Order parameter and magnetic field of a vortex line pinned at a point defect: Ginzburg-Landau theory

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Recent theoretical work has derived the correct form of the Ginzburg-Landau differential equations, for the superconducting order parameter and vector potential, in the presence of a small defect. Here, these equations are applied to the case of a single vortex line pinned on such a defect. We develop the coupled set of partial differential equations, and show how to derive analytic solutions for the order parameter and magnetic field perturbations in the region of space near the defect. Certain properties of the unperturbed vortex solution are needed to totally specify our result; these are evaluated numerically, and compared with those deduced from Clem's approximate solution. [S0163-1829(98)02305-4]

I. INTRODUCTION

A vortex line in a type-II superconductor induces spatial variations of the order parameter $\eta(\mathbf{R})$ and magnetic field $\mathbf{B}(\mathbf{R})$. These quantities can be studied, for temperatures close to T_c (the superconducting transition temperature), and on length scales greater than ξ_0 (the zero temperature correlation length), by using the Ginzburg-Landau (GL) theory. When a single small defect or impurity is present, the vortex line can lower its free energy by positioning its core at the impurity site; this effect is known as vortex pinning.

Recent work by Thuneberg[1,2] and others[3,4] has shown how to correctly include into the GL framework a localized impurity potential which is not necessarily weak. The pinning energy[1–3] and pinning potential[1] have already been calculated in several situations; such quantities are the principle ingredients of macroscopic pinning theories. However, the impurity will also influence the superconductor in other interesting ways, which can be observed experimentally, using microscopic probes. For instance, both the order parameter $\eta(\mathbf{R})$ and magnetic field $\mathbf{B}(\mathbf{R})$ are altered near the impurity. These perturbations therefore provide important insight into the nature of pinning. From a theoretical perspective, the calculation of the perturbations in $\eta(\mathbf{R})$ and $\mathbf{B}(\mathbf{R})$ constitutes a nontrivial application of the Thuneberg theory.

In this work, we investigate the changes of the order parameter $\delta\eta(\mathbf{R})$ and magnetic field $\delta\mathbf{B}(\mathbf{R})$ due to the impurity, when a vortex core is placed on a defect. Near the defect these quantities can be calculated analytically. Away from the defect, $\delta\eta(\mathbf{R})$ decays exponentially over the correlation length scale $\xi(T)$ while $\delta\mathbf{B}(\mathbf{R})$ decays exponentially over the penetration length scale $\lambda(T)$.

The paper is organized as follows. In Sec. II we review the appropriate GL theory, and set up the general equations for our problem. These equations, (21) and (22), are the main results of this section. They are a pair of coupled, linear, partial differential equations for the impurity-induced changes in the order parameter and vector potential.

In Sec. III we consider in particular the spatial region close to the impurity, where $\delta\eta(\mathbf{R})$ and $\delta\mathbf{B}(\mathbf{R})$ are largest. In this region we are able to derive explicit expressions for the perturbations—the simplicity of the result for $\delta\mathbf{B}(\mathbf{R})$ is somewhat remarkable. Equations (25)–(27) contain our main results. In Sec. IV we discuss the results, and estimate the magnitude of the perturbation effects. In the Appendix we calculate, numerically, the GL solutions for vortices in the absence of impurities.

II. GL EQUATIONS

A. General formulation

For simplicity, in this paper we consider a superconductor with a spin singlet, isotropic (i.e., $\hat{\mathbf{k}}$-independent) energy gap. The GL free energy, in terms of the complex order parameter $\eta(\mathbf{R})$ and vector potential $\mathbf{A}(\mathbf{R})$, is given, in the absence of the impurity, by

$$\Omega_{\text{pure}}=\int d^3R\left\{\frac{1}{2}K|\boldsymbol{\mathcal{D}}\eta|^2+\alpha|\eta|^2+\beta|\eta|^4+\frac{1}{8\pi}(\nabla_{\mathbf{R}}\times\mathbf{A})^2\right\}, \tag{1}$$

Here, $D=\nabla_{\mathbf{R}}+2ie\mathbf{A}/\hbar c$ is the gauge-invariant derivative, and the local magnetic field is given by $\mathbf{B}=\nabla_{\mathbf{R}}\times\mathbf{A}$. The coefficients K, α, and β can be evaluated by using the microscopic theory of a superconducting Fermi liquid. The results are

$$K=\frac{7\zeta(3)N(0)\hbar^2v_F^2}{24(\pi k_BT_c)^2}, \tag{2}$$

$$\alpha=N(0)(T-T_c)/T_c, \tag{3}$$

$$\beta=\frac{7\zeta(3)N(0)}{16(\pi k_BT_c)^2}, \tag{4}$$

where $N(0)$ is the density of states at the Fermi surface, and v_F^2 represents the Fermi surface average of the square of the Fermi velocity. Note that K can be more generally represented as a tensor K_{ij}. However, we have considered here the isotropic case $K_{ij}=K\delta_{ij}$.

