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SOLUTION OF THE LINEARIZED ENERGY-GAP EQUATION IN NONHOMOGENEOUS SUPERCONDUCTORS

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Boundary conditions are derived for the generalized energy-gap function in nonhomogeneous superconducting systems. The problem of obtaining an exact solution is discussed and several approximations are compared.

INTRODUCTION

A problem of current interest is the investigation of properties of nonhomogeneous superconductors, especially the proximity effect between different metals in contact. Such systems can be analyzed by the Green's function method developed by Gor'kov[1], but in general the resulting equations cannot be solved exactly. A major problem is that of determining appropriate boundary conditions at the intermetallic interface.

In this paper the boundary conditions are derived and the problem of calculating the exact Green's function is investigated. Different approximation schemes are discussed and compared.

BASIC EQUATIONS[2]

The properties of a nonhomogeneous superconductor are determined by the energy-gap function:

$$\Delta(\mathbf{r}) = V(\mathbf{r})F(\mathbf{r}, \mathbf{r}'), \tag{1}$$

where $V(\mathbf{r})$ is the electron-electron interaction and $F(\mathbf{r}, \mathbf{r}') = \langle\psi_{\uparrow}(\mathbf{r})\psi_{\downarrow}(\mathbf{r}')\rangle$. Close to the critical temperature the difference between the thermodynamic potentials of the normal and superconducting states can be expanded in even powers of Δ. The critical temperature is determined by the vanishing of the quadratic term:

$$\Omega = \int \Phi(\mathbf{r})[\Delta(\mathbf{r}) - V(\mathbf{r})\Phi(\mathbf{r})]\,d\mathbf{r},$$

where

$$\Phi(\mathbf{r}) = \int K(\mathbf{r}, \mathbf{r}')\Delta(\mathbf{r}')\,d\mathbf{r}'$$

and $K(\mathbf{r}, \mathbf{r}')$ is the one-electron correlation function in the normal state.[3] The function $\Delta(\mathbf{r})$, which is determined by minimization of $\Omega[\Delta]$, satisfies the equation $\Delta(\mathbf{r}) - V(\mathbf{r})\Phi(\mathbf{r}) = 0$. Since $\Phi(\mathbf{r}) = F(\mathbf{r}, \mathbf{r})$, this result agrees with Eq. (1). Therefore the equation:

$$\Delta = V\Phi[\Delta] \tag{2}$$

is called the consistency condition.

It is rarely possible to solve the consistency condition exactly. In general an arbitrary trial function can be chosen for $\Delta(\mathbf{r})$; since the exact solution of Eq. (2) minimizes Ω, the condition $\Omega[\Delta] < 0$ is a sufficient one for superconductivity. The temperature at which $\Omega[\Delta]$ vanishes is therefore a lower bound of the exact transition temperature of the system.

BOUNDARY CONDITIONS

A complete set of boundary conditions for metallic contacts have been derived by de Gennes.[3] Our discussion follows de Gennes' reasoning, but the actual calculation and results are somewhat different.

We write the kernel as an imaginary-time Fourier transform:

$$K(\mathbf{r}, \mathbf{r}') = kT \sum_{\omega} K_{\omega}(\mathbf{r}, \mathbf{r}'), \tag{3}$$

where $\omega = (2n + 1)\pi kT$.

Since $K_{\omega}(\mathbf{r}, \mathbf{r}')$ is the one-electron correlation function, the situation is similar to neutron diffusion.[4] We therefore identify the quantity

$$v\Phi_{\omega}(\mathbf{r}) = v \int K_{\omega}(\mathbf{r}, \mathbf{r}')\Delta(\mathbf{r}')\,d\mathbf{r}'$$

where v is the Fermi velocity, with the neutron flux in an absorbing medium, and $\Delta(\mathbf{r}')$ plays the role of the source function; l corresponds to the scattering mean free path and $\Xi_{\omega} = \hbar_{v}/2|\omega|$ to the mean free path for absorption, i.e., the absorption time corresponds to the lifetime of Cooper pairs, which is on the order of $\hbar/2\pi kT$.

The Fourier transform of the kernel can be written in the form (see[4], p. 56):

$$K_{\omega}(q) = \frac{2\pi N}{v}\left[\frac{q}{\operatorname{arctg}\zeta_{\omega}q} - \frac{1}{b}\right]^{-1}, \tag{4}$$

where N is the density of states at the Fermi surface and $\zeta_{\omega}^{-1} = l^{-1} + \Xi_{\omega}^{-1}$. Equation (4) agrees with the result of the microscopic theory.[2]

The exact boundary conditions on Φ_{ω} are (see[4], pp. 98–99):

$$q_{\omega}^{-2}\zeta_{\omega}^{-1}\Phi_{\omega}, \quad q_{\omega}^{-2}\operatorname{grad}\Phi_{\omega} \text{ — continuous.}$$
$$\mathbf{n}\operatorname{grad}\Phi_{\omega} = 0 \text{ on free surfaces.}$$

