The Influence of the Transverse Width on the Andreev Bound States and Self-Consistent Gap Function in Clean SNS System

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INTRODUCTION

In clean layered structure of normal metal and superconductor, Andreev-bound states are formed in the normal metallic part through multiple Andreev reflections (Andreev, 1964 & 1967) of the electron and hole waves. In the Andreev approximation (AA) (Andreev, 1964 & 1967), the incident electron towards a normal metal-superconductor (NS) interface will be reflected as a hole. Exact analysis, however, shows a small amplitude of a normally reflected electron (Sipr & Gyorffy, 1996). In most studies (Larkin & Yu, 1975), Andreev-bound states are described using the quasiclassical description, which can be shown to be equivalent to AA (Ashida et al., 1982). Interestingly, Andreev approximation works remarkably well (Blaauboer et al., 1996). In this paper, we want to investigate the reliability of AA by varying the transverse dimensions (dimensions perpendicular to the flow of current) of a mesoscopic superconductor-normal metal-superconductor (SNS) sample (Bagwell, 1999). In most systems considered so far (Tanaka & Tsukada, 1991), the transverse dimensions which the breakdown of the Andreev approximation can hardly show up are considered infinite.

THEORY

Throughout the paper, Rydberg atomic units are used– the energy is in Rydberg, the distance is in Bohr (1 Bohr ~ 0.5Å), $\hbar = 1$, and the electronic mass is 1/2. The Green's function formalism is outlined extensively by Koperdraad et al. (1995). It is an extension of the microscopic theory used by Tanaka & Tsukada (1991), in that the electron-hole scattering properties are treated exactly.

The matrix Green's function satisfies the equation

$$\begin{pmatrix} i\omega_n + \nabla^2 + \mu & -\Delta(r) \\ -\Delta^*(r) & i\omega_n - \nabla^2 - \mu \end{pmatrix} G(r, r', i\omega_n)$$

$$= \delta(r - r')1 \qquad (1)$$

in which the differential operator is closely related to the operator in the Bogoliubov-de Gennes (BdG) equations

$$\begin{pmatrix} -\nabla^2 - \mu & \Delta(r) \\ \Delta^*(r) & \nabla^2 + \mu \end{pmatrix} \Psi(r) = E\Psi(r)$$

$$\equiv E \begin{pmatrix} u(r) \\ v(r) \end{pmatrix} \qquad (2)$$

apart from the replacement of E by $i\omega_n$. The quantity ω_n, which is equal to $\omega_n = \pi n k_B T$, is called the Matsubara frequency. For a system of fermions, n is an odd integer. Possible inhomogeneities of the system are fully represented by the r dependence of the gap function. The spinor wave function $\Psi(r)$ describes quasiparticle excitations, and the energy E is measured with respect to the Fermi energy μ. Eq. (1) is derived using the finite

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temperature Green's function formalism (Abrikosov et al., 1963 & 1965) by manipulating the equations of motion instead of the often used diagrammatic analysis. The SNS system we consider is shown in Fig. 1. The gap function Δ has a constant complex value in the superconducting part and zero in the normal part. This model of the gap ignores the proximity effect. As far as the transverse directions are concerned, the general solution of Eq. (1) can be expressed as a Fourier series expansion in $\sin\ k_y y$ and $\sin\ k_z z$ in which $k_y = \frac{n_y \pi}{L_y}$ and $k_z = \frac{n_z \pi}{L_z}$. The functions $\sin k_y y$ and $\sin k_z z$ are in fact the transverse solutions of the BdG equations with the boundary conditions $\Psi(x,0,0) = \Psi(x, L_y, L_z) = 0$. Thus, we have

$$G(r,r',i\omega_n) = \frac{4}{L_y L_z}\sum G\left(x,x',k_y,k'_y,k_z,k'_z,i\omega_n\right) \times \sin k_y y \sin k'_y\ y' \sin k_z z \sin k'_z\ z' \tag{3}$$

