Spatial variations of the order parameter in superconductors containing a magnetic impurity

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The spatial variation of the superconductor order parameter in the presence of a classical spin has been analyzed by solving self-consistently the Gorkov equation for the one-particle Green's function. In the vicinity of the impurity the deviations from the bulk pair potential Δ is of the form $\Delta A(T)\sin^2 k_F r/(k_F r)^2$, where $A(T)$ is a temperature-dependent factor. At large distances from the impurity, $r \gg \xi_0$ (ξ_0 is the superconductor coherence length at zero temperature), $\Delta(r)$ varies like $1/r$ near the transition temperature, as is expected from the Ginzburg-Landau theory. At low temperatures the spatial dependence is oscillatory and decreases as $1/r^3$.

I. INTRODUCTION

The problem of magnetic impurities in superconductors has been of interest for a long time. The presence of magnetic impurities in a superconductor breaks the time-reversal symmetry of the electron system and prevents the formation of Cooper pairs. As a consequence the phase-transition temperature and the discontinuity of the specific heat are reduced, and gapless superconductivity, critical concentrations, and reentrant phase boundaries at larger impurity concentrations have been found. In 1960 Abrikosov and Gorkov[1] developed a theory, in which the basic features are correctly described. Their treatment does not consider the Kondo effect, and several authors extended their calculation to include Kondo properties of the system within all known approximation schemes. Only a few of the papers are relevant and are able to explain a reentrant phase boundary as well as the spin-fluctuation limit.[2-4]

The presence of a magnetic impurity in a superconductor breaks the translational invariance of the system and causes a change in the order parameter Δ. There is a homogeneous change in Δ, which can be neglected if we are dealing with very small impurity concentrations, and also a spatial variation of the pair potential Δ is induced. It is originated since the pair breaking, caused by the electron-impurity interaction, is a function of position; it is large in the vicinity of the impurity and it vanishes far away from the scattering center.

Three characteristic distance scales play a role in the problem. The smallest one is $1/k_F$, k_F being the Fermi momentum, which arises from breaking the translational invariance of the Fermi gas. The largest one is the superconductor coherence length at 0 °K, $\xi_0 = \epsilon_F/\Delta_0 k_F$, where ϵ_F is the Fermi energy and Δ_0 is the bulk order parameter at zero temperature. The third one is $\eta = \epsilon_F/\omega_D k_F$, ω_D being the Debye energy, which is originated from the cutoff of the electron-phonon interaction.

There exist several calculations of the spatial dependence of the order parameter due to a magnetic impurity. The first attempt is due to Tsuzuki and Tsuneto,[5] who calculated $\Delta(r)$ near the transition temperature for distances from the impurity much larger than ξ_0, the superconductor coherence length at 0 °K. With some approximations they obtain a spatial variation, which decreases like $(1/r^2)\exp(-r/\xi_0)$ and is in contradiction to the $1/r$ dependence expected from a Ginzburg-Landau theory.[6] A more careful treatment of the dependence of Δ on r is due to Heinrichs.[7] His calculation is restricted to the first Born approximation in the electron-impurity spin coupling and to temperatures near the transition temperature. He obtains the correct $1/r$ dependence for large distances and numerically a useful result for intermediate distances. The work of Heinrichs was then extended by Kitamura[8] to include some Kondo divergencies. Kuroda[9] discussed the variation of the order parameter for a classical spin in connection with an isolated bound state inside the energy gap of the superconductor. A more detailed calculation of $\Delta(r)$ for a classical spin in a superconductor has been presented by Kümmel.[10] His analysis is valid for the whole temperature regime. Kümmel applied to the problem the method of Bardeen, Kümmel, Jacobs, and Tewordt[11] for spatially varying superconductivity. The Bogoliubov equations are transformed into spin-decoupled equations and these are formally solved using a WKBJ approximation. It seems to be a hard task to calculate $\Delta(r)$ self-consistently within this scheme. His results are valid for $r \ll \xi_0$, since for $r \gg \xi_0$ the spatial dependence has to be obtained self-consistently. For small r the main contribution to $\Delta(r)$ comes from the s-wave pair breaking; for larger distances, however, all partial waves play an important role. His result is not analytic in the electron-impurity coupling; this can be seen to be a consequence of approximations made in his calculation.

The motivation for the analysis of $\Delta(r)$ in the earlier works was to estimate the corrections to the decrease of the transition temperature due to spatial inhomogeneities. These corrections have been found to be small and can be neglected. For the calculation of the spin relaxation of a Kondo impurity in a superconductor[12] it was thought that the spatial variation of Δ near the impurity plays a significant role. A satisfactory result for $\Delta(r)$ for all temperatures with the correct coupling parameter dependence was desirable. It turned out, however, that the spatial variation of Δ contributes to the spin relaxation only in higher orders of the coupling parameter than the usual direct relaxation process, and may be neglected.