Here $\pm q_{\omega}$ are the poles of $K_{\omega}(q)$. An approximate form of these conditions is:

$$v\Phi_{\omega} \text{ continuous,} \tag{5a}$$

$$\xi^{2}\operatorname{grad}\Phi_{\omega} \text{ continuous,} \tag{5b}$$

$$\mathbf{n}\operatorname{grad}\Phi_{\omega} = 0 \text{ on free surfaces,} \tag{5c}$$

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where

$$\xi^2 = \zeta_{\omega(n=0)}\Xi_{\omega(n=0)} = \frac{lv/2\pi kT}{1+(2\pi kTl/v)}.$$

Equation (5a) does not agree with the condition of de Gennes,[3] Φ_ω/N continuous, except in the case when the Fermi surfaces of the two metals are equal. The discrepancy arises from an assumption of de Gennes about the transmission coefficient which does not take into account properly the Pauli exclusion principle.

Conditions (5b) and (5c) are related to the de Gennes sum rule:

$$\int K_\omega(\mathbf{r},\mathbf{r}')\,d\mathbf{r}' = \pi N(\mathbf{r})/|\omega|.$$

Multiplication by $\Delta(\mathbf{r})$ and integration with respect to r yield[2)]

$$\int \Phi_\omega(\mathbf{r})\,d\mathbf{r} = \frac{\pi}{|\omega|}\int N(\mathbf{r})\Delta(\mathbf{r})\,d\mathbf{r}. \tag{6}$$

These conditions are of course idealized and must be modified for real surfaces as discussed in[2].

KERNEL

The kernel K(r, r′) is given by Eqs. (3) and (4). The summation is taken over all ω such that $\hbar|\omega| < k\Theta$, where Θ is the effective Debye temperature of the combined system. The cut-off frequency is the frequency at which the electron-electron interaction becomes repulsive. If the electron-phonon interaction in one of the metals is large, that metal dominates and its Debye temperature is approximately Θ.[3)]

Upon summing we obtain in the limit $lq \ll 1$,

$$K(q) = N\sum_{n=0}^{\Theta/2\pi T}\frac{1}{n+1/2+\xi^2q^2/2} = N\left[\chi\left(\frac{\Theta}{2\pi T}\right)-\chi(\xi^2q^2)\right];$$
$$\chi(z) = \psi(^1/_2 + {^1/_2}z) - \psi(^1/_2), \tag{7}$$

and ψ is the logarithmic derivative of the Γ-function. The function $\chi(z)$ is shown in Fig. 1.

CONSISTENCY CONDITION

When making use of the equation for Φ,

$$\Phi(q) = K(q)\Delta(q)$$

it is necessary to observe that this equation does not define $\Phi(q)$ if q is one of the poles of K(q), i.e., if $\xi^2q^2 = -1, -3, -5, \ldots$. The magnitude of $\Phi(q)$ in this case is determined by the boundary conditions (5). Since $\Delta(q_\omega)$ must vanish, it follows that $\Phi(q_\omega) = 0$ for all q_ω, following from the consistency condition:

$$\Delta(q) = V\Phi(q) = VK(q)\Delta(q).$$

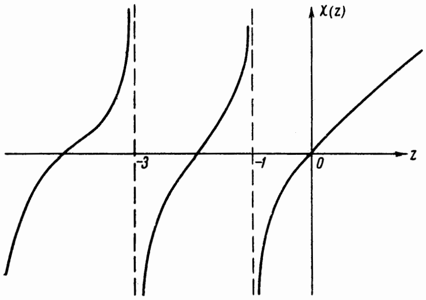

FIG. 1. Plot of $\chi(z)$ vs. z.

There therefore exist two general conditions to be satisfied by the exact solution of the consistency condition:

(a) $\Delta(q) = 0$ unless $|q| = q_i$, where q_i are the roots of the equation $VK(q) = 1$.

(b) All Φ_ω satisfy the boundary conditions (5) subject to the additional restriction that $\Phi_\omega(|q| = q_\omega) = 0$.

The second condition is very difficult to fulfill, and at the present time there exists no exact solution of a proximity effect problem. It is known that $\Phi(\mathbf{r})$ becomes singular near the interface,[5)] and therefore it is not possible to neglect the values of $\Delta(q_i)$ for $\xi^2q_i^2 \ll -1$.

SUPERPOSED FILM PROBLEM

We consider a system of two superposed metal films; the geometry is shown in Fig. 2. A useful class of trial functions is of the form:

$$\begin{aligned}\Delta(z>0) &= A_+\cos q_+(z-z_+),\\ \Delta(z<0) &= A_-\cos q_-(z-z_-),\end{aligned} \tag{8}$$

where $q_\pm$ can be real or imaginary.

The case $q_+ = q_- = 0$ was considered in[2]. With a trial step-function surprisingly good results are obtained, which can in part be understood by noting that the actual $\Delta(\mathbf{r})$ also changes rapidly near the interface.[2] In the calculation with a constant Δ it was incorrectly assumed that Φ_ω/N is continuous. If we use instead the boundary condition (5a), that $v\Phi_\omega$ is continuous, we find that the simplest trial function is obtained by requiring that $Nv\Delta$ be constant. In this case we obtain the following result, valid for any geometry:

$$T_c > 1{,}14\exp\left\{-\int N^{-1}v^{-2}\,d\mathbf{r}\Big/\int Vv^{-2}\,d\mathbf{r}\right\}. \tag{9}$$

This inequality for T_c is useful only when the dimensions of the system are small.

