Microscopic theory of vortex pinning: Impurity terms in the Ginzburg-Landau free energy

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In the presence of a single impurity, the Ginzburg-Landau free-energy functional for a superconductor acquires extra terms. Using microscopic theory, we determine the structure of these terms and their coefficients. Our calculation is very general: we assume a $\hat{\mathbf{k}}$-dependent order parameter $\Delta(\hat{\mathbf{k}})$, which transforms according to any one-dimensional irreducible representation of the crystalline point group. This representation may be conventional or unconventional, as appropriate to the current models of high-T_c superconductors. We treat an arbitrary Fermi surface. The physical significance of the theory is discussed, with emphasis on vortex pinning. We estimate the pinning energy of a single vortex. [S0163-1829(96)50418-2]

I. INTRODUCTION

The Ginzburg-Landau (GL) free-energy functional, Ω_{GL}, is widely used to analyze problems in superconductivity, particularly situations in which the order parameter is spatially varying. Microscopic theory shows that certain types of disorder, such as small pinning centers, can be taken into account by adding extra terms to Ω_{GL}. These terms can then be given a physical interpretation. For example, an extra term proportional to $|\Delta|^2$, where Δ is the order parameter, is referred to as T_c disorder. An extra term involving $|\boldsymbol{\nabla}\Delta|^2$ is referred to as mean free path ($=\ell$) disorder.

Some years ago, Thuneberg presented a microscopic theory which showed how small scattering centers were reflected in Ω_{GL}.[1,2] For the case of a $\mathbf{k}$-independent, s-wave order parameter, he found that a single impurity induced an extra term in Ω_{GL} of the $|\boldsymbol{\nabla}\Delta|^2$ form. A further calculation, involving a particular type of d-wave order parameter, found that in this more complex situation, Ω_{GL} acquired both $|\Delta|^2$ and $|\boldsymbol{\nabla}\Delta|^2$ terms, revealing both T_c disorder and mean free path disorder.

From this theory it is possible to estimate pinning energies of single vortices. In a conventional pinning theory, small defects of size $d \ll \xi_0$, with ξ_0 the zero-temperature coherence length, cause pinning energies proportional to d^3. However, the Thuneberg theory suggests much stronger pinning,[3] proportional to $d^2\xi_0$. Here, d^2 is proportional to the quantum mechanical scattering cross section σ_{sc} discussed below. The theory also predicts the temperature dependencies of the pinning energy, with distinct estimates for $\delta\ell$ and δT_c pinning.

These results have been applied in several laboratory systems. In the high-T_c superconductors, oxygen vacancies play an important role as point defects.[4] The temperature dependencies given by Thuneberg appear to be well borne out for this type of disorder.[5,6] Line defects, such as screw dislocations, have also been investigated in the high-T_c's.[7] The dependence of the pinning energy on the defect length scale d has also been confirmed.[8] In all of these experiments conclusions may only be inferred by means of collective pinning theory,[9] leaving some flexibility for their interpretation. The investigation of the pinning of single vortices has proven difficult.[10] However, the advent of tunneling and force microscopies should open new doors in this field in the near future.

The distinct temperature dependencies of vortex pinning in the presence of isotropic or anisotropic order parameters makes this issue timely due to the current debate over the symmetry of the high-T_c pairing state. It is interesting to note that the most concentrated study of the temperature dependence of collective pinning in the yttrium based compounds is consistent with exclusively isotropic symmetry.[6] Further investigation of single-vortex pinning, coupled with the results derived below, could clarify this important point.

In this paper, we extend Thuneberg's results to a more general $\hat{\mathbf{k}}$-dependent order parameter. We consider a singlet order parameter of the 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. We perform our calculation for an arbitrary function $\phi(\hat{\mathbf{k}})$, and an arbitrary Fermi surface; Eq. (11) is our main result.

