Superconducting impurity terms in the Ginzburg-Landau equations and supercurrent: A microscopic theory

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Finding the correct way to include small defects in the Ginzburg-Landau (GL) theory of superconductivity requires a microscopic analysis. In the presence of a single impurity, we compute terms which must be added to the GL free energy, supercurrent, and the GL differential equation for the order parameter. Our calculation is very general, covering any $\hat{\mathbf{k}}$-dependent order parameter $\Delta(\hat{\mathbf{k}})$ which transforms according to a one-dimensional irreducible representation of the crystalline point group. [S0163-1829(97)07401-8]

I. INTRODUCTION

The investigation of defects and their effect on superconductors is of both practical and fundamental interest. In high-T_c superconductors, localized defects, such as oxygen vacancies or impurities, and extended defects, such as twinning planes and grain boundaries, both proliferate. Analytic methods for studying these defects often rely on the Ginzburg-Landau (GL) theory, since it is well suited to describe situations where the order parameter is spatially varying. The conventional GL theory works well for the case of large defects, which can be treated by forcing the order parameter to satisfy certain boundary conditions.

A defect whose size d (characterized by its quantum-mechanical scattering cross section, $\sigma_{\rm sc}\sim d^2$) is much smaller than the zero-temperature coherence length ξ_0, presents a technical difficulty in this approach, since the GL theory involves coarse graining over length scales smaller than ξ_0. In this case, microscopic theory must be used to derive the extra terms which arise in the GL free energy when a single defect is present. In a previous paper,[1] we presented such a derivation for the case of a single defect, using a general spin-singlet order parameter of the following form:

$$\Delta(\hat{\mathbf{k}},\mathbf{r})=\eta(\mathbf{r})\phi(\hat{\mathbf{k}}). \tag{1}$$

Here $\phi(\hat{\mathbf{k}})$ is a normalized basis function for a one-dimensional representation of the crystalline point group, and $\eta(\mathbf{r})$ is the complex order parameter which appears in the GL theory. Our work generalized that of Thuneberg,[2] and is based on the microscopic theory developed by Thuneberg, Kurkijärvi, and Rainer.[3]

The Thuneberg approach leads to two types of terms in the defect free energy; one type involving the magnitude of the order parameter (δT_c terms), and the other type involving gradients of the order parameter ($\delta\ell$ terms, where ℓ is the mean free path). Both types (δT_c[4] and $\delta\ell$[5]) have been investigated as causes of vortex pinning. Another outcome of the analysis is that the vortex pinning energy of a single defect should be proportional to $d^2\xi_0$, rather than to d^3. The predicted $d^2\xi_0$ dependence has also been verified experimentally.[6] In all these experiments, the elementary pinning mechanisms are probed by transport measurements, and must therefore be interpreted in terms of a collective pinning theory.[7]

In this paper, we complete our original work by deriving and discussing the impurity terms which appear in the supercurrent $\mathbf{J}$ and in the Ginzburg-Landau differential equation (GLE). We again treat a general order parameter of the form (1), so that we cover many interesting examples of unconventional pairing, such as the d-wave order parameters recently discussed in the context of the high-T_c superconductors.[8] The GL formalism presented here allows one to compute the perturbations in the order parameter, and in $\mathbf{J}$ caused by an impurity. Particularly interesting situations arise when the order parameter is spatially varying, even in the absence of an impurity; such situations include uniform supercurrents and vortex lines.

The plan of this paper is as follows. In Sec. II, our notation is specified, and previous results, including the derivation of the impurity contribution to the GL free energy, are reviewed. In Secs. III and IV, respectively, the results for the supercurrent and the GLE are presented. Section V explains how to derive these results from microscopic theory. Section VI discusses an alternative derivation of the results, while Sec. VII contains a concluding discussion.

One interesting finding arising from this work is that, among the impurity terms in the supercurrent, there are two which are nonzero only when $\phi(\hat{\mathbf{k}})$ breaks time-reversal symmetry, as in the case of an ''$s+id$'' order parameter.[9] In particular, these terms are not proportional to the superfluid velocity. Such supercurrents are not encountered in either pure s-wave or d-wave superconductors. This point is discussed in Sec. III.