In Sec. II the basic equations are formulated. The Gorkov equation[1,13] with electron-impurity scattering should be solved self-consistently with the gap equation. Introducing a t matrix for the impurity scattering, the problem is reduced to the solution of Gorkov's equation for the "free" one-particle Green's function solved self-consistently for the pair potential $\Delta(r)$. For the sake of simplicity the present calculation is restricted to the case of a classical spin. The treatment can be easily extended to a Kondo impurity by using the approximate t matrix derived in Ref. 4. In Sec. III the solution of Gorkov's equation for a translational-invariant pair potential is used to give a first estimation for the spatial dependence of Δ. The self-consistent solution is presented in Sec. IV for distances of the order of $1/k_F$ and larger than ξ_0.

II. FORMULATION OF THE PROBLEM

The spatial dependence of the order parameter of a superconducting metal containing a magnetic impurity at the origin can be expressed by the anomalous thermodynamical one-particle Green's function $G_{12}(\vec{r}, \vec{r}\,'; z)$:

$$\Delta(\vec{r}) = \lambda \int_{-\omega_D}^{\omega_D} \frac{d\omega}{2\pi} \tanh\left(\frac{\omega}{2T}\right) G''_{12}(\vec{r}, \vec{r}; \omega) \tag{2.1a}$$

$$= 2\lambda T \sum_{n=0}^{\infty} G_{12}(\vec{r}, \vec{r}; z_n) - \lambda \int_{\omega_D}^{\infty} \frac{d\omega}{\pi} G''_{12}(\vec{r}, \vec{r}; \omega)$$

$$\simeq 2\lambda T \sum_{n=0}^{N} G_{12}(\vec{r}, \vec{r}; z_n) , \tag{2.1b}$$

where $G''(\omega)$ denotes the discontinuity of $G(z)$ on the real axis, λ is the coupling parameter of the BCS interaction, ω_D is the Debye cutoff and $z_n = i\omega_n = i\pi T(2n+1)$ are the thermodynamical fermion poles. The last equality in (2.1b) is only approximate and N is determined from the condition $\omega_N = \pi T(2N+1) \simeq \omega_D$.

We will assume that the interaction between the magnetic impurity and the conduction electrons is given by the contact exchange Hamiltonian

$$H_{sd} = J\delta(\vec{r})\vec{S}\cdot\vec{\sigma} , \tag{2.2}$$

where J is the s-d exchange coupling parameter, $\vec{S}$ is the impurity spin, and $\vec{\sigma}$ is the spin density of the conduction electrons. Only s waves with respect to the impurity site can be scattered by a contact potential, and hence $\Delta(r)$ will have spherical symmetry. The one-particle Green's function, in a 2×2 Nambu-matrix notation, expressed in terms of the t matrix for the electron scattering off a contact potential, yields

$$\hat{G}(\vec{r}, \vec{r}\,'; z) = \hat{G}^0(\vec{r}, \vec{r}\,'; z) + \hat{G}^0(\vec{r}, 0; z)\hat{t}(0, 0; z)\hat{G}^0(0, \vec{r}\,'; z), \tag{2.3}$$

where $\hat{G}^0$ is the Green's function of the superconductor calculated self-consistently with the spatially dependent pair potential $\Delta(r)$. $\hat{G}^0$ is the solution of the Gorkov equation[13]

$$[z\hat{I} - (\nabla^2/2m + \epsilon_F)\hat{\tau}_3 + \Delta(r)\hat{\tau}_1]\hat{G}^0(\vec{r}, \vec{r}\,'; z) = \delta(\vec{r} - \vec{r}\,')\hat{I} , \tag{2.4}$$

where $\hat{\tau}_1$ and $\hat{\tau}_3$ are Pauli matrices, $\hat{I}$ is the identity and ϵ_F is the Fermi energy. It is convenient to rewrite this equation by extracting from the left-hand side (lhs) the perturbation due to the impurity

$$[z\hat{I} - (\nabla^2/2m + \epsilon_F)\hat{\tau}_3 + \Delta\hat{\tau}_1]\hat{G}^0(\vec{r}, \vec{r}\,'; z) = \delta(\vec{r} - \vec{r}\,')\hat{I} + \Delta F(r)\hat{\tau}_1\hat{G}^0(\vec{r}, \vec{r}\,'; z) . \tag{2.5}$$

Here, $F(r) = 1 - \Delta(r)/\Delta$ and Δ is the pair potential of the pure superconductor, which is reached at very large distances from the impurity. It is assumed here that the change of the bulk order parameter due to one impurity is negligible. The lhs of Eq. (2.5) is obeyed by the Green's function for the translational invariant system, i.e., the pure superconductor without impurity.

It is a very hard task to calculate the t matrix for the Kondo scattering,[4,14] and in fact to the present no satisfactory result is available. Therefore, the present discussion is confined to the case of a classical spin. The t matrix for a classical spin has been exactly calculated by Shiba[15]:

$$\hat{t}(z) = \frac{(JS/2)^2\hat{G}^0(0, 0; z)}{\hat{I} - (JS/2)^2\hat{G}^0(0, 0; z)^2} . \tag{2.6}$$

The problem then consists in solving self-consistently the coupled system of equations given by (2.1), (2.3), (2.5), and (2.6).

