Form factor, standard deviation, and skewness of the field distribution in a hard type-II heavy-fermion superconductor from the Ginzburg-Landau model

P. Dalmas de Réotier and A. Yaouanc
Institut Nanosciences et Cryogénie, SPSMS, CEA and University Joseph Fourier, F-38054 Grenoble, France
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We compute the form factor and the standard deviation and skewness of the field distribution for a hard type-II heavy-fermion superconductor using an approximate analytical solution of the Ginzburg-Landau model. Our results are relevant if the temperature is such that $T > T^* = 0.56T_c$, where T_c is the superconductivity temperature. Instead of decreasing monotonically as the field is ramped up to the upper critical field as usually found, reflecting the influence of the Zeeman currents the form factor and standard deviation are predicted to display a maximum at an intermediate applied field intensity if the effective electron mass is sufficiently large. This behavior has been observed for the $CeCoIn_5$ form factor at $T \simeq T^*$ and is explained qualitatively by our computation. Contrary to the form factor and standard deviation, the skewness of the field distribution is not strongly influenced by the Zeeman currents.

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The investigation of the vortex lattice of a type-II superconductor is a method for studying the basic physical properties of the superconductor itself. Basically, two experimental types of methods exist. Either the lattice is probed, mainly with small-angle neutron-scattering (SANS), or the field distribution generated by the vortex lattice is measured. Nowadays this latter distribution can be determined using the muon spin rotation (μSR) technique. Both methods give access to information on the space-Fourier components of the magnetic field inside the vortex lattice. The SANS technique measures the modulus of the form factor associated with a Fourier component at a given location in the reciprocal vortex lattice, whereas the μSR technique enables the determination, amongst other characteristics, of the standard deviation of the field distribution. One expects a form factor and the standard deviation to monotonically decrease as a function of the applied external field intensity.[1] Contrary to this expectation, for the heavy-fermion superconductor $CeCoIn_5$ these two quantities were found to increase with the magnetic field and then to fall down as the upper critical field B_{c2} is approached. The maximum was detected very near B_{c2} at low temperature[2,3] but at 1.25 K the maximum of the measured form factor occurs around 2.5 T.[4] The purpose of this report is to study the form factors and the field distribution predicted by the Ginzburg-Landau functional, the Zeeman currents being taken into account.

Approaching T_c from below, superconductivity in a material is suppressed by the orbital currents and possibly by the Zeeman currents (i.e., the direct coupling of the magnetic field with the superconducting order parameter). This latter mechanism may exist for sufficiently heavy-fermion superconductors.

The form factor and therefore the field distribution can be described microscopically starting from a BCS-type Hamiltonian,[5] or using the BCS-Gor'kov equations in the quasiclassical limit (i.e., the Eilenberger equations). This latter method has traditionally been used to compute the form factor when the Zeeman currents are negligible. Their role has recently been considered.[6] However, for the first method diagrams need to be evaluated and the processing of the Eilenberger equations can only be performed numerically. Therefore it is still of interest to describe the vortex lattice using a Ginzburg-Landau (GL) functional because it enables an easy analytical study of the effect of the parameters entering the theory. Generally speaking, as an expansion of the free energy in terms of the superconducting order parameter and its gradient, the GL theory is expected to be valid in the vicinity of a second-order phase transition, and its range of validity is known to be broader in superconductors which are not in the clean limit.

Let us consider a superconductor with a large GL parameter $\kappa = \lambda_L/\xi_{GL} \gg 1$ (i.e., a so-called hard superconductor). Here λ_L is the London penetration depth and ξ_{GL} the GL coherence length. Let us assume an external magnetic field $\mathbf{B}_{ext}$ applied on the superconductor along the Z axis of the laboratory reference frame such that $B_{c1} < B_{ext} < B_{c2}$, where B_{c1} and B_{c2} are the lower and upper critical fields, respectively. Under such conditions a flux-line lattice (FLL) appears in the superconductor. We shall neglect any disorder of the FLL. We shall consider that the induction at the reciprocal space position specified by the vector $\mathbf{K}$ has only a component along the Z direction, and denote it as $B^Z_{\mathbf{K}}$. This is justified, for instance, when $\mathbf{B}_{ext}$ is applied along an axis of, at least, twofold symmetry. Some years ago a simple enough formula was proposed for the orbital contribution to $B^Z_{\mathbf{K}}$, that is $B^Z_{\mathbf{K};orb}$:[1]

$$B^Z_{\mathbf{K};\mathrm{orb}} = \frac{\Phi_0}{s_c}\left(1 - b_{\mathrm{nor}}^4\right)\frac{v K_1(v)}{\left(\lambda_L^X K^Y\right)^2 + \left(\lambda_L^Y K^X\right)^2}. \quad (1)$$