In Eq. (3), the summation extends over all allowed values of k_y, k'_y, k_z, k'_z. The Fourier coefficient becomes the $G\left(x,x',k_y,k'_y,k_z,k'_z,i\omega_n\right)$ Green's function of the quasiparticle motion along the *x*-direction, which can be seen by substituting Eq. (1) with Eq. (3):

$$\begin{pmatrix} i\omega_n + \frac{d^2}{dx^2} + k_{F_x}^2 & -\Delta \\ -\Delta^* & i\omega_n - \frac{d^2}{dx^2} - k_{F_x}^2 \end{pmatrix} \times G(x,x',k_y,k'_y,k_z,k'_z,i\omega_n) = \delta(x-x')\delta_{k_y,k'_y}\delta_{k_z,k'_z} \tag{4}$$

where $k_{F_x}^2 = \mu - k_y^2 - k_z^2$. Eq. (4) demonstrates that $G(x,x',k_y,k'_y,k_z,k'_z,i\omega_n)$ is diagonal to k_y and k_z. In calculating the local density of states and the self-consistent gap function, we will need the Green's function for diagonal spatial coordinates. As long as we keep $x \neq x'$, we can already take *y* = *y'* and *z* = *z'* in Eq. (3). Since we are only interested in the variations over the longitudinal direction *x*, we can average over the transverse dimensions. By that, Eq. (3) simplifies to the series:

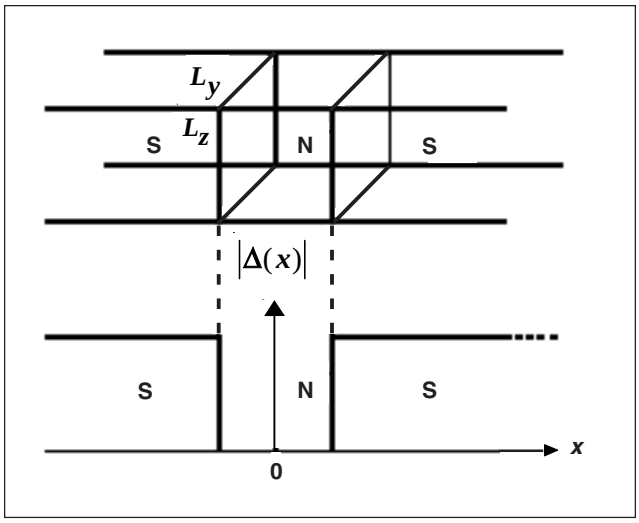

Fig. 1. The geometry of the SNS system considered.

$$G\left(x,x',i\omega_n\right) = \frac{1}{L_y L_z}\sum_{k_y,k_z} G(x,x',k_y,k_z,i\omega_n) \tag{5}$$

The solution of Eq. (4) for a superconducting bar, that is when the system shown in Fig. 1 is composed mainly of a superconducting material without the normal metal, is

$$G_S^0(x,x',k_y,k_z,i\omega_n) = \sum_\sigma d_S^\sigma \psi_S^{\sigma-}(x_<)\psi_S^{\sigma+}(x_>) = \sum_\sigma d_S^\sigma \psi_S^{\sigma+}(x_>)\psi_S^{\sigma-}(x_<) \tag{6}$$

where

$$\psi_S^{\sigma\nu} = \begin{pmatrix} u_S^\sigma e^{i\phi/2} \\ u_S^{-\sigma} e^{-i\phi/2} \end{pmatrix} e^{i\sigma\nu k_S^\sigma x} \tag{7}$$

$$\psi_S^{\sigma\nu}(x) = \left(u_S^\sigma e^{-i\phi/2} u_S^{-\sigma} e^{i\phi/2}\right) e^{i\sigma\nu k_S^\sigma x} \tag{8}$$

$$d_S^\sigma = -\frac{1}{4\Omega_S k_S^\sigma} \tag{9}$$

$$i\Omega_S = \sqrt{(i\omega_n)^2 - |\Delta|^2} \tag{10}$$

$$u_S^\sigma = \sqrt{E + \sigma\sqrt{E^2 - |\Delta|^2}} \tag{11}$$

$$k_S^\sigma = \sqrt{k_{F_x}^2 + \sigma\sqrt{E^2 - |\Delta|^2}} \tag{12}$$

$$k_{F_x}^2 = \mu - k_y^2 - k_z^2 \qquad (13)$$

ϕ is the phase of the complex constant Δ. The index σ refers to the type of particle (electronlike for σ = +1 and holelike for σ = -1), and the index *n* indicates the direction of propagation (ν = +1 to the right and ν = -1 to the left).