III. FIRST APPROXIMATION

As a first approximation we will evaluate $\Delta(r)$ neglecting the impurity perturbation $F(r)$ in Eq. (2.5), i.e., without taking care of the self-consistency condition. This is equivalent to consider the excitation spectrum of the superconductor (given by $\hat{G}^0$) as not affected by the impurity. Here, only s electrons are scattered by the impurity and contribute to the spatial dependence of Δ. By calculating $\hat{G}^0$ self-consistently with $\Delta(r)$ also other partial waves are scattered and give rise to spatial variations of Δ. Since the probability of finding non-s-electrons near the impurity is very small, this first approximation is expected to be reasonable in the vicinity of the impurity ($r \lesssim 1/k_F$), but it gives the incorrect behavior for larger and intermediate distances compared to the coherence length.

For the translational invariant superconductor [$F(r)=0$] the solution of Eq. (2.5) is given by

$$\hat{G}^0(\vec{r},\vec{r}\,';z)=\int\frac{d\vec{k}}{(2\pi)^3}e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}\frac{1}{z^2-\epsilon_k^2-\Delta^2}\times\begin{pmatrix} z+\epsilon_k & -\Delta\\ -\Delta & z-\epsilon_k\end{pmatrix}. \qquad (3.1)$$

Integrated for a parabolic band $\epsilon_k=k^2/2m$, one obtains

$$\hat{G}^0(\vec{r};z)=-[i/2(\Delta^2-z^2)^{1/2}]\{[z\hat{I}-\Delta\hat{\tau}_1][f_+(r)-f_-(r)] + i(\Delta^2-z^2)^{1/2}\,\hat{\tau}_3[f_+(r)+f_-(r)]\}, \qquad (3.2)$$

where $f_\pm=-(m/2\pi)e^{\pm ik_\pm r}/r$ and $k_\pm=[1\pm i(\Delta^2-z^2)^{1/2}/\epsilon_F]^{1/2}$. We use the notation $\hat{G}^0(\vec{r},z)=\hat{G}^0(\vec{r},0;z)=\hat{G}^0(0,\vec{r};z)$. The term in Eq. (3.2) proportional to $\hat{\tau}_3$, arises from the asymmetry of a parabolic band around the Fermi level and since no bandwidth cutoff for the electronic states was included. This term is irrelevant for the discussion of this first approximation and will be neglected in this section. The density of states of the superconductor is obtained when $\vec{r}=\vec{r}\,'$

$$\hat{G}^0(\vec{r},\vec{r};z)=\hat{G}^0(0;z)=-[\pi\rho/(\Delta^2-z^2)^{1/2}](z\hat{I}-\Delta\hat{\tau}_1), \qquad (3.3)$$

and the $\hat{t}$ matrix for the classical spin [Eq. (2.6)] yields with $\alpha=\pi J\rho S/2$

$$\hat{t}(z)=\frac{1}{\pi\rho}\frac{\alpha^2(\Delta^2-z^2)^{1/2}}{z^2(1+\alpha^2)^2-\Delta^2(1-\alpha^2)^2}[\hat{I}z(1+\alpha^2)-\hat{\tau}_1\Delta(1-\alpha^2)]. \qquad (3.4)$$

Working out explicitly the products for the Green's function of the complete system, given by Eq. (2.3), one obtains for the anomalous component

$$G_{12}(\vec{r},\vec{r}\,';z)=G_{12}^0(\vec{r},\vec{r}\,';z)+G_{11}^0(\vec{r},0;z)t_{11}(z)G_{12}^0(0,\vec{r}\,';z)+G_{11}^0(\vec{r},0;z)t_{12}(z)G_{22}^0(0,\vec{r}\,';z) + G_{12}^0(\vec{r},0;z)t_{21}(z)G_{12}^0(0,\vec{r}\,';z)+G_{12}^0(\vec{r},0;z)t_{22}(z)G_{22}^0(0,\vec{r}\,';z). \qquad (3.5)$$

For $\vec{r}=\vec{r}\,'$ we have

$$G_{12}(\vec{r},\vec{r};z)=\frac{\pi\rho\Delta}{(\Delta^2-z^2)^{1/2}}+\frac{\alpha^2}{4\pi\rho}\frac{\Delta}{(\Delta^2-z^2)^{1/2}}\frac{z^2(3+\alpha^2)+\Delta^2(1-\alpha^2)}{z^2(1+\alpha^2)^2-\Delta^2(1-\alpha^2)^2}[f_+(r)-f_-(r)]^2, \qquad (3.6)$$

and substituted into Eq. (2.1b) we arrive at

$$F_0(r)=2\lambda\rho\pi T\alpha^2\frac{\sin^2 k_F r}{(k_F r)^2}\sum_{n=0}^{\infty}\frac{\exp\{-(k_F r/\epsilon_F)[\Delta^2+\pi^2T^2(2n+1)^2]^{1/2}\}}{[\Delta^2+\pi^2T^2(2n+1)^2]^{1/2}}\frac{(3+\alpha^2)[\pi T(2n+1)]^2-(1-\alpha^2)\Delta^2}{(1+\alpha^2)^2[\pi T(2n+1)]^2+(1+\alpha^2)\Delta^2} - \lambda\rho\alpha^2\frac{3+\alpha^2}{(1+\alpha^2)^2}\frac{\sin^2 k_F r}{(k_F r)^2}\int_{\omega_D}^{\infty}d\omega\frac{\cos(k_F r\omega/\epsilon_F)}{\omega}. \qquad (3.7)$$

Here, $F_0(r)$ denotes $F(r)$ without self-consistency. The integral in (3.7) yields the cosine integral $\mathrm{Ci}(k_F r\omega_D/\epsilon_F)$.