II. NOTATION

To establish our notation, and review previous results, we recall that in the presence of a single impurity located at $\mathbf{r}=\mathbf{R}$, the GL free energy is given by

$$\Omega_{\rm GL}=\Omega_B+\Omega_I. \tag{2}$$

Here Ω_B is the usual bulk GL free energy:

$$\Omega_B = \int d^3r\left[\alpha|\eta|^2 + \beta|\eta|^4 + \frac{1}{2}\kappa_{ij}(D_i\eta)(D_j^*\eta^*) + \frac{1}{8\pi}(\boldsymbol{\nabla}\times\mathbf{A})^2\right], \tag{3}$$

where the gauge-invariant derivative is given by $\mathbf{D}\equiv\nabla+2ie\mathbf{A}/\hbar c$. The coefficients of Ω_B are given by

$$\alpha = N(0)(T-T_c)/T_c, \tag{4}$$

$$\beta = \frac{7\zeta(3)N(0)}{16(\pi k_B T_c)^2}\langle|\phi|^4\rangle, \tag{5}$$

$$\kappa_{ij} = \frac{7\zeta(3)N(0)\hbar^2}{8(\pi k_B T_c)^2}\langle v_{Fi}v_{Fj}|\phi|^2\rangle, \tag{6}$$

where $N(0)$ is the density of states at the Fermi surface, and $\mathbf{v}_F(\hat{\mathbf{k}})$ is the Fermi velocity at $\hat{\mathbf{k}}$. The Fermi-surface average is defined by

$$\langle F\rangle = \int_{\mathrm{FS}} d^2\hat{k}\, n(\hat{\mathbf{k}})F(\hat{\mathbf{k}}), \tag{7}$$

where $n(\hat{\mathbf{k}})$ is the angle-resolved density of states at $\hat{\mathbf{k}}$, normalized to 1:

$$\int_{\mathrm{FS}} d^2\hat{k}\, n(\hat{\mathbf{k}}) = 1. \tag{8}$$

To discuss impurity effects, it is convenient to write the order parameter and vector potential in the following way:

$$\eta(\mathbf{r}) = \eta_0(\mathbf{r}) + \delta\eta(\mathbf{r}), \tag{9}$$

$$\mathbf{A}(\mathbf{r}) = \mathbf{A}_0(\mathbf{r}) + \delta\mathbf{A}(\mathbf{r}); \tag{10}$$

then $(\eta_0,\mathbf{A}_0)$ is the solution to the GLE in the absence of the impurity, and $(\delta\eta,\delta\mathbf{A})$ is the change caused by the impurity. For example, $(\eta_0(\mathbf{r}),\mathbf{A}_0(\mathbf{r}))$ could represent a single vortex solution in the ordinary GL theory. The impurity free energy is given by[1]

$$\Omega_I = \frac{\sigma}{4k_BT_c}|\eta_0(\mathbf{R})|^2(1-|\langle\phi\rangle|^2) + \frac{\sigma}{192(k_BT_c)^3}|\eta_0(\mathbf{R})|^4[-3\langle|\phi|^4\rangle + 2\langle\phi\rangle\langle\phi^*|\phi|^2\rangle + 2\langle\phi^*\rangle\langle\phi|\phi|^2\rangle - 1 + 2\sigma(1-|\langle\phi\rangle|^2)^2] - \frac{\sigma\hbar^2}{192(k_BT_c)^3}\langle|\phi|^2|\mathbf{v}_F\cdot\mathbf{D_0}\eta_0(\mathbf{r})|^2\rangle_{\mathbf{r}=\mathbf{R}} + \frac{\sigma\hbar^2}{192(k_BT_c)^3}[\eta_0^*(\mathbf{R})\langle(|\phi|^2-\phi\langle\phi^*\rangle)(\mathbf{v}_F\cdot\mathbf{D_0})^2\eta_0(\mathbf{r})\rangle_{\mathbf{r}=\mathbf{R}} + \text{c.c.}]. \tag{11}$$

Here $\mathbf{D}_0$ is the gauge-invariant derivative operator, with $\mathbf{A}$ replaced by $\mathbf{A}_0$. For simplicity, we have taken the impurity potential to be an s wave, of strength v. For any particular type of defect, v is the effective potential seen by a quasiparticle, and thus is a renormalized quantity which would be difficult to calculate from first principles. However, it is directly related to normal-state transport coefficients, and so may be inferred experimentally. The parameter σ appearing in Eq. (11) is then given by

$$\sigma = \frac{N^2(0)\pi^2v^2}{1+N^2(0)\pi^2v^2}. \tag{12}$$

In this notation, the cross section of the impurity σ_{sc} is proportional to σ/k_F^2.

The theory presented in this paper applies to small defects; our basic assumption is that $\sigma_{\mathrm{sc}}\ll\xi_0^2$, where ξ_0 is the zero-temperature superconducting correlation length. Note, however, that there is no restriction on the size of v. The ratio $\sigma_{\mathrm{sc}}/\xi_0^2$ furnishes the crucial small parameter in the theoretical development. To leading order in the small ratio, then, the impurity free energy (11) is evaluated using $\eta_0(\mathbf{r})$ and $\mathbf{A}_0(\mathbf{r})$, the solutions in the absence of the impurity. Our previous paper discusses Ω_I in greater detail, using it to compute, as an example, vortex pinning energies for an order parameter of arbitrary symmetry. Finally, we note that the $|\eta_0(\mathbf{R})|^4$ term has been included in Eq. (11) for completeness, although it is always small in comparison with the preceding $|\eta_0(\mathbf{R})|^2$ term by a factor of $|\eta_0(\mathbf{R})|^2/(k_BT_c)^2$. In the analyses which follow, terms of order $|\eta_0(\mathbf{R})|^4$ will not be considered.

