattice it is convenient to introduce the Fourier components  $\mathbf{B}(\mathbf{G}) = \int \mathbf{B}(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) d^2\mathbf{r}/S$  of the periodic magnetic field  $\mathbf{B}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{B}(\mathbf{G}) \exp(i\mathbf{G} \cdot \mathbf{r})$ , where  $\mathbf{G}$  are the vectors of the reciprocal lattice and  $S$  the surface of the vortex lattice unit cell. The London equation is then easily solved for the cases of main interest, namely,  $\mathbf{B}_{\text{ext}}$  parallel to either  $\mathbf{a}$ ,  $\mathbf{b}$ , or  $\mathbf{c}$ . For these three geometries one finds

$$B_z(\mathbf{G}) = \frac{\Phi_0}{S} \frac{1}{1 + \Lambda_x G_y^2 + \Lambda_y G_x^2}, \quad (2)$$

and  $B_x(\mathbf{G}) = B_y(\mathbf{G}) = 0$ . Therefore, as expected, there is no transverse field component. Equation (2) means, for example, that if  $\mathbf{B}_{\text{ext}} \parallel \mathbf{c}$  we write this equation with  $x = a$ ,  $y = b$ , and  $z = c$ . In this way we recover the result of Ref. 17 for a uniaxial superconductor, in which two penetration lengths are equal.

Equation (1) disregards the effect of the finite size of the vortex core, which removes the logarithmic infinity of  $B_z(\mathbf{r})$  at  $\mathbf{r}_v$  and thus reduces the amplitude of the higher Fourier components. At  $B \ll B_{c2}$  this effect is accounted for by multiplication of the London solution (2) by a cutoff factor. Here a general remark seems appropriate. There is no general theory of  $\mathbf{B}(\mathbf{r})$  valid at arbitrary temperature, and even if it existed (if the BCS-Gorkov-Eliashberg theory would apply and could be solved) the material parameters entering such a theory are not known with sufficient accuracy, e.g., the anisotropic electron mean free path  $l$ , the shape of the Fermi surface, and the coupling constant. Even

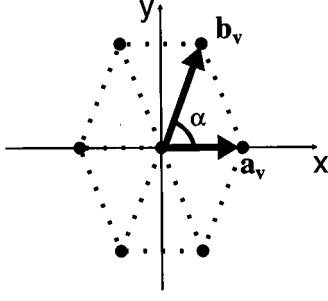


FIG. 1. Definition of the primitive cell vectors  $\mathbf{a}_v$  and  $\mathbf{b}_v$  and angle  $\alpha$  of a distorted vortex lattice in real space.  $\alpha$  is  $\pi/2$  minus the angle defined in Fig. 2 of Ref. 3.

when we use the Ginzburg-Landau (GL) theory to obtain a cutoff, we find that a general analytical solution does not exist, not even in the limit  $\kappa \rightarrow \infty$ , which would be sufficient here. If the GL theory is applicable it applies down to  $B=0$ . Below we derive the low-field cutoff factor from approximate analytical solutions of the GL theory and from a numerical solution. We are considering first an isotropic superconductor.

The best analytical GL expression available was obtained by Clem<sup>7</sup> for isotropic superconductors at low inductions  $B \ll B_{c2}$ . Using a Lorentzian trial function for the order parameter  $|\psi(\mathbf{r})|^2$  of an isolated vortex, Clem finds for large  $\kappa \gg 1$

$$B_z(G) = \frac{\Phi_0}{S} \frac{g K_1(g)}{1 + \lambda^2 G^2}, \quad g = \sqrt{2} \xi (G^2 + \lambda^{-2})^{1/2}. \quad (3)$$