In Sec. III we use our result, Eq. (11), to estimate the pinning energy of a vortex core to an impurity. This important application is given by Eq. (15). An interesting conceptual point which emerges from our work is the following. There is an intuitive method of deriving the single-impurity contribution to Ω_{GL}. In this approach, one starts with the impurity-averaged formula for Ω_{GL}, and isolates the one-impurity limit. In the cases previously considered, this approach led to the same answer as that generated by the microscopic theory. However, we find that for the more general case considered in this paper, there is an ambiguity associated with the intuitive approach, which can only be resolved via the complete single-impurity theory. This point is discussed in Sec. V.

In the context of the high-T_c superconductors, various forms for $\phi(\hat{\mathbf{k}})$ are currently of great interest. One focus is a broken symmetry state $\phi(\hat{\mathbf{k}})$ whose Fermi surface average vanishes.[11] A simple example of a function displaying this symmetry is

$$\phi_d(\hat{\mathbf{k}}) \sim (k_x^2 - k_y^2). \tag{2}$$

There is also great interest in $\phi(\hat{\mathbf{k}})$'s which have the full crystal symmetry, but change sign as a function of $\hat{\mathbf{k}}$.[12] Both symmetry types are encompassed in the following analysis.

II. RESULTS

In this section we present our results. The derivation is provided in Sec. IV. We write the GL free energy in the following form:

$$\Omega_{\mathrm{GL}}=\Omega_b+\Omega_i. \tag{3}$$

The first term, Ω_b, is the usual bulk GL free energy

$$\Omega_b=\int d^3r\{\alpha|\eta|^2+\beta|\eta|^4+\tfrac{1}{2}K_{ij}(D_i\eta)(D_j^*\eta^*)\}. \tag{4}$$

Here, the gauge-invariant derivative is defined by $\mathbf{D}\equiv\boldsymbol{\nabla}+2ie\mathbf{A}/\hbar c$.

Within the usual Fermi-liquid theory of superconductivity, we can derive the following values for the coefficients in Ω_b:

$$K_{ij}=\frac{7\hbar^2N(0)\zeta(3)}{8\pi^2k_B^2T_c^2}\langle v_{Fi}v_{Fj}|\phi|^2\rangle, \tag{5}$$

$$\alpha=N(0)\frac{T-T_c}{T_c}, \tag{6}$$

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

Here, $N(0)$ is the total 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 of a quantity $F(\hat{\mathbf{k}})$ is given by

$$\langle F\rangle\equiv\int_{\mathrm{FS}}d^2\hat{k}n(\hat{\mathbf{k}})F(\hat{\mathbf{k}}), \tag{8}$$

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

$$\int_{\mathrm{FS}}d^2\hat{k}n(\hat{\mathbf{k}})=1. \tag{9}$$

We now introduce an impurity at position $\mathbf{R}$. For simplicity, we take the impurity potential to be s wave with strength v. We define a dimensionless parameter σ as

$$\sigma=\frac{N^2(0)\pi^2v^2}{1+N^2(0)\pi^2v^2}. \tag{10}$$

In this notation the cross section of the impurity σ_{sc} is proportional to σ/k_F^2. We assume that $\sigma_{\mathrm{sc}}\ll\xi_0^2$, where ξ_0 is the zero-temperature correlation length; this furnishes the key small parameter beyond the usual assumptions of quasiclassical theory.[13]

To leading order in $\sigma_{\mathrm{sc}}/\xi_0^2$, the term Ω_i is evaluated according to the following recipe. We first obtain the solution $\eta(\mathbf{r})$ which minimizes Ω_b. This is then inserted into the following expression which is evaluated at $\mathbf{r}=\mathbf{R}$:

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

Ω_i represents the change in free energy due to the presence of the impurity located at position $\mathbf{R}$. Note that $\langle|\phi|^2\rangle=1$ by normalization, so that $|\langle\phi\rangle|\leqslant1$, and $\langle|\phi|^4\rangle\geqslant1$.

Several points are worth stressing.