Here Φ_0 is the magnetic flux quantum ($\Phi_0 = 2.06783\times10^{-15}$ T m^2), s_c the area of the vortex lattice unit cell, that is, $s_c = \Phi_0/\overline{B^Z} \simeq \Phi_0/B_{ext}$, and $b_{nor} = \overline{B^Z}/B_{c2} \simeq B_{ext}/B_{c2}$, where $\overline{B^Z}$ is the mean value of the induction in the FLL. We specify the two components of $\mathbf{K}$ in the plane perpendicular to the Z axis (i.e., K^X and K^Y), and introduce the two London penetration depths which model the superconducting anisotropy. $K_n(x)$ is the modified

Bessel function of the second kind of index n. We have defined the anisotropic cutoff factor $vK_1(v)$ with

$$v^2 = 2\left[\left(\xi_{\rm GL}^X K^X\right)^2 + \left(\xi_{\rm GL}^Y K^Y\right)^2\right] \times \left(1 + b_{\rm nor}^4\right)[1 - 2b_{\rm nor}(1 - b_{\rm nor})^2]. \quad (2)$$

The anisotropy of a vortex core is modeled by $(\xi_{\rm GL}^X, \xi_{\rm GL}^Y)$. If needed, $b_{\rm nor}$ can be written in terms of GL coherence lengths since

$$B_{c2} = \frac{\Phi_0}{2\pi\, \xi_{\rm GL}^X \xi_{\rm GL}^Y}. \quad (3)$$

It is assumed that the large κ limit applies. The result given in Eqs. (1) and (2) was obtained from an approximate solution of the GL functional based on the Clem educated guess for the functional form of the order parameter of an isolated vortex,[7] and extended to take into account the interaction between the vortices.[8] Obviously this extension is not expected to be valid very near the superconducting phase transition. The comparison between the proposed $B_{\mathbf{K}}^Z$ formula and the results of the numerical solution of the GL equations showed the formula to be a good approximation.[1] A full discussion of $B_{\mathbf{K};{\rm orb}}^Z$ has recently been given.[9]

Based on the conventional GL method, the coupling of the magnetic field with the superconducting order parameter being described, and identifying the GL parameters to microscopic parameters, according to Michal and Mineev[10] it is a fair approximation to take

$$B_{\mathbf{K}}^Z = B_{\mathbf{K};{\rm orb}}^Z + B_{\mathbf{K};{\rm Zee}}^Z, \quad (4)$$

with

$$B_{\mathbf{K};{\rm Zee}}^Z = \mathcal{C}_{\rm Zee}\left(1 - b_{\rm nor}^4\right) b_{\rm nor}^2 K_0(v), \quad (5)$$

where we have defined the $B_{\rm ext}$-independent constant,

$$\mathcal{C}_{\rm Zee} = \frac{7\zeta(3)}{\pi^3} k_{\rm F} r_{\rm e} \frac{\varepsilon_{\rm F}}{k_{\rm B}T} \frac{\mu}{k_{\rm B}T} B_{c2}^2. \quad (6)$$

According to Ref. 10 the expression for $B_{\mathbf{K};{\rm orb}}^Z$ can still be taken from the theory available for orbital currents. Here $\zeta(x)$ is the Riemann zeta function ($\zeta(3) \simeq 1.202$), $k_{\rm F}$ is the Fermi wave vector, $r_{\rm e} = e^2/(4\pi\varepsilon_0 m_{\rm e} c^2)$ is the classical radius of the electron, $\varepsilon_{\rm F} = (m_{\rm e}^* v_{\rm F}^2)/2$ denotes the Fermi energy with $m_{\rm e}^*$ the conduction electron effective mass, and $\mu = g\mu_{\rm B}/2$ ($g = 2.002$) is the electron magnetic moment assuming a free electron. Relative to Ref. 10, we take phenomenologically into account the influence of the vortex interaction with the factor $(1 - b_{\rm nor}^4)$, and the effect of the interaction and anisotropy in the vortex cores through the dependence of the argument of the Bessel function $K_0(v)$ on $b_{\rm nor}$ and $\xi_{\rm GL}^\alpha$, respectively.