It is convenient at this point to rescale our variables in order to simplify the following equations. We will measure lengths in terms of $\xi(T)$ [with $\xi^2(T)=K/2|\alpha|$], and will normalize the order parameter in terms of its bulk value $\eta_b(T)$ (with $\eta_b^2=|\alpha|/2\beta$) for a uniform superconductor. Thus we define the following dimensionless quantities:

$$\mathbf{r}=\mathbf{R}/\xi(T), \tag{5}$$

$$\psi(\mathbf{r})=\eta(\mathbf{r})/\eta_b(T), \tag{6}$$

$$\mathbf{a}(\mathbf{r})=2e\xi(T)\mathbf{A}(\mathbf{r})/\hbar c, \tag{7}$$

$$\mathbf{D}=\nabla_{\mathbf{r}}+i\mathbf{a}(\mathbf{r})=\xi(T)\boldsymbol{\mathcal{D}}, \tag{8}$$

$$\mathbf{b}(\mathbf{r})=\nabla_{\mathbf{r}}\times\mathbf{a}=2e\xi^2(T)\mathbf{B}(\mathbf{r})/\hbar c. \tag{9}$$

When an impurity is located at $\mathbf{r}=\mathbf{0}$, the (dimensionless) GL equation acquires an extra term:[1,4]

$$\psi-|\psi|^2\psi+D^2\psi=\frac{\sigma\hbar^2v_F^2}{576(k_BT_c)^3\xi^5(T)|\alpha|}\times[\mathbf{D}_0\psi_0(\mathbf{r})|_{r=0}]\cdot[\mathbf{D}_0\delta^3(\mathbf{r})]. \tag{10}$$

To understand this equation, several points should be borne in mind.

(1) The effect of an impurity on the normal state quasiparticles can be represented by a potential $v(\hat{\mathbf{k}},\hat{\mathbf{k}}')$ for scattering from $\hat{\mathbf{k}}$ to $\hat{\mathbf{k}}'$ on the Fermi surface. For simplicity, we take the potential to be of s-wave form, so that $v(\hat{\mathbf{k}},\hat{\mathbf{k}}')=v$. The impurity parameter σ, which appears in the right-hand side of Eq. (10), is defined as[5]

$$\sigma=\frac{N^2(0)\pi^2v^2}{1+N^2(0)\pi^2v^2}. \tag{11}$$

The quasiparticle scattering cross section is then proportional to σ/k_F^2. In the present theory,[1–4,6] a ''small'' impurity implies that $\sigma/k_F^2\ll\xi_0^2$. Thus, the small parameter for the expansions which follow becomes $\sigma/k_F^2\xi_0^2$. However, there is no restriction on the magnitude of v. Note that we consider here a general Fermi surface, subject only to the symmetry constraint $K_{ij}=K\delta_{ij}$. For an s-wave order parameter and for a Fermi surface with at least orthorhombic symmetry, Thuneberg has shown how to go beyond the assumption that the impurity potential satisfies $v(\hat{\mathbf{k}},\hat{\mathbf{k}}')=v$.[2] With Thuneberg's generalization, Eq. (10) remains valid, provided that Eq. (11) is generalized appropriately.

(2) To derive the GL equation (10), we coarse grain a more microscopic theory,[6] and so lose information on length scales shorter than $\xi_0=\hbar v_F/k_BT_c$. At the GL level, the small impurity appears as a δ-function driving term.