(1) In general, Ω_i contains gradient terms, and terms proportional to $|\eta|^2$ and $|\eta|^4$. Close to T_c, when the GL expansion of the free energy is valid, the $|\eta|^2$ term is always larger than the $|\eta|^4$ term, since the latter carries an additional factor of $|\eta|^2/(k_BT_c)^2$. This differs from the situation for the bulk free energy Ω_b, in which the $|\eta|^2$ and the $|\eta|^4$ terms are of comparable size.[14]

(2) When $\phi(\hat{\mathbf{k}})$ is constant and equal to 1 for all $\hat{\mathbf{k}}$, the $|\eta|^2$ and $|\eta|^4$ terms both vanish, leaving only a single gradient term. If we also consider a spherical Fermi surface we obtain in this limit

$$\Omega_i(\text{isotropic } s \text{ wave})=-\frac{\sigma\hbar^2v_F^2}{576(k_BT_c)^3}|\mathbf{D}\eta(\mathbf{r})|^2_{\mathbf{r}=\mathbf{R}}. \tag{12}$$

This is Thuneberg's original result, and reflects Anderson's theorem:[15] the thermodynamics of an isotropic s-wave superconductor is unaffected by s-wave impurity scattering.

(3) For an arbitrary $\phi(\hat{\mathbf{k}})$, one may ask which terms dominate in Ω_i, the gradient terms, or the term proportional to $|\eta|^2$? The answer is that the $|\eta|^2$ term is always more important unless $|\langle\phi\rangle|$ is close to 1 (see previous point). In that case, it is possible for the gradient term to dominate. However, the largest value $|\mathbf{D}\eta|$ can assume is typically of order $|\eta_{\mathrm{bulk}}|/\xi(T)$, where $|\eta_{\mathrm{bulk}}|=\sqrt{\alpha/2\beta}$ and $\xi(T)$ is the temperature-dependent coherence length.

(4) For an unconventional order parameter, we have $\langle\phi\rangle=0$. In this case the $|\eta|^2$ term is always the largest since $\eta(\mathbf{r})$ never varies with a characteristic length smaller than $\xi(T)$. Note that $\xi(T)$ may be anisotropic.

(5) We emphasize that the form of Ω_i in Eq. (11) should not be used to obtain GL differential equations in the usual

way, unless further justification is provided. We plan to address this point in a future publication.

III. VORTEX PINNING

We now use the result (11) to discuss the pinning energy of a vortex line. This is the energy which makes it favorable for a vortex core to be located at the impurity site **R**. The pinning energy $E_{\rm pinning}$ is defined as

$$E_{\rm pinning}=\Omega_i(\text{ vortex at }\mathbf{R})-\Omega_i(\text{ vortex at }\infty). \tag{13}$$

To estimate this, we note that near the vortex core, $|\mathbf{D}\eta|_{\mathbf{r}=\mathbf{R}}$ approximately takes on its maximum value $|\eta_{\rm bulk}|/\xi(T)$. We emphasize again that the $\eta(\mathbf{r})$ used to evaluate Ω_i is determined, to this level of approximation, in the *absence* of any pinning center at **R**. In terms of the coefficients (5)–(7), the temperature-dependent coherence length $\xi(T)$ is given by

$$\xi^2(T)\sim\frac{K_{ij}}{|\alpha|}\sim\frac{\hbar^2v_F^2}{k_B^2T_c^2(1-T/T_c)}. \tag{14}$$

We use this gradient to estimate Ω_i(vortex at **R**). However, Ω_i(vortex at $\mathbf{r}=\infty$) must be dominated by the $|\eta|^2$ term in (11) since in this case there are no local gradients near the pinning center.

Our estimate for $E_{\rm pinning}$ is finally

$$E_{\rm pinning}=-\frac{\sigma|\eta_{\rm bulk}|^2}{k_BT_c}\left[\gamma_1(1-|\langle\phi\rangle|^2)+\gamma_2\left(1-\frac{T}{T_c}\right)\right], \tag{15}$$

where γ_1 and γ_2 are dimensionless constants of order 1. γ_1 originates from the $|\eta|^2$ term in Eq. (11), and represents δT_c fluctuations. This term clearly vanishes for an isotropic (s-wave) pairing state. Its temperature dependence is due to $|\eta_{\rm bulk}|^2\sim(T_c-T)$. γ_2 originates from the gradient terms in Eq. (11), and represents $\delta\ell$ fluctuations. The temperature dependence of this term is proportional to $(T_c-T)^2$. Near T_c it is clearly weaker than the preceding term, except in the case of a (mostly) isotropic order parameter.