There are two limitations to the application of the above formalism. The description of the Zeeman effect is only strictly valid for $T > T^* = 0.56T_c$ because the GL expansion is unstable at low temperature.[10] Therefore a quantitative interpretation of data with the GL model is not justified at low temperature. In addition, as usual, the GL description is only strictly valid near the phase transition and in a larger temperature range if the sample is not too clean, preventing the effects of the electron diffraction on the vortex cores.[11]

At this juncture we need to specify $\mathbf{K}$. For simplicity we shall assume a triangular vortex lattice. It is straightforward to adapt the result given here to the case of the square lattice. Since $\mathbf{K}$ is perpendicular to $\mathbf{B}_{\rm ext}$, $\mathbf{K}_{p,q} = p\mathbf{a}^* + q\mathbf{b}^*$, where p and q are integers and $\{\mathbf{a}^*, \mathbf{b}^*\}$ define the unit cell in the reciprocal space. Introducing the anisotropy ratio,

$$t_{\rm K}^2 = \frac{3}{4}\left(\frac{\lambda_{\rm L}^X}{\lambda_{\rm L}^Y}\right), \quad (7)$$

and using the result of Ref. 12, we derive[1,9]

$$K_{p,q}^X = 2\pi p\sqrt{\frac{t_{\rm K}}{s_c}} \quad \text{and} \quad K_{p,q}^Y = 2\pi\left(q - \frac{p}{2}\right)\sqrt{\frac{1}{s_c t_{\rm K}}}. \quad (8)$$

We are now in a position to express the two components of a form factor in terms of basic parameters. As already published, but with an adapted notation, we derive[1]

$$B_{\mathbf{K}_{p,q};{\rm orb}}^Z = B_{\rm L}\, b_{p,q}(b_{\rm nor}), \quad (9)$$

where $(p,q) \neq (0,0)$. We have defined

$$B_{\rm L} = \frac{\sqrt{3}}{8\pi^2} \frac{\Phi_0}{\lambda_{\rm L}^Y \lambda_{\rm L}^X}, \quad (10)$$

and

$$b_{p,q}(b_{\rm nor}) = \left(1 - b_{\rm nor}^4\right) \frac{v_{p,q} K_1(v_{p,q})}{p^2 - pq + q^2} \quad \text{with}$$

$$v_{p,q} = \frac{2\sqrt{2\pi}}{3^{1/4}} b_{\rm nor}^{1/2} \left(1 + b_{\rm nor}^4\right)^{1/2} \times [1 - 2b_{\rm nor}(1 - b_{\rm nor})^2]^{1/2} (p^2 - pq + q^2)^{1/2}. \quad (11)$$

For the Zeeman component we derive

$$B_{\mathbf{K}_{p,q};{\rm Zee}}^Z = \mathcal{C}_{\rm Zee}\left(1 - b_{\rm nor}^4\right) b_{\rm nor}^2 K_0(v_{p,q}). \quad (12)$$

We find it convenient to write a form factor labeled by the couple of index (p,q) in a normalized form as follows:

$$\frac{B_{\mathbf{K}_{p,q}}^Z}{B_{\rm L}} = b_{p,q}(b_{\rm nor}) + \mathcal{R}\left(1 - b_{\rm nor}^4\right) b_{\rm nor}^2 K_0(v_{p,q}), \quad (13)$$

with the definition $\mathcal{R} = \mathcal{C}_{\rm Zee}/B_{\rm L}$. Since $K_0(x) \approx -\ln(x/2) - \gamma$ when $x \to 0^+$, where γ is the Euler-Mascheroni constant, as expected the second term on the right-hand side of the previous equation vanishes with $b_{\rm nor}$. The ratio $B_{\mathbf{K}_{p,q}}^Z/B_{\rm L}$ depends only on $b_{\rm nor}$ and the ratio $\mathcal{R}$. For a given temperature, this latter ratio is a material parameter.