III. SUPERCURRENT

In the presence of an impurity at $\mathbf{r}=\mathbf{R}$, the expression for the supercurrent becomes[10]

$$\mathbf{J} = \mathbf{J}_B + \mathbf{J}_I, \tag{13}$$

where $\mathbf{J}_B$ is the usual bulk supercurrent,

$$J_{Bi} = -\frac{i7\zeta(3)N(0)e\hbar}{8(\pi k_BT_c)^2}\sum_j \langle v_{Fi}v_{Fj}|\phi|^2\rangle(\eta D_j^*\eta^* - \eta^* D_j\eta) = -e\sum_i \rho_{sij}v_{si}. \tag{14}$$

The right-hand side of Eq. (14) defines the superfluid density tensor $\overleftrightarrow{\rho}_s$ in terms of the superfluid velocity $\mathbf{v}_s$,

$$\frac{2mv_{si}}{\hbar} = \frac{2eA_i}{\hbar c} + \nabla_i\theta, \tag{15}$$

where $\theta(\mathbf{r})$ is the spatially varying phase of the complex order parameter $\eta(\mathbf{r})$. The impurity term is given by

$$J_{Ii}=\frac{\sigma em}{24(k_BT_c)^3}|\eta_0|^2\sum_j v_{s0j}[3\langle v_{Fi}v_{Fj}|\phi|^2\rangle-\langle\phi\rangle \times\langle v_{Fi}v_{Fj}\phi^*\rangle-\langle\phi^*\rangle\langle v_{Fi}v_{Fj}\phi\rangle]\delta^3(\mathbf{r}-\mathbf{R}) -\frac{i\sigma e\hbar}{96(k_BT_c)^3}\sum_j (\nabla_j|\eta_0|^2)[\langle\phi\rangle\langle v_{Fi}v_{Fj}\phi^*\rangle -\langle\phi^*\rangle\langle v_{Fi}v_{Fj}\phi\rangle]\delta^3(\mathbf{r}-\mathbf{R})+\frac{i\sigma e\hbar}{96(k_BT_c)^3}\sum_j |\eta_0|^2 \times[\langle\phi\rangle\langle v_{Fi}v_{Fj}\phi^*\rangle-\langle\phi^*\rangle\langle v_{Fi}v_{Fj}\phi\rangle]\nabla_j\delta^3(\mathbf{r}-\mathbf{R}). \tag{16}$$

Here $\mathbf{v}_{s0}$ refers to the superfluid velocity evaluated using the impurity-free quantities $\mathbf{A}_{0j}$ and θ_0.

Several points are worth stressing:

(1) For consistency, $\mathbf{J}_I$ is evaluated with $\eta_0(\mathbf{r})$ and $\mathbf{A}_0(\mathbf{r})$, while $\mathbf{J}_B$ is evaluated to first order in $\delta\eta(\mathbf{r})$ and $\delta\mathbf{A}(\mathbf{r})$. Thus we see that the impurity affects the supercurrent in two ways—directly, through $\mathbf{J}_I$, and indirectly, through using a modified order parameter and vector potential in $\mathbf{J}_B$.

(2) The first two terms of $\mathbf{J}_I$ are the contributions which do not vanish upon spatial averaging. It is these terms which were considered in Ref. 10. The third term in $\mathbf{J}_I$ is of equivalent order in gradients, but does not contribute to the volume integral. Both kinds of terms must be considered in order for consistency checks, such as the continuity equation, to be satisfied [see point (4), below].

(3) The two final terms of $\mathbf{J}_I$ involve the derivatives $\nabla|\eta_0|^2$ and $\nabla\delta^3(\mathbf{r}-\mathbf{R})$, but *not* the derivative of the phase, which appears in the superfluid velocity, $\mathbf{v}_{s0}$. (Note that gauge invariance is ensured in these terms, without considering the vector potential.) These two terms are nonzero only when $\phi(\hat{\mathbf{k}})$ is a *complex* function of $\hat{\mathbf{k}}$, thus breaking time-reversal symmetry. Additionally, at least for the s-wave impurities treated in this paper, the presence of such terms requires that $\langle\phi\rangle$ must not vanish. One order parameter meeting these requirements is the "$s+id$," which has been considered recently in the context of high-temperature superconductors.[9] For a further discussion of impurity scattering in superconductors which break time-reversal symmetry, see Ref. 11.