The solution of Eq. (4) for an NS system (single interface) is,

$$G_{\nu j\nu' j}(x,x',k_y,k_z,i\omega_n) = G^0_{\nu j}(x,x',k_y,k_z,i\omega_n)\delta_{\nu\nu'} + \sum_{\sigma\sigma'} d^{\sigma}_{\nu j} d^{\sigma'}_{\nu' j} \psi^{\sigma\nu}_{\nu j}(x) t^{\sigma\sigma'\nu\nu'}_{\nu j\nu' j} \psi^{\sigma'\nu'}_{\nu' j}(x') \qquad (14)$$

where

$$G^0_{\nu j}(x,x',k_y,k_z,i\omega_n) = \sum_{\sigma} d^{\sigma}_{\nu j} \psi^{\sigma\mu}_{\nu j}(x) \psi^{\sigma,-\mu}_{\nu j}(x') \qquad (15)$$

with μ = sgn(*x*–*x'*). For multiple interfaces, that is, for arbitrary number of layers

$$G_{\nu j\nu' j'}(x,x',k_y,k_z,i\omega_n) = G^0_{\nu j\nu' j'}(x,x',k_y,k_z,i\omega_n)(\delta_{\nu\nu'}\delta_{jj'} + \delta_{-\nu\nu'}\delta_{j+\nu,j'}) + \sum_{\sigma\mu\sigma'\mu'} d^{\sigma}_{\nu j} d^{\sigma'}_{\nu' j'} \psi^{\sigma\mu}_{\nu j}(x) T^{\sigma\sigma'\mu\mu'}_{\nu j\nu' j'} \psi^{\sigma'\mu'}_{\nu' j'}(x') \qquad (16)$$

The quantities $t^{\sigma\sigma'\nu\nu'}_{\nu j\nu' j'}$ and $T^{\sigma\sigma'\mu\mu'}_{\nu j\nu' j'}$ are obtained by imposing the continuity of the Green's function and its derivative at the interfaces.

The bound-state energy is determined by looking through the local density of states (LDOS) using the formula

$$LDOS(x,E) = -\frac{1}{\pi L_y L_z} \times \lim_{\delta\to 0} \sum_{k_y,k_z} \mathrm{Im}\, G_{11}(x,x',k_y,k_z,E+i\delta) \qquad (17)$$

in which G_{11} is the upper left matrix element of the multiple scattering Green's function (Eq. (16)). At the bound-state energy, the LDOS has infinite peak. To avoid this singularity, the parameter δ is introduced to broaden the peak so that it acquires a finite height. The peaks in the plot of the LDOS against the quasiparticle energy must correspond to the Andreev-bound state energies.

In this formalism, the Andreev approximation can easily be implemented. This approximation amounts to the replacement

$$k^{\sigma}_{\nu j} \to k_{F_x} + \sigma \frac{\sqrt{E^2 - |\Delta|^2}}{2k_{F_x}} \qquad (18)$$

if $k^{\sigma}_{\nu j}$ occurs in the exponential and to $k^{\sigma}_{\nu j} \to k_{F_x}$ if $k^{\sigma}_{\nu j}$ occurs as a factor. It is valid when E, |D|<< $k^2_{F_x}$.

In the present paper, we investigate its limitation by looking at configurations in which $E,\Delta \approx k^2_{F_x}$.