It is now interesting to estimate an upper bound for $\mathcal{R}$. Since a value of 600 nm for $\lambda_{\rm L}$ is reasonable for a heavy-fermion superconductor (this is approximately the value measured at low temperature for UPt_3[13,14]), we compute $B_{\rm L} = 1.26 \times 10^{-4}$ T. Since for typical heavy-fermion superconductors $k_{\rm F} r_{\rm e}$ is on the order of 10^{-5} and $\varepsilon_{\rm F}/(k_{\rm B}T^*)$ is 10^3 at most, we get as a rough upper bound $\mathcal{C}_{\rm Zee} = 3.3 \times 10^{-2}$ T, assuming for μ the free electron magnetic moment value. This leads to $\mathcal{R}$ of about 260 for $T = T^*$.

In Fig. 1 we present $|B_{\mathbf{K}_{1,0}}^Z|^2/B_{\rm L}^2$ as a function of $b_{\rm nor}$ or $b_{\rm nor}^{1/2}$, and $\mathcal{R}$. The most striking result is the predicted maximum of $|B_{\mathbf{K}_{1,0}}^Z|^2/B_{\rm L}^2$ when $\mathcal{R}$ is large, approximately larger than 25. For example, if $\mathcal{R} = 260$ as estimated above, we find $|B_{\mathbf{K}_{1,0}}^Z|^2/B_{\rm L}^2 = 21$ at $b_{\rm nor} = 0.44$.

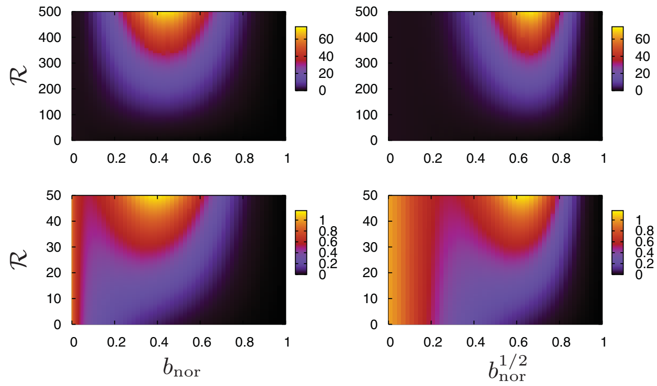

FIG. 1. (Color online) The normalized squared form factor modulus $|B^Z_{\mathbf{K}_{1,0}}|^2/B_{\rm L}^2$ as a function of either the reduced external field intensity $b_{\rm nor}$ ($b_{\rm nor} \simeq B_{\rm ext}/B_{c2}$) on the left or $b_{\rm nor}^{1/2}$ on the right, and the ratio $\mathcal{R}$ which gauges the relative weight of the Zeeman and orbital currents to a form factor. When $b_{\rm nor}$ approaches 0, the limit of $|B^Z_{\mathbf{K}_{1,0}}|^2/B_{\rm L}^2$ is 1 irrespective of the $\mathcal{R}$ value. B_{c1} is usually so small relative to B_{c2} that $B_{c1}/B_{c2} \simeq 0$ and therefore it is justified to consider very small $b_{\rm nor}$ values. The two upper panels display the data in the whole $\mathcal{R}$ range, whereas the two lower panels focus on the small $\mathcal{R}$ range.

A field map can be computed with the help of Eq. (13) and the related distribution can be derived from a histogram of the map. The result can be compared with measured distributions.[15] It is important to note that the μSR measurements only give access to the field component along the Z axis.[9] While the computation of the distribution is certainly of interest, to get a feeling of the effect of $B_{\rm ext}$ on the field distribution, it is interesting to determine its standard deviation and skewness parameter, Δ_Z and ϑ_Z, respectively.[16] While ϑ_Z is more conveniently obtained numerically from a distribution, it is possible to provide a simple analytical formula for Δ_Z, in fact, the variance Δ_Z^2.[1] We have

$$\Delta_Z^2 = \sum_{(p,q)\neq(0,0)} \left|B^Z_{\mathbf{K}_{p,q}}\right|^2. \qquad (14)$$

