# **Cutoff parameters in London theory**

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The exponential cutoff is used in London theory to calculate the magnetic field inside the vortex. In this work, using London theory and new numerical solutions of the conventional Ginzburg-Landau equations, we investigate the behavior of exponential cutoff parameter  $\alpha$  as a function of the reduced field b in the whole range of magnetic fields. We find a different behavior of this parameter for low and high magnetic fields. [S0163-1829(98)02814-8]

### I. INTRODUCTION

The effect of finite vortex core size in superconductors is very strong. Numerous publications are devoted to the study of the vortex core since this cutoff effect provides explanations for recently published experimental data without need to resort to unconventional theories. The vortex structure of type-II superconductors has been studied, using Ginzburg-Landau equations, for the cases of low and high magnetic fields H, i.e., close to  $H_{c1}$  and  $H_{c2}$  which are the lower and upper critical fields, respectively. For intermediate fields London theory has provided the only detailed phenomenological description for extreme type-II superconductors [the Ginzburg-Landau (GL) parameter  $\kappa = \lambda/\xi$  obeys  $\kappa \gg 1$ , where  $\lambda$  is the penetration depth and  $\xi$  is the coherence length]. Although London theory gives a good qualitative account of the vortex state in the restricted region  $(H_{c1} \leq H \leq H_{c2})$ , it suffers from its singular property that the magnetic flux density and the supercurrent density of an isolated vortex diverge at the center of the vortex, because the depression of the order parameter to zero in this region is not accounted by London theory.

The London equation disregards the effect of the finite size of the vortex core, which removes the logarithmic infinity of  $\mathbf{B}(\mathbf{r})$  at  $\mathbf{r}_i$ , where  $\mathbf{r}_i$  is the vortex position. At H  $\ll H_{c2}$  this effect is accounted for by multiplication of the London solution by a cutoff factor. Two common cutoffs used in reciprocal space are the Bessel and Gaussian cutoffs. The Bessel cutoff is derived from analytical approximations to Ginzburg-Landau theory near  $\underline{H}_{c1}$ . The cutoff factor in the London equation can be  $\exp(-\sqrt{2\xi}G)$ , where G is the vector of a reciprocal lattice. However, we may use the Gaussian cutoff which is less accurate but more convenient for computations, by  $\exp(-\xi_v^2 G^2)$ , where  $\xi_v = \alpha \xi$ . This factor  $\alpha$ was derived from GL theory near  $H_{c2}$  as 1/4 (Ref. 1) or 1/2 (Ref. 2) instead of 2 as proposed by Brandt at low magnetic induction.<sup>3</sup> Using London theory and a new precision Ginzburg-Landau solution, 6 we show the behavior of  $\alpha$  for all ranges of magnetic induction. We found the cutoff parameter  $\alpha = 1$  at  $H_{c1}$  and  $\alpha \approx \frac{4}{9}$  at  $H_{c2}$ .

This paper is partitioned as follows. Section II briefly reviews London theory where we show the field at the center of a single flux line. Section III describes the iteration procedure to find the precision GL solution. Section IV presents

the analytical approximation to the GL equations for isotropic superconductors at low inductions. In Sec. V our result for the parameter  $\alpha$  is discussed.

### II. LONDON THEORY

The London approximation is frequently used to describe the low-induction behavior of superconducting materials. In contrast to GL theory, London theory has an advantage in being a linear theory. However, it does have the drawback of being intrinsically divergent. London theory contains solely magnetic contributions to the free energy:

$$F_{\text{Lon}} = \int d^3 \mathbf{r} \mathbf{B}(\mathbf{r})^2 + \lambda^2 \left( \frac{\Phi_0}{2\pi} \nabla \phi(r) - \mathbf{A}(\mathbf{r}) \right)^2, \quad (1)$$

where the local magnetic field  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ .  $\phi$  is the phase of an order parameter of constant magnitude, and the presence of the flux lines is controlled by  $\nabla \phi$ . Minimizing the free energy with respect to the vector potential, the London equation is obtained,

$$\mathbf{B}(\mathbf{r}) - \lambda^2 \nabla^2 \mathbf{B}(\mathbf{r})^2 = \Phi_0 \sum_i \delta(\mathbf{r} - \mathbf{r}_i), \qquad (2)$$

which enables the free energy (1) to be written as

$$F_{\text{Lon}} = \sum_{i} \int d\mathbf{r}_{i} \mathbf{B}(\mathbf{r}_{i}). \tag{3}$$