At low temperatures [temperatures for which $\tanh(\Delta/2T)\simeq 1$] the infinite sum in (3.7) can be converted into an integral using the relation

$$2\pi T\sum_{n=0}^{\infty}\psi(\omega_n)\to\int_0^{\infty}d\omega\,\psi(\omega)+\tfrac{1}{6}\pi^2T^2\psi'(0)+O(T^4), \qquad (3.8)$$

and after some transformations one arrives at

$$F_0(r)=\lambda\rho\alpha^2\frac{\sin^2 kr}{(k_F r)^2}\left\{\frac{3+\alpha^2}{(1+\alpha^2)^2}\left[\mathrm{Ci}\left(k_F r\frac{\omega_D}{\epsilon_F}\right)+K_0\left(k_F r\frac{\Delta}{\epsilon_F}\right)\right] - 4\Delta^2\frac{1-\alpha^2}{(1+\alpha^2)^4}\int_{\Delta}^{\infty}dx\frac{\exp[-(k_F r/\epsilon_F)x]}{(x^2-\Delta^2)^{1/2}}\times\frac{1}{x^2-4\Delta^2\alpha^2/(1+\alpha^2)^2}\right\}, \quad T\ll T_c. \qquad (3.9)$$

Here, K_0 is the modified Bessel function of zeroth order.

For temperatures near the critical temperature, $T\lesssim T_c$, we have $\Delta(T)\ll T_c$, and the expression (3.7) can be reduced to

$$F_0(r)=\lambda\rho\alpha^2\frac{3+\alpha^2}{(1+\alpha^2)^2}\frac{\sin^2 k_F r}{(k_F r)^2}\times\left(\mathrm{Ci}\left(k_F r\frac{\omega_D}{\epsilon_F}\right)+2\sum_{n=0}^{\infty}\frac{\exp[-e^{\gamma}(2n+1)r/\xi_0]}{2n+1}\right), \quad T\lesssim T_c, \qquad (3.10)$$

where γ is Euler's constant and $\xi_0=\epsilon_F/k_F\Delta(T=0)$ is the superconductor coherence length. The infinite sum in (3.10) can be carried out yielding

$$F_0(r)=\lambda\rho\alpha^2\frac{3+\alpha^2}{(1+\alpha^2)^2}\frac{\sin^2 k_F r}{(k_F r)^2}\times\left[\mathrm{Ci}\left(k_F r\frac{\omega_D}{\epsilon_F}\right)-\ln\tanh\left(\frac{e^{\gamma}}{2}\frac{r}{\xi_0}\right)\right], \quad T\lesssim T_c. \qquad (3.11)$$

Finally, we want to discuss the behavior of $F(r)$

for the special cases of small and large distances from the impurity site compared with the superconductor coherence length ξ_0. For $r \ll \xi_0$ we obtain from Eq. (3.9) for $T \ll T_c$

$$F_0(r) = \lambda\rho \frac{\alpha^2}{(1+\alpha^2)^2}\left[(3+\alpha^2)\ln\frac{2\omega_D}{\Delta} - \frac{\arcsin[2\alpha/(1+\alpha^2)]}{2\alpha}\right] \times \frac{\sin^2 k_F r}{(k_F r)^2}, \quad T \ll T_c, \; k_F r \ll \omega_D/\Delta, \qquad (3.12)$$

and for $T \lesssim T_c$ from (3.11)

$$F_0(r) = \lambda\rho\alpha^2 \frac{3+\alpha^2}{(1+\alpha^2)^2}\ln\left(\frac{2\omega_D}{\Delta}\right)\frac{\sin^2 k_F r}{(k_F r)^2}, \quad T \lesssim T_c, \; k_F r \ll \omega_D/\Delta. \qquad (3.13)$$

It can be seen from expression (3.7) that the variation of Δ with r for small distances from the impurity is governed by the factor $\sin^2 k_F r/(k_F r)^2$ for all temperatures.

Since s waves should give the main contribution for small r, this is essentially the behavior in the neighborhood of the impurity. It will be shown in Sec. IV that contributions coming from a self-consistent treatment are very small in this region.