In Fig. 2 we display $\Delta_Z/B_{\rm L}$ and ϑ_Z in Fig. 3 as a function of $b_{\rm nor}$ or $b_{\rm nor}^{1/2}$, and $\mathcal{R}$. We note that the shapes of $|B^Z_{\mathbf{K}_{1,0}}|^2/B_{\rm L}^2$ and

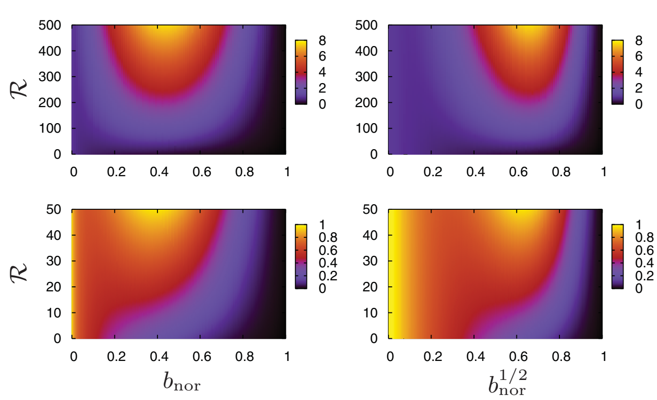

FIG. 2. (Color online) Same caption as in Fig. 1 but for the normalized standard deviation $\Delta_Z/B_{\rm L}$. By definition $\Delta_Z/B_{\rm L} = 1$ when $b_{\rm nor} \to 0$, no matter the $\mathcal{R}$ value.

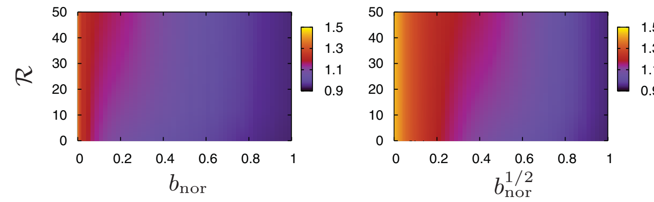

FIG. 3. (Color online) The skewness parameter ϑ_Z as a function of either the reduced external field intensity $b_{\rm nor}$ on the left or $b_{\rm nor}^{1/2}$ on the right. Here we limit the drawings to $0 \leqslant \mathcal{R} \leqslant 50$ since for $\mathcal{R} > 50$ the field dependence of ϑ_Z is similar to the one found at $\mathcal{R} = 50$. When $b_{\rm nor}$ tends to 0 we have $\vartheta_Z = 1.44$ no matter the $\mathcal{R}$ value.

$\Delta_Z/B_{\rm L}$ in Figs. 1 and 2, respectively, are quite similar. This is not surprising given the fact that Δ_Z^2 is mainly determined by the $|B^Z_{\mathbf{K}_{1,0}}|^2$ and five equivalent terms corresponding to the six nearest neighbors vectors $\mathbf{K}$ to the origin in the flux-line reciprocal lattice.[1] The skewness parameter, defined as

$$\vartheta_Z = \overline{[(B^Z - \overline{B^Z})^3]}^{1/3} \Big/ \overline{[(B^Z - \overline{B^Z})^2]}^{1/2}, \qquad (15)$$

measures the asymmetry of the FLL distribution: It would be zero if the distribution was symmetric. It is known to be strongly field dependent in the orbital limit, ϑ_Z decreasing by about 30% as $B_{\rm ext}$ varies from B_{c1} to B_{c2}.[16] We find that ϑ_Z depends on $\mathcal{R}$ for values up to $\simeq$30, and above this value it is almost $\mathcal{R}$ independent.