(4) $\mathbf{J}$ must satisfy the equilibrium continuity equation $\nabla\cdot\mathbf{J}=0$, for acceptable solutions of its fuctional variables $\eta(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$. This requirement is met naturally for $\delta\eta(\mathbf{r})$ and $\delta\mathbf{A}(\mathbf{r})$, which are determined by the equations presented in Sec. IV. For an explicit example of how all the terms in Eq. (13) conspire to enforce $\nabla\cdot\mathbf{J}=0$, see Ref. 12.

IV. EQUATIONS FOR $\delta\eta$ AND $\delta\mathbf{A}$

The differential equation for $\eta(\mathbf{r})$, in the presence of an impurity, is given by[10]

$$\alpha\eta+2\beta|\eta|^2\eta-\sum_{ij}\frac{\kappa_{ij}}{2}D_iD_j\eta =d_0\delta^3(\mathbf{r}-\mathbf{R})+\sum_i d_{1i}D_{0i}\delta^3(\mathbf{r}-\mathbf{R}) +\sum_{ij} d_{2ij}D_{0i}D_{0j}\delta^3(\mathbf{r}-\mathbf{R}). \tag{17}$$

Here the coefficients α, β, and κ_{ij} are defined as previously, while the coefficients of the impurity-induced driving terms are given by

$$d_0=\frac{\sigma\eta_0(\mathbf{R})}{4k_BT_c}(|\langle\phi\rangle|^2-1) -\sum_{ij}\frac{\sigma\hbar^2(D_{0i}D_{0j}\eta_0(\mathbf{r}))_{\mathbf{r}=\mathbf{R}}}{192(k_BT_c)^3}\langle v_{Fi}v_{Fj}(|\phi|^2-\phi\langle\phi^*\rangle)\rangle, \tag{18}$$

$$d_{1i}=-\sum_j\frac{\sigma\hbar^2(D_{0j}\eta_0(\mathbf{r}))_{\mathbf{r}=\mathbf{R}}}{192(k_BT_c)^3}\langle v_{Fi}v_{Fj}|\phi|^2\rangle, \tag{19}$$

$$d_{2ij}=-\frac{\sigma\hbar^2\eta_0(\mathbf{R})}{192(k_BT_c)^3}\langle v_{Fi}v_{Fj}(|\phi|^2-\phi^*\langle\phi\rangle)\rangle. \tag{20}$$

Equations (17)–(20) are supplemented by Maxwell's equation

$$\nabla\times(\nabla\times\mathbf{A})=\frac{4\pi}{c}(\mathbf{J}_B+\mathbf{J}_I). \tag{21}$$

In Eqs. (17) and (21), the left-hand sides should be expanded to first order in $\delta\eta(\mathbf{r})$ and $\delta\mathbf{A}(\mathbf{r})$, to give coupled equations for $\delta\eta(\mathbf{r})$ and $\delta\mathbf{A}(\mathbf{r})$, in the presence of $\eta_0(\mathbf{r})$, $\mathbf{A}_0(\mathbf{r})$, and the impurity.

Note that for an isotropic s-wave order parameter $[\phi(\hat{\mathbf{k}})=1]$, the right-hand side of Eq. (17) is zero unless $D_{0i}\eta_0$ is nonzero at the impurity site;[2] then the homogeneous superconducting state $[\eta_0=(-\alpha/2\beta)^{1/2}$, $\mathbf{A}_0=0]$ is unperturbed by the presence of the impurity. This result is not in conflict with the early work of Fetter, who did find order-parameter perturbations associated with small impurities.[13] However, these perturbations only occur over very small distances (of order $1/k_F$) from the impurity. The quasiclassical method used here, while capable of handling length scales smaller than ξ_0, coarse grains over the much smaller scale of $1/k_F$. This coarse graining is appropriate and consistent with BCS theories, since these all leave out information on this length scale.

It is instructive to apply the modified GLE, Eq. (17), in a specific example. In particular, consider the case of a homogenous superconductor, which, when unperturbed by the impurity, is described by

$$\eta_0=\sqrt{-\alpha/2\beta},\quad \mathbf{A}_0=0. \tag{22}$$

If $\langle\phi\rangle\neq 1$, then, in general, $\delta\eta(\mathbf{r})$ will be nonzero. For simplicity, we take $\langle\phi\rangle=0$, which corresponds to an unconventional (for example, d-wave) superconductor. Then $\delta\eta(\mathbf{r})$ is given by the solution to the following inhomogeneous equation:

$$\alpha\delta\eta+6\beta\eta_0^2\delta\eta-\frac{1}{2}\sum_{ij}\kappa_{ij}\frac{\partial^2\delta\eta}{\partial x_i\partial x_j}$$
$$=-\frac{\sigma\eta_0(\mathbf{R})}{4k_BT_c}\delta^3(\mathbf{r}-\mathbf{R})-\sum_{ij}\frac{\sigma\hbar^2\eta_0(\mathbf{R})}{192(k_BT_c)^3}$$
$$\times\langle v_{Fi}v_{Fj}|\phi|^2\rangle\frac{\partial^2\delta^3(\mathbf{r}-\mathbf{R})}{\partial x_i\partial x_j}. \quad (23)$$