The London equation is easily solved with  $\mathbf{B}(\mathbf{r}) = \Phi_0 \Sigma_i K_0[(|\mathbf{r} - \mathbf{r}_i|)/\lambda]$ . While this models well the flux line interaction for large  $\kappa$  systems, the intrinsic self-field is logarithmically divergent. The divergences are due to the absence of flux line cores within London theory. One approach to these divergences is to replace the  $\delta$  function in the London equation (2) by a short-ranged function, such as  $\delta(\mathbf{r} - \mathbf{r}_i) \rightarrow S(\mathbf{r} - \mathbf{r}_i) = \exp[(\mathbf{r} - \mathbf{r}_i)^2/\xi_v^2]$ .

We shall investigate some of the consequences of the cutoff chosen, and as the London free energy only contains terms involving the magnetic induction, we chose to fix any available parameters using known (or calculable) results involving the magnetic induction.

The quantity we investigate is the magnetic induction at the center of straight flux lines  $\mathbf{B}(0)$ , and investigate possible cutoffs within an isotropic system. We use cylindrical coor-

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dinates  $(\rho, \theta, z)$ , with the average magnetic induction aligned along the  $\hat{\mathbf{z}}$  axis. The Fourier transform of the magnetic induction associated with a single flux line is

$$\widetilde{B}(G) = \frac{1}{1 + \lambda^2 G^2}.\tag{4}$$

This shows the logarithmic divergence of the self-field  $B_{\text{self}}(\rho)$  when a cutoff is not used. Replacing the  $\delta$  function in the London equation as described above, the divergence can be removed,  $\widetilde{B}(G) \rightarrow \widetilde{S}(G)\widetilde{B}(G)$ , and London theory can be regularized.

We shall initially investigate an exponential cutoff  $\widetilde{S}(G) = \exp(-\xi_v^2 G^2)$ , where  $\xi_v = \alpha \xi$ ,  $\xi$  is the coherence length  $\lambda/\kappa$ , and  $\alpha$  is a constant O(1) to be determined.

The field at the center of a single flux line is then<sup>5</sup>

$$B_z(0) = \frac{\Phi_0}{2\pi\lambda^2} \int_0^\infty \frac{k \, dk}{2\pi} \, \frac{\exp(-\xi_v^2 k^2)}{1 + \lambda^2 k^2}$$

$$= \frac{1}{2\kappa^2} \exp(-\alpha^2/\kappa^2) E_1(\alpha^2/\kappa^2), \tag{5}$$

where  $E_1(x)$  is the exponential integral function  $E_1(x) = \int_x^\infty \exp(-u) du/u$ , and  $\gamma$  is the Euler constant  $\gamma = 0.577\ 21...$  For  $\kappa \gg$  and  $\alpha \sim O(1)$ , then using  $E_1(x) = -\gamma - \ln(x) - \sum_{n=1}^\infty (-1)^n x^n/(n \cdot n!)$  for  $x \ll 1$  the self-field is

$$B_z(0) = \frac{1}{2} \kappa^{-2} [-\ln(\alpha^2/\kappa^2) + \gamma].$$
 (6)

