Solvable Pair Potential for the Bogoliubov–de Gennes Equations of Space-Dependent Superconductivity*

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The Bogoliubov–de Gennes equations for the quasiparticle states of space-dependent superconductivity are solved exactly for a two-parameter pair potential representing a normal-metal-superconductor interface. For the simplest case of a superconductor filling the half-space $z > 0$, $\Delta(z,T) = [\Delta_0(T) + \Delta_1(T)e^{-z/\xi}]$, where Δ_0 is the bulk value of the gap and Δ_1 and ξ are variational parameters. For $T \sim T_c$, Δ_1 and ξ can be determined by minimizing the Ginzburg-Landau free-energy functional. In addition, the effect of self-consistency on the low-lying bound states of a superconductor–normal-superconductor junction is discussed.

It has recently been shown by Bar-Sagi and Kuper[1] that the pair potential $\Delta(z, T) = \Delta_0(T) \times \tanh[z/\xi(T)]$, for a simple-interface problem, gives rise to an exactly solvable Bogoliubov–de Gennes equation for the superconducting quasiparticle states $u_n(z)$ and $v_n(z)$. The parameter $\xi(T)$ was determined from the self-consistency condition for $T \sim T_c$ and it agreed with the Ginzburg-Landau value. Bar-Sagi and Kuper suggest that their potential will be useful for all temperatures.

In this note we present another pair potential for which the Bogoliubov–de Gennes equations are exactly solvable. For a simple interface with the superconductor in the $z > 0$ half-space, this potential is

$$\Delta(z, T) = \Theta(z)[\Delta_0(T) + \Delta_1(T)e^{-z/\xi(T)}] .$$

Note that as either of the variational parameters Δ_1 or ξ goes to zero, $\Delta(z, T)$ becomes the step potential used with success by several authors[2] for $T \sim 0$. We will see that the exponential form for $\Delta(z, T)$ is also useful for $T \sim T_c$. Although not precisely of the Ginzburg-Landau form, $\Delta_0(T) + \Delta_1(T) \times e^{-z/\xi(T)}$ represents $\Delta_0(T)\tanh[z/\xi(T)]$ exactly for $z/\xi(T) \ll 1$ if $\Delta_1 = -\Delta_0$. The variational coherence length ξ can then be determined by minimizing the Ginzburg-Landau free energy. The exponential potential therefore is sufficiently flexible that it should be useful for multiple interfaces at any temperature.

To begin the analysis we note that for the simple-interface problem the Bogoliubov-de Gennes equations in the Andreev approximation[3]

$$\left(-i\hbar v_{Fz}\frac{d}{dz} - E\right)u_n(z,\theta,T) + \Delta(z,T)v_n(z,\theta,T) = 0 ,$$
$$\left(i\hbar v_{Fz}\frac{d}{dz} - E\right)v_n(z,\theta,T) + \Delta^*(z,T)u_n(z,\theta,T) = 0 , \qquad (1)$$

can be written in the uncoupled form[1]

$$\left(-(\hbar v_{Fz})^2\frac{d^2}{dz^2} + \Delta^2(z,T) \pm \hbar v_{Fz}\frac{d}{dz}\Delta(z,T) - E_n^2\right) \times f_n(z,\theta,T) = 0 , \qquad (2)$$

where $v_{Fz} \equiv v_F\cos\theta$, E_n is the quasiparticle energy,

$$f_n^{\pm}(z,\theta,T) \equiv u_n(z,\theta,T) \pm iv_n(z,\theta,T)$$

and $u_n(z,\theta,T)$ and $v_n(z,\theta,T)$ are the particle and hole components of the quasiparticle state $\varphi(z,\theta,T)$. The pair potential must be self-consistently determined via

$$\Delta(z,T) = V_{BCS}\sum_{n,\theta} u_n(z,\theta,T)v_n^*(z,\theta,T)\tanh\left(\frac{E_n}{2kT}\right). \qquad (3)$$

In the following we will suppress all arguments except z. Consider the trial pair potential given by $\Delta(z) = \Delta_0 + \Delta_1 e^{-z/\xi}$. The necessary quantity to be used in Eq. (2) is

$$\Delta^2(z) \pm \hbar v_{Fz}\frac{d\Delta(z)}{dz} = \Delta_0^2 + \left(2\Delta_0\Delta_1 \mp \frac{\Delta_1\hbar v_{Fz}}{\xi}\right) \times e^{-z/\xi} + \Delta_1^2 e^{-2z/\xi} . \qquad (4)$$

We thus obtain

$$\left(\frac{d^2}{dz^2} - \frac{2\Delta_0\Delta_1 \mp \Delta_1\hbar v_{Fz}/\xi}{(\hbar v_{Fz})^2}e^{-z/\xi} - \frac{\Delta_1^2}{(\hbar v_{Fz})^2}e^{-2z/\xi} + \frac{E^2 - \Delta_0^2}{(\hbar v_{Fz})^2}\right)f^{\pm}(z) = 0 . \qquad (5)$$