For $r \gg \xi_0$, on the other hand, we have for all temperatures

$$F_0(r) = \lambda\rho\alpha^2 \frac{3+\alpha^2}{(1+\alpha^2)^2}\frac{\sin^2 k_F r}{(k_F r)^2}\operatorname{Ci}\left(k_F r\frac{\omega_D}{\epsilon_F}\right), \quad r \gg \xi_0. \qquad (3.14)$$

The cosine integral behaves asymptotically like

$$\operatorname{Ci}(x) \sim \frac{\sin x}{x} - \frac{\cos x}{x^2}, \quad x \gg 1. \qquad (3.15)$$

Hence, in this non-self-consistent approximation, $F_0(r)$ is an oscillating function and decreases like $(\xi_0/r)^3$ for large distances and for all temperatures. The oscillations are due to the cutoff of the superconductor coupling at ω_D. The $1/r^3$ dependence does not agree with the long-range Ginzburg-Landau result[6]; this breakdown for large distances is not surprising since the self-consistent determination of $\Delta(r)$ is fundamental here.

It should be noted that the dependence on the coupling parameter $\alpha = \pi J\rho S/2$ is analytic and that the result can be expanded in even powers of α. This contradicts the result obtained by Kümmel,[10] where $F(r)$ is a function of the absolute value of α. This different dependence on the coupling can be understood by calculating $\Delta(r)$ through (2.1a) with the discontinuity of (3.6). There are two contributions: one coming from the bound state within the gap and one from the continuum spectrum $\Delta \leq \omega \leq \omega_D$. The continuum contribution has an analytic part and one which depends on the absolute value of the coupling parameter. The latter has similar characteristics as the Kümmel result, but this nonanalytic term is exactly canceled by the contribution coming from the pole residuum of the bound state in the gap. Hence, if for the evaluation in F_0 approximations are made, these may destroy the exact cancellation of the two nonanalytic terms.

IV. SELF-CONSISTENT CALCULATION

In this section the effects of the spatial dependence of $\Delta(r)$ on the "unperturbed" Green's function $\hat{G}^0$ are considered. $F(r)$ will not be neglected in the rhs of Eq. (2.5) and is determined self-consistently through Eq. (2.1). The s electrons are scattered by the s-d potential and originate the spatial variation of $\Delta(r)$ calculated in Sec. III. This pair potential is able to scatter also non-s-partial waves, and this scattering gives rise to new contributions to $\Delta(r)$.

First we rearrange Eq. (2.5) in the absence of impurities. For the translational invariant system the solution is given by the expression (3.2). Rewriting Eq. (2.5) into equations for the function $f_\pm(r)$, we have

$$[\nabla^2/2m + \epsilon_F \pm i(\Delta^2 - z^2)^{1/2}] f_\pm(\vec{r}-\vec{r}\,'; z) = \delta(\vec{r}-\vec{r}\,'), \qquad (4.1)$$

which is the usual differential equation of a Green's function for a problem with spherical symmetry. If an impurity is present at $r=0$, we need the complete expression (2.5), which expressed for the analogous functions to $f_\pm(r)$, $\varphi_\pm(\vec{r},\vec{r}\,')$, yields

$$\left(\frac{\nabla^2}{2m} + \epsilon_F \pm i(\Delta^2 - z^2)^{1/2}\right)\varphi_\pm(\vec{r},\vec{r}\,'; z) = \delta(\vec{r}-\vec{r}\,') + F(r)\left[\pm i\frac{\Delta^2}{(\Delta^2 - z^2)^{1/2}}\varphi_\pm(\vec{r},\vec{r}\,'; z) - \left(z \pm i\frac{z^2}{(\Delta^2 - z^2)^{1/2}}\right)\varphi_\mp(\vec{r},\vec{r}\,'; z)\right]. \qquad (4.2)$$

Integrating these coupled differential equations, we obtain

$$\varphi_\pm(\vec{r},\vec{r}\,'; z) = f_\pm(\vec{r}-\vec{r}\,'; z) \pm i\frac{\Delta^2}{(\Delta^2 - z^2)^{1/2}}\int d\vec{s}\, f_\pm(\vec{r}-\vec{s}; z)F(s)\varphi_\pm(\vec{s},\vec{r}\,'; z) - \left(z \pm i\frac{z^2}{(\Delta^2 - z^2)^{1/2}}\right)\int d\vec{s}\, f_\pm(\vec{r}-\vec{s}; z)F(s)\varphi_\mp(\vec{s},\vec{r}\,'; z). \qquad (4.3)$$

We will assume that the perturbation due to the impurity is small. This is equivalent to state that the effect of $F(r)$ in Eq. (4.3) is small and only linear terms in $F(r)$ need to be taken into account.