Hu<sup>4</sup> solved the isotropic GL expressions in the limit of large  $\kappa$ . Two constants  $c_0$  and  $c_1$  were found as

$$B(0) = \kappa^{-2} (\ln \kappa + c_0) H_{c_2}, \tag{7}$$

$$H_{c_1} = \frac{1}{2} \kappa^{-2} (\ln \kappa + c_1) H_{c_2}.$$

Numerically integrating the GL equations, in the limit of large  $\kappa$  it was found that  $c_0 \sim -0.282$  and  $c_1 \sim 0.497$ . Equating Eqs. (6) and (7) the parameter  $\alpha$  can be chosen so that London theory minics well the presence of the core. Given that  $H_{c_2} = \Phi_0/2\pi\xi^2$ , then  $\alpha = \exp-(c_0 + \gamma/2) \sim 1.0$ .

## III. ITERATION PROCEDURE

The calculation by Hu involves numerically integrating the isotropic GL equations for a single flux line. An iteration procedure proposed by Brandt<sup>6</sup> allows the evaluation of properties within a spatially periodic structure. The GL free energy is written in terms of the density  $w = |\varphi|^2$  and the supervelocity  $\mathbf{Q} = \mathbf{A} - \nabla \phi / \kappa$ . These real invariant functions are expressed as Fourier series

$$w(\mathbf{r}) = \sum_{\mathbf{K}} a_{\mathbf{K}} [1 - \cos(\mathbf{K} \cdot \mathbf{r})],$$

$$B(\mathbf{r}) = \overline{B} + \sum_{\mathbf{K}} b_{\mathbf{K}} \cos(\mathbf{K} \cdot \mathbf{r}),$$

$$\mathbf{Q}(\mathbf{r}) = \mathbf{Q}_A(\mathbf{r}) + \sum_{\mathbf{K}} b_{\mathbf{K}} \frac{\hat{\mathbf{z}} \times \mathbf{K}}{K^2} \sin(\mathbf{K} \cdot \mathbf{r}),$$

(8)

with  $\mathbf{r}=(x,y)$ ; the sums are over all reciprocal lattice vectors  $\mathbf{K}_{mn}\neq 0$ ,  $\bar{B}$  is the average induction, and  $\mathbf{Q}_A(\mathbf{r})$  is the supervelocity of the Abrikosov solution, correct at  $H_{c_2}$ . Rather than trying to find a solution by minimizing  $f(B,\kappa,a_{\mathbf{K}},b_{\mathbf{K}})$  with respect to a finite number of Fourier components  $a_{\mathbf{K}}$  and  $b_{\mathbf{K}}$ , Brandt proposes an iteration procedure for the parameters  $a_{\mathbf{K}}$  and  $b_{\mathbf{K}}$ . This procedure is very stable with fast convergence for any  $\bar{B}$  and  $\kappa$ .

We use this procedure to calculate the field at the center of a vortex,  $B_{GL}(0)$ . GL theory models the core well, and we use the GL result to help us determine the appropriate cutoff in a similar manner to the previous section.

Unlike GL theory, London theory is linear, and the induction at the center of a flux line can be separated into two components

$$B_{\text{Lon}}(\mathbf{r}_i) = B_{\text{self}}(\mathbf{r}_i) + B_{\text{int}}(\mathbf{r}_i), \tag{9}$$

where  $B_{\rm self}$  is the self-induction and  $B_{\rm int}$  is the interaction field. The interaction field does not diverge, and is the sum of all the contributions from the flux lines,  $B_{\rm int}({\bf r}_i) = \sum_{j \neq i} K_0(|{\bf r}_j - {\bf r}_i|/\lambda)$ . For simplification we take  ${\bf r}_i = 0$ .