Another convenient choice is to take q_+ and q_- to be roots of the equation $V_\pm K_\pm(q) = 1$. In particular, we pick the "principal roots," defined as follows: in the case $NV > 0$ (attractive interaction) this is the root for which $\xi^2q^2 > -1$, and for $NV < 0$ (repulsion) we require $-1 > \xi^2q^2 > -3$ (cf. Fig. 1). The "principal root" defined in this way gives consistent results in the limits $NV \to +0$ and $NV \to -0$ and does not take large real values.

Such a function was used by Werthamer,[6] who took it to be an exact solution of the consistency condition;

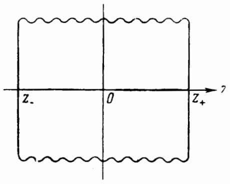

FIG. 2. System of two superposed films.

[2)] Note that in Ref. [2] a factor of N(r) was incorrectly omitted from Eq. (23).

[3)] The question of different θ_D is discussed in [6].

this is not the case, since such a Δ satisfies only part of the full consistency condition (cf. Appendix).

The method of Werthamer[6] and the more sophisticated single-frequency approximation of de Gennes[3] determine the critical temperature by applying special boundary conditions to Δ. Their methods are based on the following assumption:

If at some temperature T there exists a function of the form of Eq. (8) such that $q_\pm$ are the principle roots of the equation $V_\pm K_\pm(q) = 1$ and Δ satisfies the following boundary conditions at the interface:

$$(v/V)\Delta \text{ continuous},$$
$$(\xi^2/V)\,\mathrm{grad}\,\Delta \text{ continuous},$$

then T is approximately equal to T_c. The meaning of the expression "approximately" here is of course arbitrary. In any case, it is necessary that the free energy difference

$$\Omega = \int_{z_-}^{z_+} \Phi(z)[\Delta(z) - V(z)\Phi(z)]\,dz$$

be small. Since the quantity in square brackets depends only on terms of the form $\cos[(q_\omega)_\pm(z - z_\pm)]$, the assumption is valid only in the case where such terms are negligible. This can be checked by the calculation described in the Appendix.

CONCLUSION

In nonhomogeneous superconducting systems the energy-gap function cannot generally be exactly determined. Sometimes a simple trial function gives a close lower bound to the critical temperature; for example, Eq. (9) for systems of small dimension. Generally there are two possibilities: we can do an exact calculation with a crude trial function, or an approximate calculation with a more realistic function. The latter procedure is really intuitive, since the trial function does not behave like the exact solution near the interface, and therefore the imposition of boundary conditions is of questionable validity.

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APPENDIX

We show a sample calculation of the contribution of the poles of K(q) to $\Phi(q)$. In particular we consider the n = 0 term. The trial function is of the form of Eq. (8). The general form of Φ_ω for n = 0 is:

$$kT[\Phi_{\omega(n=0)}(z)]_\pm = \frac{N_\pm \Delta(z)}{1 + \xi_\pm^2 q_\pm^2} + B_\pm \operatorname{ch} \frac{(z - z_\pm)}{\xi_\pm}. \tag{A.1}$$

Applying the boundary conditions, Eq. (5), we obtain the restrictions:

$$\frac{N_+ v_+ A_+ \cos q_+ z_+}{1 + \xi_+^2 q_+^2} + v_+ B_+ \operatorname{ch}\frac{z_+}{\xi_+} = \frac{N_- v_- A_- \cos q_- z_-}{1 + \xi_-^2 q_-^2} + v_- B_- \operatorname{ch}\frac{z_-}{\xi_-},$$

$$\frac{N_+ \xi_+^2 q_+ A_+ \sin q_+ z_+}{1 + \xi_+^2 q_+^2} - \xi_+ B_+ \operatorname{sh}\frac{z_+}{\xi_+} = \frac{N_- \xi_-^2 q_- A_- \sin q_- |z_-|}{1 + \xi_-^2 q_-^2} - \xi_- B_- \operatorname{sh}\frac{|z_-|}{\xi_-}. \tag{A.2}$$

Equations (A.2) are sufficient to determine B_+ and B_-. For example, in the previously considered case $q_+ = q_- = 0$, $N_+ v_+ A_{++} = N_- v_- A_-$, we obtain $B_+ = B_- = 0$; from this we obtain the inequality (9).

Replacing ξ by $(i/q_\omega) = \xi/\sqrt{2|n|+1}$ we obtain a system of equations which, generally speaking, has no solution for B_+ and B_-.

It is clear that a function of the form of Eq. (8) cannot satisfy the consistency condition, and that for an exact solution it is necessary to include all roots of the equation $VK(q) = 1$. In this case, equations similar to Eqs. (A.2) and the restrictions B = 0 can be used to determine the coefficients $(A_i)_\pm$.

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