We can replace $\varphi_\pm$ in the in the rhs of Eq. (4.3) by the unperturbed function $f_\pm(\vec{s}-\vec{r}\,';z)$. For $\vec{r}=\vec{r}\,'$ the spatial integrations in the rhs of (4.3) are single convolutions and the Fourier transform of $\delta\varphi_\pm=\varphi_\pm - f_\pm$ becomes

$$\delta\tilde{\varphi}_\pm(p,z)=\left[\pm i\,\frac{\Delta^2}{(\Delta^2-z^2)^{1/2}}\mathfrak{F}[f_\pm^2](p) - \left(z\pm i\,\frac{z^2}{(\Delta^2-z^2)^{1/2}}\right)\mathfrak{F}[f_\pm f_\mp](p)\right]\tilde{F}(p)\;, \tag{4.4}$$

where $\delta\tilde{\varphi}$ and $\tilde{F}$ are the Fourier transforms of $\delta\varphi$ and $F(r)$, respectively, and $\mathfrak{F}[g]$ denotes the Fourier transform of g. The evaluation of $\mathfrak{F}[f_\pm^2]$ and $\mathfrak{F}[f_\pm f_\mp]$ is straightforward:

$$\mathfrak{F}[f_\pm^2](p)=i\,\frac{m^2}{2\pi p}\ln\left(\frac{+ip\pm 2ik_F-k_F(\Delta^2-z^2)^{1/2}/\epsilon_F}{-ip\pm 2ik_F-k_F(\Delta^2-z^2)^{1/2}/\epsilon_F}\right) \tag{4.5}$$

and

$$\mathfrak{F}[f_\pm f_\mp](p)=i\,\frac{m^2}{2\pi p}\ln\left(\frac{+ip-k_F(\Delta^2-z^2)^{1/2}/\epsilon_F}{-ip-k_F(\Delta^2-z^2)^{1/2}/\epsilon_F}\right). \tag{4.6}$$

The Green's function $\hat{G}^0$ is obtained by inserting $\varphi_\pm$ into Eq. (3.2). Inserting into Eq. (2.1b), we arrive at the equation

$$\tilde{F}(p)=\tilde{F}_0(p)\Bigg/\Bigg\{1-i\lambda\rho\,\frac{\pi m}{k_F}\,T\sum_{n=0}^{N}\frac{1}{\Delta^2-z_n^2}\,\frac{1}{p}\times\left[\Delta^2\ln\left(\frac{4k_F^2+[ip-k_F(\Delta^2-z_n^2)^{1/2}/\epsilon_F]^2}{4k_F^2+[-ip-k_F(\Delta^2-z_n^2)^{1/2}/\epsilon_F]^2}\right) - 2z_n^2\ln\left(\frac{ip-k_F(\Delta^2-z_n^2)^{1/2}/\epsilon_F}{-ip-k_F(\Delta^2-z_n^2)^{1/2}/\epsilon_F}\right)\right]\Bigg\}\;, \tag{4.7}$$

where $\tilde{F}_0(p)$ is the Fourier transform of $F_0(r)$ calculated in Sec. III. The expression (4.7) should be Fourier antitransformed in order to get the spatial dependence of Δ. This is a hard task and we will consider only the special cases of large distances from the impurity and the vicinity of the impurity.

A. Large distances from the impurity

The behavior at large distances from the impurity is given by the small-p behavior of Eq. (4.7). Expanding the denominator in powers of p, we obtain

$$\tilde{F}(p)=\tilde{F}_0(p)/[A(T)+(p\xi_0)^2B(T)]\;, \tag{4.8}$$

with

$$A(T)=\lambda\rho 2\pi T\sum_{n=0}^{N}\frac{\Delta^2}{(\Delta^2-z_n^2)^{3/2}} \tag{4.9}$$

and

$$B(T)=-\lambda\rho\tfrac{2}{3}\pi T(\pi T_c e^{-\gamma})^2\sum_{n=0}^{\infty}\frac{z_n^2}{(\Delta^2-z_n^2)^{5/2}}\;. \tag{4.10}$$

Both constants $A(T)$ and $B(T)$ are positive. Transformed to real space, Eq. (4.8) leads to an equation of the Ginzburg-Landau type extended to all temperatures:

$$[-B(T)\xi_0^2\nabla^2+A(T)]F(r)=F_0(r)\;. \tag{4.11}$$

The interesting solution is the inhomogeneous one, since for $F_0=0$ no perturbation from the impurity exists and $F(r)$ should vanish identically. Defining $\Omega=[A(T)/B(T)]^{1/2}/\xi_0$, the Fourier antitransform of Eq. (4.8) yields

$$F(r)=\frac{1}{8rB(T)\xi_0^2\Omega}\int_0^\infty dx\,xF_0(x)\times\{\exp[-\Omega|r-x|]-\exp[-\Omega|r+x|]\}\;. \tag{4.12}$$

Near the critical temperatures, $T\lesssim T_c$, one sees from (4.9) that $A(T)$ vanishes like $(1-T/T_c)$ and $B(T)$ reaches the value $B(T_c)=\frac{7}{12}\lambda\rho\,e^{-2\gamma}\zeta(3)$, where ζ is the Riemann zeta function. Since Ω vanishes, we can perform a Taylor expansion in powers of Ω in Eq. (4.12)

$$F(r)=\frac{1}{4B(T_c)\xi_0^2}\left(\frac{1}{r}\int_0^r dx\,x^2F_0(x)+\int_r^\infty dx\,xF_0(x)\right)\;,\qquad T\lesssim T_c\;, \tag{4.13}$$