Here  $K_1(x) = -K'_0(x)$  is a modified Bessel function with the limits  $K_1(x) = 1/x - (x/2) \ln(1.7139/x)$  ( $x \ll 1$ ) and  $K_1(x) = (\pi/2x)^{1/2} \exp(-x)$  ( $x \gg 1$ ). From Eq. (3) we recover the London solution if the cores size shrinks to zero. The cutoff factor  $g K_1(g)$  in Eq. (3) may be approximated for all  $g$  values by  $\exp(-\sqrt{2} \xi G)$  or, less accurate but convenient for computations, by  $\exp(-2 \xi^2 G^2)$  as suggested in Ref. 18. The cutoff  $\exp(-\xi^2 G^2/4)$  given in Ref. 19 was derived from the GL solution near  $B_{c2}$ , and is not valid at low  $B$  ( $B \ll B_{c2}$ ). At intermediate fields the cutoff should interpolate between these two expressions. Therefore, the argument of the Gaussian cutoff used recently is smaller than the one we propose:  $1/4$  (Ref. 13) or  $1/2$  (Ref. 14) instead of two valid at low  $B$ . The correct low-field cutoff yields a stronger field dependence of the SANS intensity than predicted for example in Ref. 13.

Clem's approximate analytical theory of the dilute vortex lattice was extended to larger fields and to anisotropic superconductors by Hao *et al.*<sup>9</sup> using the same type of variational approach. The resulting Fourier components for an isotropic superconductor may be written as

$$B_z(\mathbf{G}) = \frac{\Phi_0}{S} \frac{f_\infty K_1 \left[ \frac{\xi_v}{\lambda} (f_\infty^2 + \lambda^2 G^2)^{1/2} \right]}{(f_\infty^2 + \lambda^2 G^2)^{1/2} K_1 \left( \frac{\xi_v}{\lambda} f_\infty \right)}, \quad (4)$$

where  $\xi_v$  and  $f_\infty$  are two variational parameters representing the effective core radius of a vortex and the depression of the

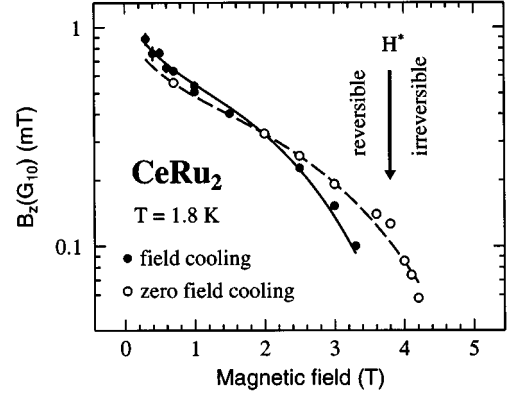


FIG. 2. Form factor for the reflection  $[1,0]$  from the vortex lattice of  $\text{CeRu}_2$  as a function of the applied field. The points taken from Ref. 6 have been obtained using either a field cooling or zero-field cooling procedure. The lines are fits to Eq. (7).

order parameter due to the overlap of vortex cores, respectively. For the cases of interest here ( $\kappa > 10$ ) the two variational parameters have simple functional dependences on  $b \equiv B/B_{c2}$  and  $\kappa$ :<sup>9,7</sup>

$$f_\infty^2 = 1 - b^4, \quad (5a)$$

$$\xi_v = \xi \left( \sqrt{2} - \frac{0.75}{\kappa} \right) (1 + b^4)^{1/2} [1 - 2b(1 - b)^2]^{1/2}. \quad (5b)$$

In Eqs. (5)  $\Phi_0/S = B = bB_{c2}$  is the mean induction, which for  $2b\kappa^2 > 1$  may be equated to  $B_{\text{ext}}$ .