IV. DERIVATION

In this section we sketch the microscopic derivation of the main result, Eq. (11). Thuneberg, Kurkijärvi, and Rainer (TKR) have explained the basic method for computing the free energy of a superconductor in the presence of an impurity.[3] For our purposes, we generalize their formulation to the case of a $\hat{\mathbf{k}}$-dependent order parameter and a general Fermi surface.

In the quasiclassical approach of TKR, the single-particle propagator $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ is the key quantity. $\mathbf{r}$ represents the mean coordinate $(\mathbf{r}_1+\mathbf{r}_2)/2$ as the particle propagates from $\mathbf{r}_1$ to $\mathbf{r}_2$, while $\mathbf{k}$ is the Fourier transform of the relative coordinate $\mathbf{r}_1-\mathbf{r}_2$. The primary achievement of the quasiclassical formulation is the coarse graining of irrelevant information, which leads to $\mathbf{k}$ being evaluated only at the Fermi surface.[16] We denote this as $\hat{\mathbf{k}}$. The ε are Matsubara energies. For singlet pairing, the spin indices become redundant, and we may take $\hat{g}$ to be a 2×2 matrix in particle-hole space.

To determine $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ with an impurity at $\mathbf{r}=\mathbf{R}$, we solve the following equation of motion:

$$\left[\left(i\varepsilon-\frac{e}{c}\mathbf{v}_F(\hat{\mathbf{k}})\cdot\mathbf{A}(\mathbf{r})\right)\hat{\tau}_3-\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r}),\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\right] + i\hbar\mathbf{v}_F(\hat{\mathbf{k}})\cdot\nabla\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=[\hat{t}(\varepsilon),\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)]\delta^3(\mathbf{r}-\mathbf{R}), \tag{16}$$

along with the normalization condition

$$\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=-\hbar^2\pi^2. \tag{17}$$

We now explain the ingredients of Eq. (16). The $\hat{\tau}_i$ are Pauli matrices in particle-hole space. The self-energy $\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r})$ is given by

$$\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r})=i\Delta_1(\hat{\mathbf{k}},\mathbf{r})\hat{\tau}_1+i\Delta_2(\hat{\mathbf{k}},\mathbf{r})\hat{\tau}_2, \tag{18}$$

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

$$\hat{t}(\varepsilon)=v+\frac{N(0)v}{\hbar}\int d^2\hat{k}n(\hat{\mathbf{k}})\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r}=\mathbf{R},\varepsilon)\hat{t}(\varepsilon). \tag{19}$$

The impurity potential v is taken to be purely s wave. Finally, the "intermediate" progagator $\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ is determined from the impurity-free equations of motion

$$\left[\left(i\varepsilon-\frac{e}{c}\mathbf{v}_F(\hat{\mathbf{k}})\cdot\mathbf{A}(\mathbf{r})\right)\hat{\tau}_3-\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r}),\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\right] + i\mathbf{v}_F(\hat{\mathbf{k}})\cdot\nabla\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=0, \tag{20}$$

$$\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)=-\hbar^2\pi^2. \tag{21}$$

The change in the free energy due to the impurity is determined from the following expression:

$$\Omega_i=\frac{N(0)k_BT}{\hbar}\int_0^1d\lambda\sum_\varepsilon\int_{\rm FS}d^2\hat{k}n(\hat{\mathbf{k}}) \times\int d^3r\ {\rm Tr}_\tau[\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon,\lambda)\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r})], \tag{22}$$

where ${\rm Tr}_\tau$ is a trace in particle-hole space, and $\delta\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon,\lambda)\equiv\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon,\lambda)-\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon,\lambda)$.

Note the following points.

(1) In evaluating both $\hat{g}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ and $\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ via Eqs. (16)–(17) and (20)–(21), and in evaluating Ω_i with Eq. (22), we use the order parameter $\Delta(\hat{\mathbf{k}},\mathbf{r})$ which minimizes the free energy in the *absence* of the impurity. That is, the $\Delta(\hat{\mathbf{k}},\mathbf{r})$ which we require is obtained by minimizing Ω_b from Eq. (4). This provides the leading contribution to Ω_i in terms of the small parameter $\sigma_{\rm sc}/\xi_0^2$.