In the remaining part of this report we apply the $|B^Z_{\mathbf{K}_{1,0}}(B_{\rm ext})|^2$ prediction for the data obtained at $T = 1.25$ K for $CeCoIn_5$.[4] Since $T = 1.25\ {\rm K} = 0.545 T_c \simeq T^*$, the superconducting phase transition is second order at that temperature and the FLL lattice is rhombic,[17,18] it is reasonable to attempt the comparison of the data with the model in Eq. (13). The result is presented in Fig. 4. At first sight, the GL model provides a fair description of the measurements, in particular, a description of the observed $|B^Z_{\mathbf{K}_{1,0}}(B_{\rm ext})|^2$ maximum. This analysis clearly shows that the Zeeman currents rather than the orbital currents drive the field contrast in the mixed phase of $CeCoIn_5$. The curve is obtained with $\lambda_{\rm L} = 570$ nm and $\mathcal{R} = 85$, but also with

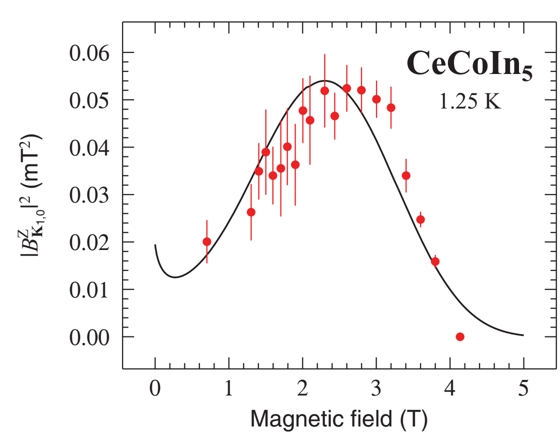

FIG. 4. (Color online) Comparison of the measured squared form factor $|B^Z_{\mathbf{K}_{1,0}}|^2$ for $CeCoIn_5$ at 1.25 mT (Ref. 4) with the prediction of the approximate analytical solution of the GL model developed in this report.

$B_{c2} = 5.5$ T. Our λ_L value is consistent with μSR estimates,[3,19] but not with values derived from microwave surface impedance and tunnel diode oscillator methods.[20,21] This may be due to the fact that SANS and μSR are bulk methods, in contrast to the other two techniques. While $\mathcal{R}$ is also reasonable, the inferred B_{c2} value at 1.25 K is somewhat large, as clearly seen in Fig. 4 which indicates $B_{c2} \simeq 4.2$ T. As possible reasons for this discrepancy in the higher critical field, one may suggest that the temperature of the measurement is not high enough. We recall that $T \simeq T^*$ rather than $T > T^*$. Another possibility is to suppose our solution of the GL equations to be too rough. While we believe that measurements closer to T_c would certainly be more relevant for a comparison with the GL prediction, and a numerically exact solution of the GL model with the Zeeman currents included would be useful, as it was done for the GL functional in the absence of Zeemen currents,[22] the main reason for the failure is probably rooted in the inadequacy of the GL model for modeling the physics of $CeCoIn_5$. The compound is in fact extremely clean with a mean-free path ℓ which is much larger than the coherence length.[20,23] Therefore ℓ is also much larger than the FLL parameter $a_\triangle \approx \sqrt{\Phi_0/B_{ext}} \simeq 30$ nn for $B_{ext} = 2.5$ T (i.e., the field at which $|B^Z_{\mathbf{K}_{1,0}}(B_{ext})|^2$ displays a maximum). This means that the electron diffraction due to the vortex cores should be strong.[11] This is not described by the GL functional.

In this work we have shown that Zeeman currents can be at the origin of a dramatic increase in the value of $|B^Z_{\mathbf{K}}|$ or Δ_Z. Hence, it is possible that even if these parameters are so small as to preclude the detection of a signal at low field, they may sufficiently increase in an intense field to yield a measurable signal. The heavy-fermion superconductor UBe_{13} could offer such a possibility.[24] The fact that B_{c2} is only $\sim$9 T is quite favorable in inducing a Zeeman contribution for $|B^Z_{\mathbf{K}}|$ and Δ_Z at a currently available field intensity.

In conclusion, we provide a simple method for obtaining the FLL form factors and field distribution of a hard heavy-fermion superconductor. Our results are quantitatively valid if the temperature is sufficiently large or if the superconductor is not too clean. The field dependence of the measured form factor for $CeCoIn_5$ at high temperature is explained qualitatively. Following our work, it seems worthwhile to attempt an extension of Delrieu's analytical work[11] to the case of a heavy-fermion superconductor. Relative to the works which focus on the numerical solution of the Eilenberger equations, Delrieu found an approximate analytical solution valid for a clean superconductor at any temperature for B_{ext} relatively close to B_{c2}.

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