Note that we have simplified our problem, using $\delta\mathbf{A}=0$, since other broken symmetry solutions are expected to have higher energies. To solve Eq. (23), it is easiest to work in a coordinate system for which κ_{ij} is diagonal. The anisotropic GL coherence lengths are given by

$$\xi_x^2=\frac{\kappa_{xx}}{4|\alpha|},\quad \xi_y^2=\frac{\kappa_{yy}}{4|\alpha|},\quad \xi_z^2=\frac{\kappa_{zz}}{4|\alpha|}, \quad (24)$$

which allows dimensionless coordinates to be defined as

$$x'=\frac{x}{\xi_x},\quad y'=\frac{y}{\xi_y},\quad z'=\frac{z}{\xi_z}. \quad (25)$$

Equation (23) is finally solved by Fourier transform. Making use of Eqs. (4)–(6), the result can be expressed as

$$\frac{\delta\eta(\mathbf{r})}{\eta_0}=-\frac{\sigma}{8|\alpha|\xi_x\xi_y\xi_zk_BT_c}\left(1+\frac{2\pi^2(T_c-T)}{21\zeta(3)T_c}\right)\frac{e^{-|\mathbf{r}'-\mathbf{R}'|}}{4\pi|\mathbf{r}'-\mathbf{R}'|}, \quad (26)$$

where $\mathbf{R}'$ is the location of the impurity in reduced variables. We point out that the divergence of $\delta\eta(\mathbf{r}')$, as $\mathbf{r}'\to\mathbf{R}'$, is an ignorable artifact of our solution, since Eq. (23) is valid only on length scales greater than ξ_0. The divergence will be cut off when $|\mathbf{r}-\mathbf{R}|$ is of order ξ_0.

V. MICROSCOPIC DERIVATION

A. General formalism

We now discuss how to derive our two main results, Eq. (16) for $\mathbf{J}_I$, and the inhomogeneous GLE, Eq. (17). Our previous paper[1] already gave the details of the free-energy calculation, so in this paper we do not review the derivation of Eq. (11).

We use the quasiclassical version of Gor'kov's equations,[14,15] in the presence of a single impurity,[3] to perform our calculations. The key quantity is the propagator $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$, which for spin-singlet pairing can be taken to be a 2×2 matrix in particle-hole space. Here $\hat{\mathbf{k}}$ is a unit vector on the Fermi surface, $\mathbf{r}$ is a position in real space, and ε is a Matsubara frequency. It is convenient to expand $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ in terms of Pauli matrices $\hat{\tau}_i$:

$$\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=\sum_{i=1}^{3}g_i(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\hat{\tau}_i. \quad (27)$$

Note that no unit matrix ($\hat{\tau}_0$) term appears in this sum.

Then the electric current density is given by

$$\mathbf{J}(\mathbf{r})=-\frac{2eN(0)k_BT}{\hbar}\sum_{\varepsilon}\langle\mathbf{v}_F(\hat{\mathbf{k}})g_3(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\rangle. \quad (28)$$

The self-consistency equation for the order parameter also involves $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$. We take the pairing interaction $V(\hat{\mathbf{k}},\hat{\mathbf{k}}')$ to be given by

$$V(\hat{\mathbf{k}},\hat{\mathbf{k}}')=V_p\phi(\hat{\mathbf{k}})\phi^*(\hat{\mathbf{k}}'), \quad (29)$$

where $\phi(\hat{\mathbf{k}})$ is the same function which appears in Eq. (1), and V_p is the attractive BCS pairing energy. Then the self-consistency equation is

$$\Delta(\hat{\mathbf{k}},\mathbf{r})=\frac{N(0)k_BT}{2\hbar}\sum_{\varepsilon}\langle V(\hat{\mathbf{k}},\hat{\mathbf{k}}')\mathrm{Tr}_\tau[\hat{g}(\hat{\mathbf{k}}',\mathbf{r},\varepsilon)(\hat{\tau}_1-i\hat{\tau}_2)]\rangle, \quad (30)$$

where Tr_τ is a trace over the Pauli matrices. Solving for $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ in terms of $\Delta(\hat{\mathbf{k}},\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$, as described below, and substituting this into Eq. (30), leads to the GLE, Eq. (17).