For  $\kappa \gg 1$  the argument of  $K_1$  in the denominator of Eq. (4) is much smaller than 1, thus we may use  $K_1(x) \approx 1/x$ . Since for high- $T_c$  superconductors and typical  $B_{\text{ext}}$  values,  $b$  is never larger than a few %, we may also neglect the field dependence of  $f_\infty$  and  $\xi_v$ , putting  $f_\infty \approx 1$  and  $\xi_v \approx \sqrt{2} \xi$ . For the analysis of measurements performed on heavy fermion superconductors, the field dependence of  $f_\infty(b)$  can thus be disregarded [usually  $B_{\text{ext}} \leq 1$  T (Ref. 3)] but this may not be true for  $\xi_v(b)$ . For example, with  $\text{UPt}_3$  at  $B_{\text{ext}} = 1$  T one has  $b \approx 0.4$  (Ref. 3) and therefore  $\xi_v \approx 0.854 \times \sqrt{2} \xi$ .

The smallest nonzero reciprocal vector for an equilateral triangular lattice is  $G_{10} = G_{\text{min}} = a_v^* = (2\pi/S)a_v$  (see Fig. 1 for the definition of  $a_v$ ), thus  $G_{\text{min}}^2 = (8\pi^2/\sqrt{3})(B/\Phi_0)$ . This means that for the high- $T_c$  compounds at  $B = B_{\text{ext}} = 20$  mT one has  $\Lambda G_{\text{min}}^2 \approx 10 \gg 1$ , if  $\Lambda^{1/2} = \lambda = 1500$  Å is used. For  $\text{UPt}_3$   $\lambda$  is even larger.<sup>3</sup> Accounting for the large value of  $\Lambda G_{\text{min}}^2 = (4\pi/\sqrt{3})b\kappa^2$  we may write

$$B_z(\mathbf{G}) = \frac{\Phi_0}{S} \frac{f_\infty^2}{\Lambda G^2} (\xi_v G) K_1(\xi_v G). \quad (6)$$

In this paper we test the applicability of formula (6) to recently published SANS results on  $\text{CeRu}_2$ .

The conventional superconductor  $\text{CeRu}_2$  has attracted some interest because of its complex phase diagram in the  $(B_{\text{ext}}, T)$  plane. Notably, a reversible-irreversible line is observed. The form factor  $B_z(G)$  is easily obtained from the SANS cross section.<sup>20</sup> The  $\text{CeRu}_2$  measurements of  $B_z(G_{10})$  as a function of  $B_{\text{ext}}$  are presented in Fig. 2. Because

$\Lambda$  is scalar, we derive from Eq. (6)

$$B_z(G_{10}) = \frac{3^{1/4}}{2\pi\sqrt{2}} \frac{\sqrt{\Phi_0 B_{\text{ext}}} f_{\infty}^2 \xi_v}{\lambda^2} K_1 \left( \frac{2\pi\sqrt{2}}{3^{1/4}} \xi_v \sqrt{B_{\text{ext}}/\Phi_0} \right). \quad (7)$$

This expression depends only on the two parameters  $\lambda$  and  $\xi$ . The fits yield for the data recorded either in the field cooling (FC) or zero-field cooling (ZFC) procedure,  $\lambda = 1870 \text{ \AA}$  and  $\xi = 84 \text{ \AA}$  and  $\lambda = 2090 \text{ \AA}$  and  $\xi = 74 \text{ \AA}$ , respectively. Taking the traditional point of view, the FC data reflect the equilibrium properties of the vortex lattice. From these data  $\kappa = 22$  is larger than the previously estimated  $\kappa = 14.5$ .<sup>21,22</sup> From the  $\xi$  value we compute  $B_{c2} = \Phi_0 / (2\pi\xi^2) = 4.7 \text{ T}$ . Magnetization measurements at 1.8 K give  $B_{c2} = 5.3 \text{ T}$ .<sup>21</sup> The values deduced from the FC neutron data are satisfactory in view of the well known difficulty to extract a reliable  $\kappa$  value from magnetization measurements.

The traditional Gaussian cutoff predicts  $\ln[B_z(G_{10})] \propto B_{\text{ext}}$ , i.e., a straight line in Fig. 2. This is not observed.