(3) Equation (10) should be expanded to first order in our small parameter $\sigma/k_F^2\xi_0^2$. This amounts to the following linearization procedure. We write $\psi(\mathbf{r})=\psi_0(\mathbf{r})+\delta\psi(\mathbf{r})$, $\mathbf{a}(\mathbf{r})=\mathbf{a}_0(\mathbf{r})+\delta\mathbf{a}(\mathbf{r})$, and $\mathbf{D}_0=\nabla_{\mathbf{r}}+i\mathbf{a}_0$, where $\psi_0(\mathbf{r})$ and $\mathbf{a}_0(\mathbf{r})$ solve Eq. (10) in the absence of the impurity (i.e., with $\sigma=0$). We then expand the left-hand side of Eq. (10) to first order in $\delta\psi$ and $\delta\mathbf{a}$, and set this first order piece equal to the right-hand side. $\delta\psi$ and $\delta\mathbf{a}$ then represent the parts of the GL solution proportional to σ. Consistent with this linearization procedure, the right-hand side of Eq. (10) involves only the unperturbed terms $\psi_0(\mathbf{r})$ and $\mathbf{a}_0(\mathbf{r})$.

In the presence of the impurity, the (dimensionless) Maxwell equation also picks up an additional term ($\mathbf{J}_2$):

$$\nabla_{\mathbf{r}}\times\nabla_{\mathbf{r}}\times\mathbf{a}=4\pi(\mathbf{J}_1+\mathbf{J}_2), \tag{12}$$

$$\mathbf{J}_1=-\frac{ie^2K^2}{2\hbar^2c^2\beta}(\psi\mathbf{D}^*\psi^*-\psi^*\mathbf{D}\psi), \tag{13}$$

$$\mathbf{J}_2=\frac{i\sigma e^2v_F^2K}{576(k_BT_c)^3c^2\xi^3(T)\beta}(\psi_0\mathbf{D}_0^*\psi_0^*-\psi_0^*\mathbf{D}_0\psi_0)\,\delta^3(\mathbf{r}). \tag{14}$$

Equation (12) should also be linearized in $\delta\psi(\mathbf{r})$ and $\delta\mathbf{a}(\mathbf{r})$, with $\mathbf{J}_1$ evaluated to first order in these quantities and $\mathbf{J}_2$ evaluated using $\psi_0(\mathbf{r})$ and $\mathbf{a}_0(\mathbf{r})$.

For a given $[\psi_0(\mathbf{r}),\mathbf{a}_0(\mathbf{r})]$, Eqs. (10) and (12) constitute a pair of linear, coupled, differential equations for $\delta\psi$ and $\delta\mathbf{a}$. For an application of these equations in a simpler context, see Ref. 7.

B. Application to a single vortex line

We now specialize, and apply Eqs. (10) and (12) to the case of a single vortex line which is centered on an impurity at the origin. $\psi_0(\mathbf{r})$ and $\mathbf{a}_0(\mathbf{r})$ then represent the solutions of the $\sigma=0$ GL equations, with a single vortex at the origin. These unperturbed vortex solutions are well studied.[8] (Some aspects of the computations are discussed in the Appendix.) The following gauge choice is most convenient:

$$\psi_0(\mathbf{r})=f_0(\rho)e^{-i\phi}, \tag{15}$$

$$\mathbf{a}_0(\mathbf{r})=a_0(\rho)\hat{\boldsymbol{\phi}}, \tag{16}$$

where we have used polar coordinates (ρ,ϕ,z) and taken the vortex line to be along the z axis.[9] At large ρ, we have $f_0(\rho)\to1$, while in the limit $\rho\to0$, we have

$$\lim_{\rho\to0}\{f_0(\rho)=\gamma\rho,\quad a_0(\rho)=\tau\rho\}. \tag{17}$$

γ and τ are constants which depend on β and K through the Ginzburg-Landau parameter $\kappa^2=\lambda^2(T)/\xi^2(T)=\hbar^2c^2\beta/4\pi e^2K^2$. ($\gamma$ and τ should be determined numerically, as described in the Appendix.)

According to Eqs. (10) and (12), the impurity perturbations to $\psi_0(\mathbf{r})$ and $a_0(\mathbf{r})$ take on the following form:

$$\delta\psi(\mathbf{r})=f_1(\rho,z)e^{-i\phi}, \tag{18}$$

$$\delta\mathbf{a}(\mathbf{r})=a_1(\rho,z)\hat{\boldsymbol{\phi}}. \tag{19}$$

Thus, the order parameter magnitude will depend on z as well as ρ. Further, we find

$$\delta\mathbf{b}(\mathbf{r})=\nabla_{\mathbf{r}}\times\delta\mathbf{a}=-\frac{\partial a_1}{\partial z}\hat{\boldsymbol{\rho}}+\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho a_1)\hat{\mathbf{z}}. \tag{20}$$

So, the magnetic field in the presence of the impurity will now have a $\hat{\boldsymbol{\rho}}$ component, in addition to a perturbed $\hat{\mathbf{z}}$ component.