It was shown in the previous section that London theory could be regularized in a manner that gave results equivalent to GL expressions. With this motivation we choose the cut-off such that  $B_{\rm Lon}(0) = B_{\rm GL}(0)$ . Using a fast convergent expansion for the interaction field, it is found that the self-induction behaves as

$$B_{\text{self}}(0) = B_{\text{GL}}(0) - B_{\text{int}}(0) = \kappa^{-2} H_{c_2}(\ln \kappa + \delta)$$
 (10)

for all fields in the limit of large  $\kappa$ . The parameter  $\delta$  is a function of the reduced average magnetic induction  $\overline{B(\mathbf{r})}/H_{c_2}=b$ . The exponential cutoff  $\widetilde{S}(k)$  then contains a parameter  $\alpha$  that must also depend on b. Comparing Eqs. (6) and (10) we chose  $\alpha(b)=\exp{-(\delta(b)+\gamma/2)}$ . This parameter is shown in Fig. 1, and is approximately 1 in the limit of small b but reduces to  $\approx \frac{4}{9}$  as  $b \to 1$ .

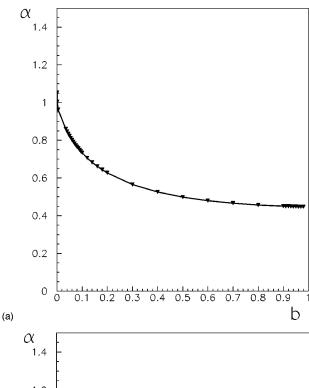
# IV. ANALYTICAL GL EQUATION

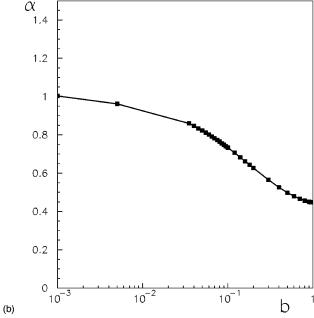
Clem has used a variational trial wave function to provide a good analytical approximation to the Ginzburg-Landau equations for isotropic superconductors at low induction. Writing the normalized order parameter in the form  $\Psi(\rho) = f(\rho) \exp(-i\phi)$  where  $f(\rho) = \rho/R = \rho/(\rho^2 + \xi_v^2)^{1/2}$ , an inhomogeneous equation for the vector potential can be obtained, whose solution is

$$A_{\phi}(\rho) = \frac{\Phi_0}{2\pi\rho} \left[ 1 - \frac{RK_1(R/\lambda)}{\xi_v K_1(\xi_v/\lambda)} \right],\tag{11}$$

where  $K_n(x)$  is a modified Bessel function. The corresponding magnetic field is then

$$B_z(\rho) = \frac{\Phi_0}{2\pi\lambda \xi_n} \frac{K_0(R/\lambda)}{K_1(\xi_n/\lambda)}.$$
 (12)





<u>FIG.</u> 1. The cutoff parameter  $\alpha$  as a function of the reduced field  $b = \overline{B(r)}/H_{c_2}$  for the Ginzburg-Landau constant,  $\kappa = 70$ , on (a) linear scale and (b) logarithmic scale.

This method has been extended to larger fields and anisotropic superconductors by Hao *et al.*<sup>9</sup>.

Here, we initially investigate Clem's expression for the magnetic field. The magnetic field at the center of a vortex is just

$$B_z(0) = \frac{\Phi_0}{2\pi\lambda\xi_v} \frac{K_0(\xi_v/\lambda)}{K_1(\xi_v/\lambda)}.$$
 (13)

Using  $K_0(x) \sim -\ln(x) - \gamma + \ln(2)$  and  $K_1(x) \sim 1/x$  when  $x \ll 1$ , for large  $\kappa$  systems the magnetic field at the center of the vortex becomes  $B_z(0) = \kappa^{-2} H_{c_2}[-\ln(\alpha/\kappa) - \gamma + \ln 2]$ . The variational parameter  $\xi_v$  is written in the form  $\xi_v = \alpha \xi$  and  $\gamma$  is the Euler constant.

Again, using Hu's expression for  $B_z(0)$  we can determine the appropriate value of the variational constant  $\beta$ . A single flux line then requires  $\beta = \exp(\gamma + C_0 - \ln 2) \sim 3/2$ .