The generalization of Eq. (6) to anisotropic penetration length tensors reads for  $\kappa \gg 1$

$$B_z(\mathbf{G}) = \frac{\Phi_0}{S} (1-b^4) \frac{uK_1(u)}{\Lambda_x G_y^2 + \Lambda_y G_x^2}. \quad (8a)$$

Here  $uK_1(u)$  is an anisotropic cutoff factor with

$$u^2 = 2(\xi_x^2 G_x^2 + \xi_y^2 G_y^2)(1+b^4)[1-2b(1-b)^2], \quad (8b)$$

$$uK_1(u) \approx 1 - (u^2/4)\ln(2.937/u^2) \quad \text{for } u \ll 1. \quad (8c)$$

For the computation of  $B_z(\mathbf{G})$  we need to specify the geometry of the vortex lattice. As shown by Kogan<sup>24</sup> for  $B \gg B_{c1}$ , the angle characterizing this lattice (see Fig. 1) depends only on the penetration-length ratio

$$\tan \alpha = \sqrt{3}(\lambda_x/\lambda_y). \quad (9)$$

Using Kogan's formula (9), the form factor factorizes,  $B_z(G_{pq}) = B_0 b_{pq}(b)$ , where

$$B_0 = \frac{1}{\pi^2} \left( \frac{3}{64} \right)^{1/2} \frac{\Phi_0}{\lambda_x \lambda_y} \quad (10)$$

and  $b_{pq}(b)$  is a universal function,

$$b_{pq}(b) = (1-b^4) \frac{v_{pq} K_1(v_{pq})}{p^2 - pq + q^2}, \quad (11a)$$

$$v_{pq} = \frac{2\sqrt{2}\pi}{3^{1/4}} b^{1/2} [1+b^4]^{1/2} [1-2b(1-b^2)^2]^{1/2} \times (p^2 - pq + q^2)^{1/2}. \quad (11b)$$

In Fig. 3 we present  $b_{10}(b)$  computed from the variational solution (11), the Gaussian cutoff (Ref. 19), and the numerical solution of the GL equations.<sup>23</sup> Remarkably, the comparison between the variational and the numerical solutions shows that for  $b \leq 0.05$  the first three Fourier coefficients  $B_z(G)$  deviate by  $< 10\%$  and for  $b \leq 0.01$  by  $< 4\%$ ; even for  $b = 0.2$  (0.3) the  $B_z(G_{10})$  Eqs. (4) with (5) falls below the

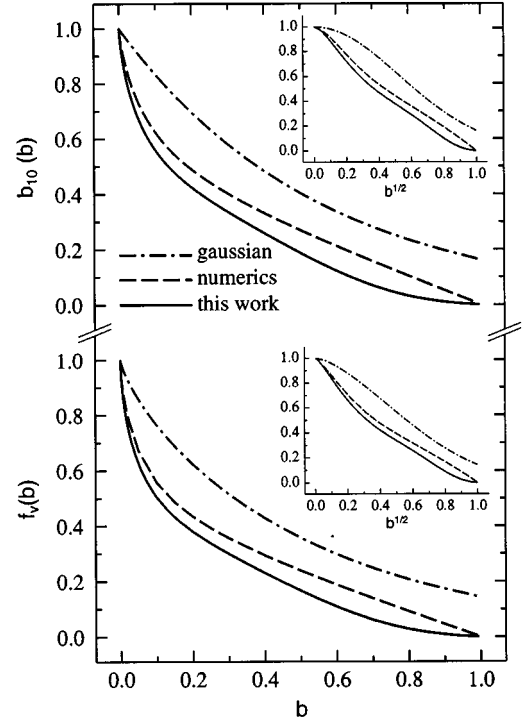


FIG. 3. The universal functions  $b_{10}(b)$  Eq. (11a) (the largest reduced form factor, top) and  $f_v(b)$  Eq. (14) (the reduced variance, bottom) calculated in three ways: From this work (solid lines), from the Gaussian cutoff (dash-dotted lines), and from the exact Ginzburg-Landau solution (dashed lines). The insets plot these functions versus  $\sqrt{b}$  to stretch the cusplike  $b$  dependence of the correct cutoff at low reduced inductions  $b=0$ . Note the strong deviation of the previously used Gaussian from the correct cutoff.

exact value by only 14% (18%), and even for small  $\kappa = 5$  this Clem-Hao approximation is reasonable.