To determine $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ in the presence of an impurity located at $\mathbf{r}=\mathbf{R}$, we must solve the following equation of motion:[3]

$$\left[\left(i\varepsilon-\frac{e}{c}\mathbf{v}_F(\hat{\mathbf{k}})\cdot\mathbf{A}(\mathbf{r})\right)\hat{\tau}_3-\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r}),\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\right]$$
$$+i\hbar\mathbf{v}_F(\hat{\mathbf{k}})\cdot\nabla\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$$
$$=[\hat{t}(\varepsilon),\hat{g}_{\mathrm{int}}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)]\delta^3(\mathbf{r}-\mathbf{R}), \quad (31)$$

along with the normalization condition

$$\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=-\hbar^2\pi^2. \quad (32)$$

The self-energy $\Delta(\hat{\mathbf{k}},\mathbf{r})$ is given by

$$\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r})=i\Delta_1(\hat{\mathbf{k}},\mathbf{r})\hat{\tau}_1+i\Delta_2(\hat{\mathbf{k}},\mathbf{r})\hat{\tau}_2, \quad (33)$$

where $\Delta_1(\hat{\mathbf{k}},\mathbf{r})$ and $\Delta_2(\hat{\mathbf{k}},\mathbf{r})$ are, respectively, the imaginary and real parts of the order parameter $\Delta(\hat{\mathbf{k}},\mathbf{r})$. The impurity $\hat{t}$ matrix is determined from the following equation:

$$\hat{t}(\varepsilon)=v+\frac{N(0)v}{\hbar}\int d^2\hat{k}\; n(\hat{\mathbf{k}})\hat{g}_{\mathrm{int}}(\hat{\mathbf{k}},\mathbf{r}=\mathbf{R},\varepsilon)\hat{t}(\varepsilon). \quad (34)$$

Here v is the impurity potential, as discussed in Sec. II. Since we have taken a purely s-wave impurity potential, $\hat{t}(\varepsilon)$ has no $\hat{\mathbf{k}}$ dependence; it does, however, have a frequency dependence.

Finally, the intermediate propagator $\hat{g}_{\mathrm{int}}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ is determined from the "impurity-free" equations of motion:

$$\left[\left(i\varepsilon-\frac{e}{c}\mathbf{v}_F(\hat{\mathbf{k}})\cdot\mathbf{A}(\mathbf{r})\right)\hat{\tau}_3-\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r}),\hat{g}_{\mathrm{int}}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\right]$$
$$+i\hbar\mathbf{v}_F(\hat{\mathbf{k}})\cdot\nabla\hat{g}_{\mathrm{int}}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=0, \quad (35)$$

$$\hat{g}_{\mathrm{int}}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\hat{g}_{\mathrm{int}}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=-\hbar^2\pi^2. \quad (36)$$

While these equations for $\hat{g}_{\mathrm{int}}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ do not explicitly reflect the impurity's presence, its effects are implicitly contained in the self-energy $\Delta(\hat{\mathbf{k}},\mathbf{r})$. In general, the $\Delta(\hat{\mathbf{k}},\mathbf{r})$ used in this equation should be the fully self-consistent solution to the gap Eq. (30) in the presence of the impurity.

B. Solving the quasiclassical equations

We have presented the quasiclassical framework for our microscopic calculations. In general, however, it is a formidable task to solve self-consistently for $\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$, $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$, $\hat{t}(\varepsilon)$, $\Delta(\hat{\mathbf{k}},\mathbf{r})$, and $\mathbf{A}(\mathbf{r})$. [The latter quantity is obtained self-consistently from Maxwell's Eq. (21), with $\mathbf{J}(\mathbf{r})$ given by Eq. (28).] Our task can be lightened, however, by several appropriate simplifications. First, since we are working in the Ginzburg-Landau limit, close to T_c, we may expand various quantities to leading powers in $\Delta(\hat{\mathbf{k}},\mathbf{r})$. Second, we are interested in situations (again near T_c) for which $\eta_0(\mathbf{r})$, defined in Sec. II, varies slowly on the length scale of ξ_0, the zero-temperature correlation length. This allows us to make gradient expansions at several key points. Finally, we are interested in impurities for which the ratio $\sigma_{\rm sc}/\xi_0^2$ is small. This small ratio plays a key role in allowing analytic progress in the calculation.

We write the order parameter in the following form:

$$\Delta(\hat{\mathbf{k}},\mathbf{r})=\Delta_0(\hat{\mathbf{k}},\mathbf{r})+\delta\Delta(\hat{\mathbf{k}},\mathbf{r}). \tag{37}$$

Here $\Delta_0(\hat{\mathbf{k}},\mathbf{r})$ is the full solution in the absence of the impurity, and $\delta\Delta(\hat{\mathbf{k}},\mathbf{r})$ is the change due to the impurity. [Note that $\Delta_0(\hat{\mathbf{k}},\mathbf{r})=\eta_0(\mathbf{r})\phi(\hat{\mathbf{k}})$, where $\eta_0(\mathbf{r})$ was introduced in Eq. (9).] To leading order in $\sigma_{\rm sc}/\xi_0^2$, we may compute $\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ with $\Delta_0(\hat{\mathbf{k}},\mathbf{r})$. Since we assume that $\Delta_0(\hat{\mathbf{k}},\mathbf{r})$ is a slowly varying function of $\mathbf{r}$ [although in general, $\delta\Delta(\hat{\mathbf{k}},\mathbf{r})$ is not], we may solve for $\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ in terms of a gradient expansion

$$\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=\hat{g}_{\rm int}^{(0)}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)+\hat{g}_{\rm int}^{(1)}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)+\cdots. \tag{38}$$

Here $\hat{g}_{\rm int}^{(n)}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ is nth order in gauge-invariant gradients of $\Delta_0(\hat{\mathbf{k}},\mathbf{r})$.