Using the preceding definitions (15), (16), (18), and (19), we arrive at the following pair of coupled, linear, differential equations for $f_1(\rho,z)$ and $a_1(\rho,z)$:

$$\frac{\partial^2 f_1}{\partial z^2}+\frac{1}{\rho}\frac{\partial f_1}{\partial \rho}+\frac{\partial^2 f_1}{\partial \rho^2}-\left(a_0-\frac{1}{\rho}\right)^2 f_1 - 2a_1 f_0\left(a_0-\frac{1}{\rho}\right)+f_1-3f_0^2 f_1 = \frac{\gamma\sigma\hbar^2 v_F^2 e^{i\phi}}{576(k_B T_c)^3\xi^5(T)|\alpha|}(\hat{\mathbf{x}}-i\hat{\mathbf{y}})\cdot\nabla_{\mathbf{r}}\delta^3(\mathbf{r}), \tag{21}$$

$$\frac{\partial^2 a_1}{\partial z^2}+\frac{1}{\rho}\frac{\partial a_1}{\partial \rho}+\frac{\partial^2 a_1}{\partial \rho^2}-\frac{a_1}{\rho^2}=\frac{1}{\kappa^2}\left\{f_0^2 a_1+2f_0 f_1\left(a_0-\frac{1}{\rho}\right)\right\}. \tag{22}$$

Note that the magnitudes of f_1 and a_1 are determined by the δ-function driving term in Eq. (21), particularly through the impurity parameter σ. We also note that since the unperturbed vortex line has a vanishing current density at the impurity site, the explicit impurity term (14) in Maxwell's equation is zero. Thus, the changes in the magnetic field are due solely to the changes in the order parameter caused by the impurity.

III. SOLUTION CLOSE TO THE IMPURITY

The rather formidable set of equations for $f_1(\rho,z)$ and $a_1(\rho,z)$ simplifies greatly, at distances much closer to the impurity than $\xi(T)$; in our rescaled variables, this means that the results of this section are meant to cover the region $\rho^2+z^2\ll 1$. Recalling that $f_0(\rho)$ and $a_0(\rho)$ both vanish linearly as $\rho\to 0$, the proper short distance versions of Eqs. (21) and (22) become

$$\frac{\partial^2 f_1}{\partial \rho^2}+\frac{1}{\rho}\frac{\partial f_1}{\partial \rho}+\frac{\partial^2 f_1}{\partial z^2}-\frac{f_1}{\rho^2} = \frac{\gamma\sigma\hbar^2 v_F^2 e^{i\phi}}{576(k_B T_c)^3\xi^5(T)|\alpha|}(\hat{\mathbf{x}}-i\hat{\mathbf{y}})\cdot\nabla_{\mathbf{r}}\delta^3(\mathbf{r}), \tag{23}$$

$$\frac{\partial^2 a_1}{\partial \rho^2}+\frac{1}{\rho}\frac{\partial a_1}{\partial \rho}+\frac{\partial^2 a_1}{\partial z^2}-\frac{a_1}{\rho^2}=-\frac{2\gamma}{\kappa^2}f_1. \tag{24}$$

One advantage of the formulation we have chosen is that the equations become decoupled in the following sense: we can now solve Eq. (23) independently for f_1, and then use this result in Eq. (24) to find a_1. Remarkably enough, when the analytic form for $f_1(\rho,z)$ is inserted into Eq. (24), a simple, analytic solution for $a_1(\rho,z)$ may also be found, leading to a simple solution for $\delta\mathbf{b}(\mathbf{r})$. The following results are obtained:

$$\delta\psi(\mathbf{r})=\frac{\gamma\sigma\hbar^2 v_F^2}{2304\pi(k_B T_c)^3\xi^5(T)|\alpha|}\frac{\rho e^{-i\phi}}{(\rho^2+z^2)^{3/2}}, \tag{25}$$

$$\delta\mathbf{b}(\mathbf{r})=\frac{\gamma^2\sigma\hbar^2 v_F^2}{2304\pi(k_B T_c)^3\xi^5(T)|\alpha|\kappa^2}\times\left\{\frac{z\rho\hat{\boldsymbol{\rho}}}{(\rho^2+z^2)^{3/2}}+\frac{(2z^2+\rho^2)\hat{\mathbf{z}}}{(\rho^2+z^2)^{3/2}}\right\}, \tag{26}$$

$$\delta\mathbf{a}(\mathbf{r})=\frac{\gamma^2\sigma\hbar^2 v_F^2}{2304\pi(k_B T_c)^3\xi^5(T)|\alpha|\kappa^2}\frac{\rho\hat{\boldsymbol{\phi}}}{(\rho^2+z^2)^{1/2}}. \tag{27}$$