We shall not analyze the SANS data of UPT<sub>3</sub> (Ref. 3) with Eq. (8) because the conventional GL theory discussed here does not describe the phase diagram of this compound. We argue that the effect of the vortex cores in UPT<sub>3</sub> is stronger than suggested by Joynt.<sup>13</sup>

We now consider the field distribution (probability) of the vortex lattice which is measured by  $\mu$ SR (Ref. 25) and can be computed from the Fourier coefficients, Eq. (8). Its variance is  $\Delta_v^2 = \langle B_z^2 \rangle - \langle B_z \rangle^2$ , where  $\langle \dots \rangle$  means the spatial average. One has

$$\Delta_v^2 = \sum_{\mathbf{G} \neq 0} |B_z(\mathbf{G})|^2. \quad (12)$$

$\Delta_v$  separates into two factors,  $\Delta_v = \Delta_0 f_v(b)$  where

$$\Delta_0 = 0.06092 \frac{\Phi_0}{\lambda_x \lambda_y} \quad (13)$$

is the London limit ( $\xi_x, \xi_y \rightarrow 0$ ) (Ref. 17) and  $f_v(b)$  is a universal function which accounts for the core size,

$$f_v^2(b) = 0.12968 \sum_{(p,q) \neq (0,0)} b_{pq}^2; \quad (14)$$

see Fig. 3. The functions  $b_{10}$  and  $f_v$  are very similar since in the sum (14) the six  $b_{10}$  equivalent terms dominate.

Quite unexpectedly, the functions  $b_{10}$  and  $f_v$  are *strongly field dependent even at low reduced fields*  $b$ , where the London model predicts constant  $b_{pq}=1$  and  $f_v=1$ . One has approximately  $1-b_{pq}(b)\propto 1-f_v\propto b^{1/2}$ , see Fig. 3. This finding is confirmed by the exact numerical solution of the GL theory,<sup>23</sup> depicted as dashed lines in Fig. 3. This strong  $b$  dependence originates from the limit (8c) with  $u^2=\xi_v^2 G^2=(8\pi/\sqrt{3})b(G/G_{10})^2$ , which means that the cutoff factor  $uK_1(u)$  is considerably less than unity except at very small  $b\ll\sqrt{3}/(8\pi)=1/14.5$  even for  $G=G_{10}$ .

We are aware of only one investigation on a single crystal of the field dependence of the vortex lattice field distribution.<sup>2</sup> From this  $\mu$ SR study of  $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$  and

the value  $B_{c2}=90$  (10) T (Ref. 26) we estimate  $\Delta_v\approx 5.04$  and 5.73 mT at  $B_{\text{ext}}=0.5$  and 1.5 T, respectively. This leads to a ratio  $\mathcal{R}_{\text{exp}}\equiv\Delta_v(1.5\text{ T})/\Delta_v(0.5\text{ T})=0.88$  while our computation (see Fig. 3) predicts  $\mathcal{R}_{\text{GL}}=0.90$ . Therefore the conventional GL theory provides a simple and natural explanation of the observed field dependence of the observed field distribution in  $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$ .

In conclusion, we have shown that the effect of the finite core size on the Fourier components of the magnetic field in a conventional superconductor with large  $\kappa$  is strong, even at low fields  $B_{c1}<B\ll B_{c2}$ , since the cutoff factor in Eqs. (6) and (8) is  $uK_1(u)<1$ . This cutoff effect provides a natural explanation for recently published neutron and  $\mu$ SR data without the need to resort to unconventional theories.

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