Defining the scaled variable $\bar{z} \equiv z/\xi$ and the quantities

$$b_{\mp} \equiv \xi^2(2\Delta_0\Delta_1 \mp \Delta_1\hbar v_{Fz}/\xi)/(\hbar v_{Fz})^2 ,$$
$$a^2 \equiv \xi^2\Delta_1^2/(\hbar v_{Fz})^2 , \qquad (6)$$
$$c^2 \equiv \xi^2(\Delta_0^2 - E^2)/(\hbar v_{Fz})^2 ,$$

Eq. (5) becomes

$$\left(\frac{d}{dz^2} - b_{\mp} e^{-\bar{z}} - a^2 e^{-2\bar{z}} - c^2\right) f^{\pm}(z) = 0 \ . \tag{7}$$

In terms of the variable $y \equiv 2\, ae^{-\bar{z}}$ and the functions $g^{\pm} \equiv y^{1/2} f^{\pm}$,

$$\left(\frac{d^2}{dy^2} - \frac{1}{4} - \frac{b_{\mp}/2a}{y} - \frac{c^2 - \frac{1}{4}}{y^2}\right) g^{\pm}(y) = 0 \ , \tag{8}$$

where

$$b_{\mp}/2a = (\xi \Delta_0/\hbar v_{Fz}) \mp \tfrac{1}{2} \ .$$

Equation (8) is Whittaker's differential equation[4] and the solution appropriate to the present analysis (i.e., regular at $z=0$) can be written in terms of the confluent hypergeometric function $M(c+\frac{1}{2}+b_{\mp}/2a,\ 1+2c,\ y)$:

$$g^{\pm}_{-b_{\mp}/2a, c}(y) = e^{-1/2y} y^{1/2+c} M(c+\tfrac{1}{2}+b_{\mp}/2a,\ 1+2c,\ y) \tag{9}$$

Because Eq. (8) is invariant to changing the sign of c, a degeneracy exists and the general solution is a linear combination of the solutions for $\pm c$.

We are now equipped to display the general form for $f^{\pm}(\bar{z})$:

$$f^{\pm}(\bar{z}) = (e^{-ae^{-\bar{z}}})[A_1^{\pm} e^{-c\bar{z}} M(c+\tfrac{1}{2}+b_{\mp}/2a,\ 1+2c,\ 2ae^{-\bar{z}}) + A_2^{\pm} e^{c\bar{z}} M(-c+\tfrac{1}{2}+b_{\mp}/2a,\ 1-2c,\ 2ae^{-\bar{z}})] \ . \tag{10}$$

The four coefficients $A_1^{\pm}$, $A_2^{\pm}$ are determined by inserting $u = \frac{1}{2}(f^+ + f^-)$ and $v = (1/2i)(f^+ - f^-)$ back into the first-order Bogoliubov–de Gennes equations, Eqs. (1), and then applying the boundary conditions.

For $E > \Delta_0$ we see that $c^2 < 0$ and the asymptotic form of Eq. (10) for either f^+ or f^- is

$$f(\bar{z}) \to e^{\pm c\bar{z}} = e^{\pm i(\epsilon/\hbar v_{Fz})z} \ , \tag{11}$$

where $\epsilon^2 \equiv E^2 - \Delta_0^2$. For $E < \Delta_0$ we have $c^2 > 0$ and the appropriate asymptotic form of f is exponentially damped,

$$f(\bar{z}) \to e^{-c\bar{z}} = e^{-(|\epsilon|/\hbar v_{Fz})z} \ . \tag{12}$$

We return now to the self-consistency problem. The parameters Δ_1 and ξ are determined in general by minimizing the free energy.[5] In what follows, a simplified version of this prescription will be carried out for the Ginzburg-Landau regime. Before doing this, however, we present a brief discussion of how self-consistency affects the bound states that arise due to a normal-metal–superconductor (NS) interface for $T \sim 0$.

Bardeen and Johnson[2] (BJ) studied the bound-state contribution to the Josephson current through an SNS junction for $T \ll T_0$. Their wave functions were calculated with the step-potential model and are given by

$$\begin{pmatrix} u \\ v \end{pmatrix} = A \begin{pmatrix} e^{i(qz+\eta_1)/2} \\ e^{-i(qz+\eta_1)/2} \end{pmatrix} e^{i\vec{k}_F\cdot\vec{r}} \qquad \text{for } 0 < z < d$$

$$\begin{pmatrix} u \\ v \end{pmatrix} = A' \begin{pmatrix} e^{i\eta_0^+/2} \\ e^{-i\eta_0^+/2} \end{pmatrix} e^{-(z-d)/2\xi_{BJ}} e^{i\vec{k}_F\cdot\vec{r}} \qquad \text{for } z > d \ , \tag{13}$$

where $2d$ is the normal-metal thickness and the wave function for $z < 0$ is given by symmetry. Since $k_F \gg q$ the quasiparticle energy relative to E_F is $E = \frac{1}{2}\hbar v_{Fz} q = \Delta_0 \cos\eta_0$, and $(2\xi_{BJ})^{-1} = (\Delta_0/\hbar v_{Fz})\sin\eta_0$. Bardeen and Johnson consider only the low-lying states $E \ll \Delta_0$. In this case the eigenvalues are given by $E_n = \frac{1}{2}\hbar v_{Fz} q_n$, where $n = 0, 1, 2 \ldots$ and

$$q_n = (n+\tfrac{1}{2})\pi/(d + \hbar v_{Fz}/2\Delta_0) \equiv (n+\tfrac{1}{2})\pi/d^* \ . \tag{14}$$

The normalization, $\int d^3r(|u|^2 + |v|^2) = 1$, requires that $|A|^2 = |A'|^2 = 1/4d^*$, and accounts for the quasiparticle penetration of the interface.