IV. DISCUSSION

Equations (25)–(27) are the main results of this paper. They reflect the changes in the order parameter, magnetic field, and vector potential due to the impurity. We now discuss important points concerning these equations.

(1) The results hold for distances from the impurity greater than ξ_0, but less than $\xi(T)$. Close enough to T_c, this range of validity can be reasonably large, since $\xi(T)\sim\xi_0[(T_c-T)/T_c]^{-1/2}$. Furthermore, any anomalies which appear in Eqs. (25)–(27) as $\rho,z\to 0$ are not physical, since these solutions are not valid at short distances.

(2) The magnitude of the order parameter near the vortex core actually increases from its unperturbed value, when the impurity is taken into account. This is consistent with the idea that scattering from nonmagnetic impurities lowers the free energy cost of gradients of the order parameter.[1] The situation is analogous to the case of a finite concentration of impurities, where the GL coefficient K is reduced from its impurity-free value.

(3) Associated with the increase in $|\psi|$, circulating vortex currents are also enhanced near the defect site, causing the $\hat{\mathbf{z}}$ component of $\mathbf{b}(\mathbf{r})$ to increase. We may estimate the largest deviation of the magnetic field from its unperturbed value, $\delta B_{\max}$. To do this, we estimate $\delta\mathbf{b}$ at a distance ξ_0 from the impurity. Note that in real units, $\mathbf{B}=H_{c2}(T)\mathbf{b}$, where $H_{c2}(T)=\hbar c/2e\xi^2(T)$. If we take γ^2 and σ to be of order one, we finally get

$$\frac{\delta B}{H_{c2}}\simeq\frac{2(k_B T_c)^2}{\kappa^2 E_F^2}\frac{(T_c-T)}{T_c}. \tag{28}$$

It should be possible to test both the magnitude and temperature dependence of this prediction using a suitable microscopic probe.[10]

(4) In spite of the local perturbations to the magnetic field, impurities do not affect the quantization of vorticity; the net flux associated with a pinned vortex remains Φ_0 in the $\hat{\mathbf{z}}$ direction. However, the vortex field lines, which are parallel to $\hat{\mathbf{z}}$ for the unperturbed vortex, now acquire a new $\hat{\boldsymbol{\rho}}$ component near the defect. The perturbation to the magnetic field is largest inside a radius ξ_0 of the defect [see Eq. (28)]. At a distance of order $\xi(T)$ from the vortex core, the perturbation field lines begin to close on themselves. Full screening of $\delta\mathbf{B}(\mathbf{r})$ occurs at distances of order $\lambda(T)$. Note that neither the screening of $\delta\mathbf{B}(\mathbf{r})$, nor the decay of $\delta\psi(\mathbf{r})$ over length

scale $\xi(T)$, can emerge from Eqs. (23) and (24), since those apply only very near the impurity.

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APPENDIX: DETERMINATION OF γ AND τ

In Sec. IV of this paper, an estimate was made for the magnitude of δB, near the defect site, for which it was found that $\delta B \propto \gamma^2$. In general, many quantities calculated near the vortex core depend sensitively on the parameter $\gamma = \partial f_0/\partial\rho|_{\rho\to 0}$, regardless of the presence of a perturbing defect. To the best of our knowledge, there exists in the literature no general calculation of this important quantity, nor of the quantity $\tau = \partial a_0/\partial\rho|_{\rho\to 0}$. Such a calculation is therefore presented here. The results are found to agree quite well with the approximate solution of Clem.[11]