This variational calculation indicates a possible improvement for the cutoff function used within London theory. The Fourier transform of the magnetic field (12) is

$$\widetilde{B}_{z}(G) = \frac{\Phi_{0}K_{1}(G\xi_{v})}{k\lambda K_{1}(\xi_{v}/\lambda)}.$$
(14)

In the limit  $\xi_v \leq \lambda$  this expression resembles London theory as

$$B_z(G) = \frac{\Phi_0}{S} \frac{gK_1(g)}{1 + \lambda^2 G^2}, \quad g = \beta \xi (G^2 + \lambda^{-2})^{1/2}. \quad (15)$$

This is the London expression with the cutoff function  $\widetilde{S}(k) = gK_1(g)$  and shows for large  $\kappa$  that the divergent London expression can be regularized using a "Bessel function" cutoff. However, we now have the situation were the variational GL parameter is exactly the same as the London theory cutoff parameter. We follow the same method as the previous section to determine the cutoff parameter. The cutoff parameter is chosen so that the correct magnetic field at the center of the flux line is obtained within London theory. Therefore, using similar methods to the previous section, London theory can be made to mimic GL theory using a Bessel function cutoff  $\widetilde{S}(G) = gK_1(g)$  when  $\beta(b) = \exp{-[\gamma + \delta(b) - \ln 2]}$ . This is related to the cutoff parameter used with the exponential cutoff,  $\beta(b) = 2\exp(-\gamma/2)\alpha(b)$ . For small fields,  $\beta(b) \sim 3/2$  but smoothly varies until  $\beta \sim 2/3$  for  $b \rightarrow 1$ .

The calculation by Clem determines  $\alpha$  by ensuring the correct critical field  $H_{c1}$ . We have calculated the total field at the center of a vortex, and then calculated exactly the non-divergent contribution within London theory. As the London theory free energy only contains terms containing the magnetic field, the London theory cutoff parameters  $\alpha$  are chosen to obtain the correct magnetic field. To make the London free energy more like the GL free energy, extra terms can be added, whose parameters are determined by the required energy of a flux line, and hence  $H_{c}$ :

$$F_{\text{Lon}} = \sum_{i} \int d\mathbf{r}_{i} \cdot \mathbf{B}(r_{i}) + \sum_{i} c \int \epsilon_{0} |d\mathbf{r}_{i}|, \qquad (16)$$

where  $\epsilon_0$  is the line energy of the flux line.

The two parameters in this free energy are related to the two parameters calculated by  $\mathrm{Hu.}^4$  The cutoff parameter is calculated above and is obtained by calculating the field at the center of the flux lines. The other parameter c is obtained by calculating  $H_{c_1}$  and is the difference between the two parameters calculated by  $\mathrm{Hu}$ :

$$c = c_1 - c_0 = 0.497 - (-0.282) \sim 0.78.$$
 (17)

To calculate the explicit divergent terms we have used a cutoff function within London theory (previous section) or used a simple variational wave function within GL theory that can be solved. These are both self-consistent, and show that the cutoff or variation GL parameters must contain an

element of just being a fitting parameter. The correct low-field cutoff<sup>11</sup> yields a stronger field dependence, which is in agreement with our result.

# V. CONCLUSION

In this paper the parameter  $\alpha$  of the Gaussian cutoff is studied. Using London theory and a precision Ginzburg-Landau solution we analyzed the behavior of this parameter as a function of reduced field. Here we have analyzed the isotropic extreme type-II superconductors,  $\kappa \gg 1$ . We found a sensible b dependence of this parameter for b below 0.3. It is shown in Fig. 1. We find that for a large value of the mag-

netic induction the b dependence is not strong and near  $H_{c2}$  the cutoff parameter  $\alpha \approx \frac{4}{9}$ . For sufficiently low values of the magnetic induction we find  $\alpha = 1.0$ . In summary, our systematic method gives results at variance with the normal assumption of a fixed cutoff parameter and thus calls into question much of the earlier work on this problem.

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