The gap function can be determined self-consistently, using the formula

$$\Delta(x) = -\frac{V}{\beta L_y L_z} \sum_{\omega_n,k_y,k_z} F(x,x',k_y,k_z,i\omega_n) \qquad (19)$$

where $F(x,x',k_y,k_z,i\omega_n)$ is the upper right element of the matrix Green's function $G_{\nu j\nu' j'}(x,x',k_y,k_z,i\omega_n)$ and *V* is the pairing interaction amplitude. In carrying out the calculation, we first substitute in $F(x,x',k_y,k_z,i\omega_n)$ the step-like gap profile shown in Fig. 1. We can determine a new value of the gap by using Eq. (19). This new value is again substituted in $F(x,x',k_y,k_z,i\omega_n)$, and another new value is again obtained using Eq. (19). The iteration is continued until the difference in the gap values between two successive iterations is negligibly small.

RESULTS

Local density of states

To investigate the reliability of the Andreev approximation, we focus on the choice of the transverse dimensions which we choose to be $L_y = L_z = L_t$. The transverse components of the solutions of the BdG equations are $\sin(k_y y)\ \sin(k_z z)$ in which $k_y = \frac{n_y \pi}{L_y}$ and $k_z = \frac{n_z \pi}{L_z}$. The different combinations of (k_y, k_z)

or (n_y, n_z) are called modes whose allowed values are determined by

$$k_{F_x}^2 = \mu - \left(\frac{\pi}{L_t}\right)^2 \left(n_y^2 + n_z^2\right) > 0 \ . \qquad (20)$$

When the transverse dimension is small, the second term in the right becomes large, and as a result of which, only a few modes will be allowed. If this term exceeds the chemical potential μ, k_{F_x} becomes imaginary, the wave-function is damped, and consequently, such mode cannot exist. For larger transverse dimensions, the second term is smaller whereupon more modes are allowed. Most of our calculations will be done for small L_t so that only few modes will exist. We will tune L_t such that $k_{F_x}^2$ is of the same order of magnitude as the gap energy Δ, in which regime the Andreev approximation (Eq. (18)) is not valid, and call such L_t value a critical width.

Figs. 2 and 3 show the results for a configuration in which $(n_y, n_z) = (2,2)$ is the highest allowed mode. The chemical potentials in the superconductor and in the normal metal, μ_S and μ_N, respectively, are assumed equal with magnitude 0.5. The longitudinal dimension *L* of the normal-metal part is 4,000 Bohr and the gap Δ is treated as real, with magnitude 0.0001 Ry. The LDOS in the normal-metal part at *x* = 1,000 Bohr is plotted against *E*/Δ. The peaks represent discrete energy states (Blaauboer et al., 1996). We make the width curves, determined by the parameter δ in $E + i\delta$, wide enough so that the fundamental features can be seen. The numbers in parentheses denote the mode to which the energy belongs. In Fig. 3, the transverse width is determined by the condition that $k_{F_x}^2 = \Delta$ for the mode (2,2) in which one finds that L_t = 12.5676 Bohr; and in Fig. 2 the transverse width is L_t = 13 Bohr, which is slightly larger than the critical width, but has the same allowed modes. In Fig. 2, the exact results and the AA results coincide and only three states are found, one for each mode. For the critical width shown in Fig. 3, the states for the first two modes are almost unchanged, but for the (2,2) mode many states are found. The peaks corresponding to the AA are split in the exact treatment.