Next we write the full $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ as

$$\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)+\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon). \tag{39}$$

This defines $\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$. To leading order in $\sigma_{\rm sc}/\xi_0^2$, the equations for $\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ are then given by

$$\begin{aligned}\left[\left(i\varepsilon-\frac{e}{c}\mathbf{v}_F(\hat{\mathbf{k}})\cdot\mathbf{A}_0(\mathbf{r})\right)\hat{\tau}_3-\hat{\Delta}_0(\hat{\mathbf{k}},\mathbf{r}),\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\right]&\\ +i\hbar\mathbf{v}_F(\hat{\mathbf{k}})\cdot\boldsymbol{\nabla}\,\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)&\\ =\left[\frac{e}{c}\mathbf{v}_F(\hat{\mathbf{k}})\cdot\delta\mathbf{A}(\mathbf{r}),\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\right]&\\ +[\,\delta\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r}),\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)]&\\ +[\hat{t}(\varepsilon),\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)]\,\delta^3(\mathbf{r}-\mathbf{R}),&\end{aligned} \tag{40}$$

$$0=\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)+\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\,\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon). \tag{41}$$

To compute the *explicit* impurity terms in both $\mathbf{J}$ and the GLE (i.e., $\mathbf{J}_I$ and the GLE δ-function driving terms) we only need to solve for the piece of $\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ which is due to the $[\hat{t}(\varepsilon),\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)]$ term on the right-hand side of Eq. (40). Equations (40) and (41) then comprise a set of linear equations for $\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$. The solution is a strong function of $\mathbf{r}$ near the impurity location $\mathbf{R}$.

As they stand, these equations are not amenable to solution by Fourier transform, since they contain products of $\mathbf{r}$-dependent functions. To remedy this, we expand near $\mathbf{R}$ as follows:

$$\begin{aligned}\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=\hat{g}_{\rm int}^{(0)}(\hat{\mathbf{k}},\mathbf{R},\varepsilon)+(\mathbf{r}-\mathbf{R})\cdot\boldsymbol{\nabla}_{\mathbf{R}}\hat{g}_{\rm int}^{(0)}(\hat{\mathbf{k}},\mathbf{R},\varepsilon)+\cdots&\\ +\hat{g}_{\rm int}^{(1)}(\hat{\mathbf{k}},\mathbf{R},\varepsilon)+\cdots,&\end{aligned} \tag{42}$$

$$\Delta_0(\hat{\mathbf{k}},\mathbf{r})=\Delta_0(\hat{\mathbf{k}},\mathbf{R})+(\mathbf{r}-\mathbf{R})\cdot\boldsymbol{\nabla}_{\mathbf{R}}\Delta_0(\hat{\mathbf{k}},\mathbf{R})+\cdots, \tag{43}$$

$$\hat{t}(\varepsilon)=\hat{t}^{(0)}(\varepsilon)+\hat{t}^{(1)}(\varepsilon)+\cdots. \tag{44}$$

[In the last equation, we have indicated that we solve for $\hat{t}(\varepsilon)$ in terms of $\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$, using the gradient expansion (38).] After these expansions, it is quite straightforward to solve for $\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$, and then use this solution to compute the impurity terms already presented in Secs. III and IV.

To compute $\mathbf{J}_I$ of Eq. (16), for example, we need to determine $\delta g_3(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ to second order in $\Delta_0(\mathbf{r},\hat{\mathbf{k}})$, and to first order in gradients. To compute the GLE impurity driving terms (18)–(20), we need $\delta g_1(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ and $\delta g_2(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ to first order in $\Delta_0(\mathbf{r},\hat{\mathbf{k}})$, and to second order in gradients.