(2) Equation (22) employs a dimensionless coupling-constant integration over λ. $\hat{g}(\lambda)$ and $\hat{g}_{\rm int}(\lambda)$ here denote propagators which are determined using the rescaled order parameter $\Delta(\hat{\mathbf{k}},\mathbf{r})\to\lambda\Delta(\hat{\mathbf{k}},\mathbf{r})$.

To evaluate (22), we adopt the GL assumption that $\Delta(\hat{\mathbf{k}},\mathbf{r})$ is a slowly varying function of $\mathbf{r}$. This allows us to solve for $\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ in terms of a gradient expansion of $\Delta(\hat{\mathbf{k}},\mathbf{r})$. The expression for $\hat{g}_{\rm int}(\hat{\mathbf{k}},\mathbf{r},\varepsilon)$ is then used to compute the $\hat{t}$ matrix. We also employ a gradient expansion of $\hat{\Delta}(\hat{\mathbf{k}},\mathbf{r})$ in Eq. (22). In these expansions short distance details are lost, but information is retained on length scales suitable to the GL theory. The algebra in all of these steps is considerably simplified by keeping only terms of lowest order.

V. DISCUSSION

The main result of this paper is Eq. (11), which expresses the correction to the free energy due to an isolated impurity. This formula is valid for a small impurity, whose cross section $\sigma_{\rm sc}$ satisfies $\sigma_{\rm sc}\ll\xi_0^2$. However, there is no requirement that the impurity potential v be small. Equation (11) allows us to estimate the pinning energy of a vortex line, as given by Eq. (15).

As a final point, we note that there is a second way to derive Eq. (11), as discussed by Thuneberg.[1,9] In this intuitive method, we start with the formula for the impurity-averaged GL free energy, and take its low concentration limit. We then replace the impurity concentration c by the single-impurity form: $c\to\delta^3(\mathbf{r}-\mathbf{R})$. We illustrate this method for one of the terms in Eq. (11), namely the gradient term.

In the presence of a density c of impurities, and for a singlet order parameter, the coefficient K_{ij} in Eq. (4) is replaced by[17]

$$K_{ij}=N(0)\pi k_B T_c\hbar^2\sum_{\varepsilon>0}\frac{\langle v_{Fi}v_{Fj}|\phi+\hbar\langle\phi\rangle/2\tau\varepsilon|^2\rangle}{(\varepsilon+\hbar/2\tau)^3}, \tag{23}$$

where

$$\frac{\hbar}{2\tau}=\frac{N(0)\pi v^2}{1+N^2(0)\pi^2v^2}c=\frac{\sigma}{N(0)\pi}c. \tag{24}$$

To obtain the single impurity limit of (23), we expand to first order in $\hbar/2\tau$. This gives our previous "bulk" result of Eq. (5) plus an additional impurity correction δK_{ij}. Making the single-impurity substitution for c, δK_{ij} becomes

$$\delta K_{ij}\to\frac{\sigma\hbar^2\delta^3(\mathbf{r}-\mathbf{R})}{96(k_BT_c)^3}\langle v_{Fi}v_{Fj}(\phi\langle\phi^*\rangle+\phi^*\langle\phi\rangle-3|\phi|^2)\rangle. \tag{25}$$

This correction term, inserted into (4), becomes the gradient contribution to Ω_i.

Note however that a further "integration by parts" is required to convert this "intuitive" correction into the combination of gradient terms of Eq. (11). A weakness of the intuitive approach is that this decomposition is not unique; the fraction of $(D_i\eta)(D_j^*\eta^*)$ which should be transformed into $\eta^*(D_jD_i\eta)$, via the integration by parts, can only be specified by microscopic theory. However, in spite of these limitations, the intuitive derivation of Ω_i remains instructive, and even provides the correct result in the limit considered by Thuneberg.

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