Using dimensionless variables, the equations satisfied by $f_0(\rho)$ and $a_0(\rho)$ become

$$\frac{d^2 f_0}{d\rho^2} + \frac{1}{\rho}\frac{df_0}{d\rho} - \left(a_0 - \frac{1}{\rho}\right)^2 f_0 + f_0 - f_0^3 = 0, \qquad \text{(A1)}$$

$$\frac{d^2 a_0}{d\rho^2} + \frac{1}{\rho}\frac{da_0}{d\rho} - \frac{a_0}{\rho^2} - \frac{1}{\kappa^2} f_0^2 \left(a_0 - \frac{1}{\rho}\right) = 0, \qquad \text{(A2)}$$

while the boundary conditions, appropriate for a vortex core located at $\rho = 0$, are $f_0(\rho) = a_0(\rho)\rho = 0$ when $\rho \to 0$, and $f_0(\rho) = a_0(\rho)\rho = 1$ when $\rho \to \infty$. Equations (A1) and (A2) cannot be solved exactly, in the general case. We therefore solve the equations numerically, for fixed values of κ. To characterize our results, we show the resulting κ dependences of γ and τ in Fig. 1, with $\kappa > 1/\sqrt{2}$ for a type-II superconductor.

The results of Fig. 1 reflect an exact treatment of the vortex, within the GL description. An approximate, but analytic, treatment has also been provided by Clem.[11] In this scheme, only the second GL equation (A2) is solved. This is accomplished by using the variational form $f_0 \simeq \rho/(\rho^2 + \xi_v^2)^{1/2}$, which permits an exact solution for a_0. The GL free energy is then constructed for the vortex line, and minimized, in terms of the variational parameter ξ_v. Clem's model thus improves and regularizes the London vortex solution, by introducing a vortex core. Indeed, the results for the quantity τ (which emerges from the conventional London theory only through *ad hoc* regularization) are quite impressive; Fig. 1 shows Clem's approximate, transcendental solution for τ, as well as its large-κ asymptotic behavior: $\tau \simeq (\ln\sqrt{2}\kappa - \gamma_E)/2\kappa^2$, where $\gamma_E \simeq 0.577$ is Euler's constant. Although the model is not designed to provide accurate information in the vicinity of $\xi(T)$, we may still use it to calculate γ as shown in Fig. 1. It is interesting that the outcome has the correct qualitative behavior, but is slightly too large.

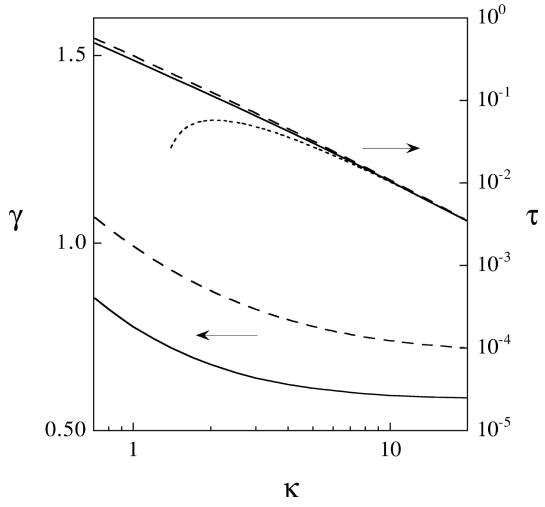

FIG. 1. Results are shown for γ (bottom two curves) and τ (top three curves), defined in Eq. (17), as a function of the Ginzburg-Landau parameter κ. Exact numerical solutions of Eqs. (A1) and (A2) are given as solid lines. Approximate solutions, due to Clem, are shown as dashed lines; these describe τ very accurately for all κ. The large-κ asymptotic form of Clem's result, $\tau \simeq (\ln\sqrt{2}\kappa - \gamma_E)/2\kappa^2$, is shown as a dotted line, and is accurate in the range $\kappa \gtrsim 5$.

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[5] The normal state impurity scattering time τ_i is also described in terms of v, as $(2\tau_i)^{-1} = cN(0)\pi v^2/\{1 + [N(0)\pi v]^2\}$, where c is the density of impurities.

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[8] For example, see, M. Tinkham, *Introduction to Superconductivity* (McGraw-Hill, New York, 1980).

[9] In the exponent of Eq. (15), we have chosen the minus sign convention which produces a vortex with **B** parallel to $+\hat{z}$. The reader is cautioned that some standard textbooks and references state results with inconsistent conventions, especially regarding the charge of the electron. Here, we assume $e = |e|$, so the electronic charge becomes $-e$.

[10] For example, the magnetic force microscope can probe the local magnetic structure of a vortex at the surface of a sample, allowing Eqs. (26) and (28) to be tested; see H. J. Hug *et al.*, Physica C **235-240**, 2695 (1994).

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