We will now discuss the wave functions of the exponential potential for the SNS junction. We will also consider only the bound states. Because of symmetry it will be sufficient to work with the region $z > 0$. In addition, the normal-metal states are the same as in Eq. (13), but with different q_n, so that we need consider only the region $z > d$. We will see that the self-consistency correction amounts simply to a redefinition of the penetration or renormalization constant d^*.

By observing the behavior of $M(c+\frac{1}{2}+b_{\mp}/2a,\ 1+2c,\ 2ae^{-(z-d)/\xi})$ for $E_n \ll \Delta_0$, one can show that the wave function modified for self-consistency is pproximately[6]

$$\begin{pmatrix} u \\ v \end{pmatrix} = (4d^*_{SC})^{-1/2} \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{-a} e^{-c(z-d)/\xi} \exp(ae^{-(z-d)/\xi}) \ , \tag{15}$$

where d^*_{SC} is given by

$$d^*_{SC} = d + (\hbar v_{Fz}/2\Delta_0)\int_0^\infty d\bar{z}\, e^{-\bar{z}}\, \frac{\exp(2ae^{-\xi_{BJ}\bar{z}/\xi})}{e^{2a}} \tag{16}$$

and $\xi_{BJ} \approx \hbar v_{Fz}/2\Delta_0$. It is evident from Eq. (16) that $d^*_{SC} > d^*$, since the integral is always greater than unity for Δ_1, and therefore a, negative. The bound-state energy modified for self-consistency can now be written

$$E_n^{SC} = \hbar v_{Fz}(n+\tfrac{1}{2})\pi/2d^*_{SC} < E_n^{BJ} \ . \tag{17}$$

Since $d^*_{SC} > d^*$ the self-consistency correction lowers all of the bound-state energies by allowing a larger effective "box size" for the motion of the quasiparticles in N.

We will now determine the parameters Δ_1 and ξ in the $T \sim T_c$ regime by minimizing the Ginzburg-

Landau (GL)[7] free-energy functional. This procedure is different from the method of Bar-Sagi and Kuper who insure that their trial potential, $\Delta(z)=\Delta_0 \tanh z/\xi$, is self-consistent [i.e., satisfies Eq. (3)] to second order in Δ_0 for $T\sim T_c$. However, since the exponential potential does not solve the GL equation, it is necessary to take this alternate route of minimizing the free energy.

The GL free-energy functional, in a conventional notation,[8] is

$$F_s = F_n + \alpha \int d^3r\, |\psi(\vec{r})|^2 + (\tfrac{1}{2}\beta)\int d^3r\, |\psi(\vec{r})|^4 + (\tfrac{1}{2}m)\int d^3r\, |(-i\hbar\vec{\nabla} - (2e/c)\vec{A})\psi(\vec{r})|^2 + (1/8\pi)\int d^3r\, |\vec{H}-\vec{H}_a|^2 , \quad (18)$$

and the order parameter $\psi(\vec{r})$ is proportional to the gap parameter $\Delta(\vec{r})$. We therefore express our variational or trial function as

$$\psi(z) = \psi_0 + \psi_1 e^{-z/\xi}, \text{ for } z > 0 . \quad (19)$$

We also impose boundary conditions such that the exponential potential fits $\Delta_0 \tanh(z/\xi)$ for $z/\xi \ll 1$. We choose

$$\psi_1 = -\psi_0 . \quad (20)$$

In the absence of a magnetic field, the free energy relative to a bulk superconductor in the half-space $z>0$ can be written

$$\Delta F = \alpha \int d^3r(|\psi|^2 - |\psi_0|^2) + \tfrac{1}{2}\beta \int d^3r(|\psi|^4 - |\psi_0|^4) + (\hbar^2/2m)\int d^3r\, |\vec{\nabla}\psi|^2 . \quad (21)$$

The optimum value of ξ is of course determined from the condition $\partial\Delta F/\partial\xi = 0$. A moderate amount of algebraic manipulation results in

$$\xi^2 = \hbar^2 / \tfrac{11}{6} m|\alpha| = \tfrac{12}{11}\xi_{GL}^2 , \quad (22)$$

where we have used $\psi_0^2 = -\alpha/\beta$.

The above simple calculation leads to the conclusion that when using the quasiparticle wave functions of Eq. (10) for $T\sim T_c$ one can use the Ginzburg-Landau coherence length and a value of Δ_1 suggested by the boundary condition of Eq. (20), i.e., $\Delta_1 = -\Delta_0$. This conclusion of course is only valid when one is interested in effects that are operative over distances of the order of $\xi_{GL}(T)$.

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