$F_0(x)$ is given by Eq. (3.11). The fast oscillations of $F_0(r)$ with period π/k_F are not essential for large distances and $\sin^2 k_F r$ can be replaced by its spatial mean value $\frac{1}{2}$. Now Eq. (4.13) can be integrated yielding

$$F(r)=\tfrac{3}{14}\alpha^2\,\frac{3+\alpha^2}{(1+\alpha^2)^2}\,\frac{1}{\zeta(3)}\,\frac{1}{(k_F\xi_0)^2}\times\left(\frac{\pi^2}{4}e^{\gamma}\,\frac{\xi_0}{r}-2e^{2\gamma}\,\frac{\cos(k_F r\omega_D/\epsilon_F)}{(k_F r\,\omega_D/\epsilon_F)^2}+\cdots\right)\qquad T\lesssim T_c\;,\quad r\gg\xi_0\;, \tag{4.14}$$

for the leading terms. The dominant term decreases like $1/r$ as is expected from a Ginzburg-Landau theory and as it has been derived by Heinrichs.[7]

For small temperatures, such that $\tanh(\Delta/2T)\simeq 1$, on the other hand, we obtain from (4.9) $A(T)=\lambda\rho$ and from (4.10) $B(T)=\lambda\rho/9$. Hence, $\Omega=3/\xi_0$ and $F_0(r)$ is given by Eq. (3.9). The factor $\sin^2 k_F r$ will again be replaced by its spatial average $\frac{1}{2}$, since these fast oscillations do not play a relevant role for distances larger than the coherence length. Only the cosine-integral term of $F_0(r)$ is important; all the other decrease exponentially for large r. Neglecting exponentially small terms, we have then for $F(r)$

$$F(r)=\tfrac{3}{8}\alpha^2\,\frac{3+\alpha^2}{(1+\alpha^2)^2}\,\frac{1}{\xi_0 r k_F^2}\left[e^{-3r/\xi_0}\int_0^r dx\,\frac{\sinh(3x/\xi_0)}{x}\times\mathrm{Ci}\left(\frac{x\omega_D}{\xi_0\Delta}\right)+\sinh\frac{3r}{\xi_0}\int_r^\infty dx\,\frac{e^{-3x/\xi_0}}{x}\mathrm{Ci}\left(\frac{x\omega_D}{\xi_0\Delta}\right)\right]\;,\qquad T\ll T_c\;. \tag{4.15}$$

The integrals can be estimated approximately using the fact that a function ψ, which equals $\lambda r e^{-\lambda r x}$ for $x \geq 0$ and equals 0 for $x < 0$, approaches a $\delta(x)$ function as r tends to infinity. Neglecting terms, which decrease exponentially, we arrive at

$$F(r) \simeq \tfrac{1}{8}\alpha^2 \frac{3+\alpha^2}{(1+\alpha^2)^2} \frac{\Delta^2}{\epsilon_F^2} \left(\frac{\xi_0}{r}\right)^2 \mathrm{Ci}\left(\frac{r}{\xi_0}\frac{\omega_D}{\Delta}\right)$$

$$\simeq \tfrac{1}{8}\alpha^2 \frac{3+\alpha^2}{(1+\alpha^2)^2} \frac{\Delta^3}{\epsilon_F^2 \omega_D} \left(\frac{\xi_0}{r}\right)^3 \sin\frac{r}{\xi_0}\frac{\omega_D}{\Delta} + O\left(\frac{\xi_0}{r}\right)^4 ,$$

$$T \ll T_c , \quad r \gg \xi_0 . \qquad (4.16)$$

Hence, for small temperatures, $F(r)$ is an oscillating function which decreases as $1/r^3$.

B. Vicinity of the impurity

The spatial dependence in the vicinity of the impurity is mainly given by the large-p behavior in Eq. (4.7). Expanding the denominator of Eq. (4.7) for large p, we have

$$\tilde{F}(p) = \tilde{F}_0(p) + \frac{\lambda\rho(k_F/\epsilon_F)^2 2\pi T \sum_{n=0}^{N}(\Delta^2 - z_n^2)^{1/2}}{p^2 + \lambda\rho(k_F/\epsilon_F)^2 2\pi T \sum_{n=0}^{N}(\Delta^2 - z_n^2)^{1/2}} \tilde{F}_0(p) . \qquad (4.17)$$

Calling

$$\Omega^2 = \lambda p \left(\frac{k_F}{\epsilon_F}\right)^2 2\pi T \sum_{n=0}^{N} (\Delta^2 - z_n^2)^{1/2} ,$$

we have that the Fourier antitransform of (4.17) is

$$F(r) = F_0(r) + (\Omega/8r)\int_0^\infty dx\, x F_0(x)\{\exp[-\Omega\,|r-x|\,] - \exp[-\Omega(r+x)]\} . \qquad (4.18)$$

The coefficient Ω has only a small temperature dependence and its value is approximately $\Omega^2 \sim \lambda\rho(\omega_D/\epsilon_F)k_F^2$. Hence, $\Omega \ll k_F$ and the expression (4.18) can be reduced to

$$F(r) = F_0(r) + \frac{\Omega^2}{4}\left(\frac{1}{r}\int_0^r dx\, x^2 F_0(x) + \int_r^\infty dx\, x F_0(x) e^{-\Omega x}\right) . \qquad (4.19)$$