VI. ALTERNATIVE DERIVATION

In Sec. V, we explained how to derive the basic equations (16) and (17) by starting with microscopic theory. One may ask, however, if it is possible to obtain these results directly, starting with Eq. (11). The answer to this question is ''yes;'' it is possible, if Ω_I is properly interpreted. Recall that, to evaluate the change in the free energy to leading order in $\sigma_{\rm sc}/\xi_0^2$, we use the impurity-free order parameter $\eta_0(\mathbf{r})$ in Ω_I. One can show, by using microscopic theory, that if $\eta_0(\mathbf{r})$ is replaced by $\eta_0(\mathbf{r})+\delta\eta(\mathbf{r})$ in Ω_I, then the terms which are first order in $\delta\eta(\mathbf{r})$ are correctly reproduced. These additional terms are second-order in $\sigma_{\rm sc}/\xi_0^2$. This procedure leaves out other second order terms which do not involve $\delta\eta(\mathbf{r})$; these omitted terms play no role in generating the GLE or the supercurrent.

To derive the GLE, Eq. (17), we proceed as anticipated above. In Ω_B, replace $\eta(\mathbf{r})$ by $\eta_0(\mathbf{r})+\delta\eta(\mathbf{r})$, expanding to second order in $\delta\eta(\mathbf{r})$. [The first order terms in $\delta\eta(\mathbf{r})$ vanish, since Ω_B is stationary at $\eta_0(\mathbf{r})$.] In Ω_I, replace $\eta_0(\mathbf{r})$ by $\eta_0(\mathbf{r})+\delta\eta(\mathbf{r})$, keeping first order terms in $\delta\eta(\mathbf{r})$. Then Eq. (17) is the consequence of the following variational procedure:

$$\frac{\delta(\Omega_B+\Omega_I)}{\delta\,\delta\eta^*(\mathbf{r})}=0. \tag{45}$$

To perform the differentiation, it is best to rewrite Ω_I in the following form:

$$\Omega_I = \int d^3 r f_I[\eta(\mathbf{r}), \eta^*(\mathbf{r}), \mathbf{A}(\mathbf{r})], \tag{46}$$

where f_I explicitly contains a factor of $\delta^3(\mathbf{r}-\mathbf{R})$, to reproduce Eq. (11).

To obtain Maxwell's equation (21), we now replace $\mathbf{A}(\mathbf{r})$ in Ω_B, by $\mathbf{A}_0(\mathbf{r})+\delta\mathbf{A}(\mathbf{r})$, working to second order in $\delta\mathbf{A}(\mathbf{r})$. Likewise, we replace $\mathbf{A}_0(\mathbf{r})$ in Ω_I, by $\mathbf{A}_0(\mathbf{r})+\delta\mathbf{A}(\mathbf{r})$, linearizing to first order in $\delta\mathbf{A}(\mathbf{r})$. Maxwell's equation is the result of the variation

$$\frac{\delta(\Omega_B+\Omega_I)}{\delta\delta A_i(\mathbf{r})}=0. \tag{47}$$

This leads to the following identification:

$$J_{Ii} = -c\frac{\partial f_I}{\partial A_{0i}} + c\sum_j \nabla_j \frac{\partial f_I}{\partial(\nabla_j A_{0i})}. \tag{48}$$

We conclude this section by discussing an additional point of interest. In a previous paper, we pointed out that one could derive Ω_I by starting with the impurity-averaged free energy, and then taking the one-impurity limit. We showed, however, that there is not a unique way of taking this limit, due to ambiguities introduced by possible partial integrations. Only a single-impurity, microscopic calculation, such as the one performed here, can resolve this ambiguity. Ambiguities of this type also affect attempts to derive $\mathbf{J}(\mathbf{r})$ and the GLE from impurity-averaged results.

VII. DISCUSSION

Our goal in this paper has been to discuss all aspects of how a single, localized defect can be correctly treated in a Ginzburg-Landau theory for an order parameter of the form (1). After reviewing our previously derived expression for the free energy, Eq. (11), we presented and derived the main results of this paper; the GLE, Eq. (17), and the supercurrent, Eq. (16). On length scales greater than ξ_0, these formulas represent a complete theory which involves only a spatially varying complex order parameter $\eta(\mathbf{r})$ and vector potential $\mathbf{A}(\mathbf{r})$. The complicated details concerning quasiparticle scattering from the impurity have been incorporated into the various impurity terms. The coarse graining over length scales shorter than ξ_0 causes the impurity terms to show up as δ functions or derivatives of δ functions.

In our previous paper, we showed how Ω_I, Eq. (11), could be used to compute vortex pinning energies. In the present paper, we used the GLE, Eq. (17), to compute $\delta\eta(\mathbf{r})$ near an impurity, for the class of order parameters satisfying $\langle\phi\rangle=0$. Many other applications of these equations can be envisioned. For example, one could take $\eta_0(\mathbf{r})$ and $\mathbf{A}_0(\mathbf{r})$ to be either a single vortex solution, or the Abrikosov vortex lattice; in either case, the changes $\delta\eta(\mathbf{r})$, $\delta\mathbf{A}(\mathbf{r})$, and $\delta\mathbf{J}(\mathbf{r})$, caused by an impurity, could be computed. We hope to address such problems in the future.

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