Expression (4.19) shows that the corrections to $F_0(r)$ coming from the self-consistency condition contain the factor $(\Omega/k_F)^2$, and are negligibly small (several orders of magnitude) compared to $F_0(r)$ in the neighborhood of the impurity. Assuming that $F_0(r)$ behaves like $F_0(r) = A(T)\sin^2 k_F r/(k_F r)^2$ for all r, the integrals in (4.19) can be overestimated

$$F(r) = A(T)\left[\frac{\sin^2 k_F r}{(k_F r)^2} + \frac{\Omega^2}{4k_F^2}\left(\frac{1}{2} - \frac{1}{4}\frac{\sin 2k_F r}{k_F r} + \ln\frac{4k_F^2}{\Omega^2} + [\mathrm{Ci}(2k_F r) - \gamma - \ln k_F r]\right)\right] . \qquad (4.20)$$

As mentioned before, the corrections are negligible and finally

$$F(r) = F_0(r) = A(T)\frac{\sin^2 k_F r}{(k_F r)^2} , \quad r \ll \xi_0 \frac{\omega_D}{\epsilon_F} . \qquad (4.21)$$

V. SUMMARY AND CONCLUDING REMARKS

The spatial variation of the superconductor order parameter in the presence of a classical spin has been analyzed for large distances from the impurity and in its vicinity. The distortion in the superconductor due to the impurity is expressed by the local deviations of the order parameter from the bulk value $\Delta F(r)$. The Gorkov equation for the one-particle Green's function has been solved self-consistently with the "gap" equation by taking only first-order effects in $F(r)$ into account. This is equivalent to assume that the distortions due to the impurity are small.

The electron-impurity interaction has been assumed to be given by a contact s-d Hamiltonian. Only s electrons are scattered by this potential. The s-wave scattering generates a spatial variation of the pair potential, which induces a scattering of other partial waves. This non-s-electron scattering is taken into account by solving the Gorkov equation consistently with the spatial-dependent pair potential.

In the vicinity of the impurity only s waves are important and corrections due to a self-consistent treatment of Gorkov's equation are negligible. The deviation from the bulk pair potential Δ is of the form $\Delta F(r) = \Delta A(T)\sin^2 k_F r/(k_F r)^2$, $A(T)$ being an analytic and even function of the exchange coupling (for a classical spin). The general expression for $A(T)$ is given by Eq. (3.7).

Far away from the impurity, $r \gg \xi_0$, on the other hand, the spatial variation of $\Delta(r)$ is determined by the scattering of all partial waves and a self-consistent treatment of $\Delta(r)$ is fundamental. Near the transition temperature the deviations from the bulk value vary like $1/r$ as is expected from the Ginzburg-Landau theory. At low temperatures the variation is oscillatory with period $2\pi\xi_0\Delta/\omega_D$ and decreases as $(\xi_0/r)^3$.

Finally, it should be pointed out that qualitatively the same results are expected by including the Kondo effect. For instance, the approximate $\hat{t}$ matrix for a Kondo impurity in a superconductor derived in Ref. 4 can be used

$$\hat{t}(z) = \hat{K}(z)/[\hat{I} - \hat{G}^0(0,0;z)\hat{K}(z)] , \qquad (5.1)$$

with

$$\hat{K}(z) = \hat{G}^0(0,0;z)R\big(i(\Delta^2 - z^2)^{1/2}\big)/\pi\rho \qquad (5.2)$$

and

$$R(z) = \frac{\pi}{4}J^2\rho\frac{S(S+1)}{3}\left\{1 + \frac{2}{i}T(J\rho, z) + 4J\rho\left[\ln\frac{D}{2\pi T} - \psi\left(\frac{1}{2} - i\frac{z}{2\pi T}\right)\right]\frac{1}{i}T(\tfrac{3}{4}J\rho, z)\right\}, \qquad (5.3)$$

where

$$T(x,z)=i\left(\frac{D}{4\pi T}\right)^{2x}2\,\frac{\Gamma(2x)}{\Gamma(x)\Gamma(1+x)}\times F(1,2x;1+x;\tfrac{1}{2}+iz/4\pi T)\ . \qquad (5.4)$$

Here, Γ, ψ, and F are the gamma, digamma, and hypergeometric function, respectively, and D is a cutoff for the electronic excitations. The only change in $F_0(r)$, given by Eq. (3.7), is obtained by equating $\alpha^2=\pi^2\rho^2 R(i(\Delta^2-z_n^2)^{1/2})$ and by taking α as frequency dependent. Hence, the spatial variation of $\Delta(r)$ in the neighborhood of the impurity is still given by $\sin^2 k_F r/(k_F r)^2$ and the only change is in the factor $A(T)$ and in its temperature dependence. In the same way it can be seen through Eq. (4.12) that no qualitative change is expected for large distances ($r \gg \xi_0$).

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