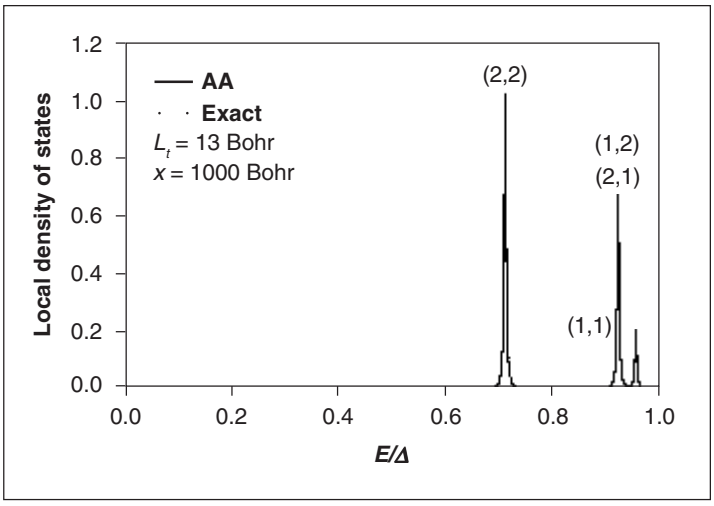

Fig. 2. The LDOS against *E*/Δ for an SNS system in which L_t = 13 Bohr.

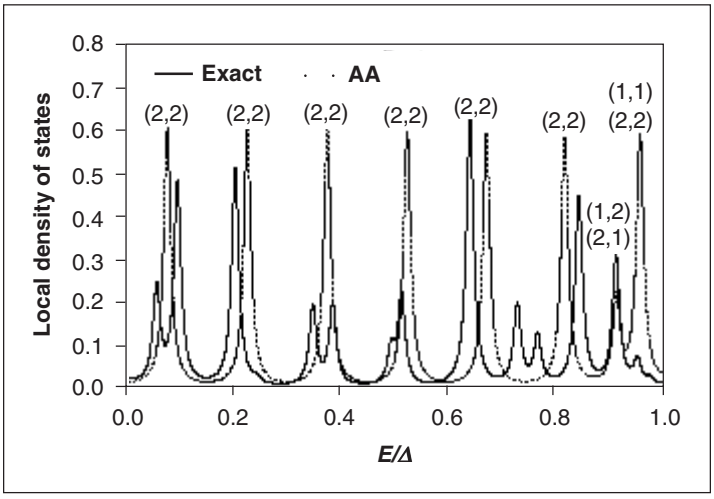

Fig. 3. The LDOS against *E*/Δ for *x* = 1,000 Bohr, L_t = 12.5676 Bohr, *L* = 4,000 Bohr, and Δ = 0.0001 Ry.

Finally, we want to make a comment on our choices of the transverse widths. It will come out in the next section that superconductivity is suppressed for transverse widths in the order of 20 Bohr or less. This means that our choices of L_t are not at all appropriate. We made those choices to illustrate with clarity the fundamental features of the Andreev-bound states. If we choose a larger transverse width in which no suppression of superconductivity occurs, many states will appear and the picture would have been quite crowded. The fundamental features, however, remain unchanged.

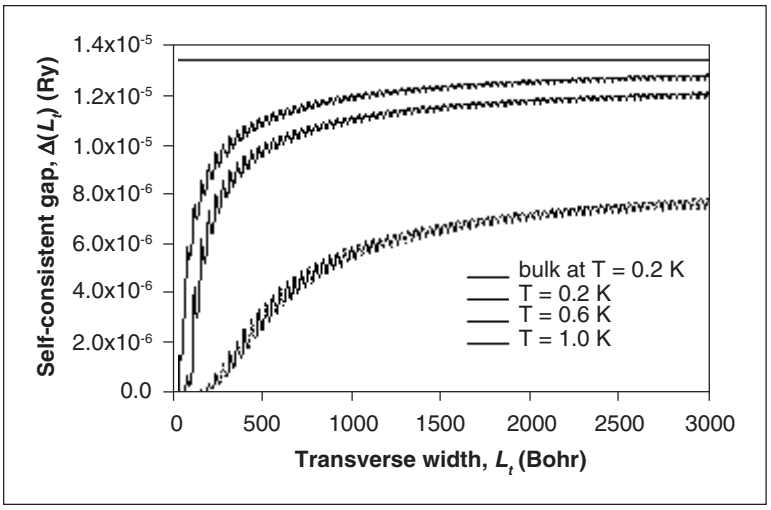

Fig. 4. The self-consistent gap function against the transverse width, L_t, for a bar-shaped superconductor at different temperatures. The number of iterations is 100.

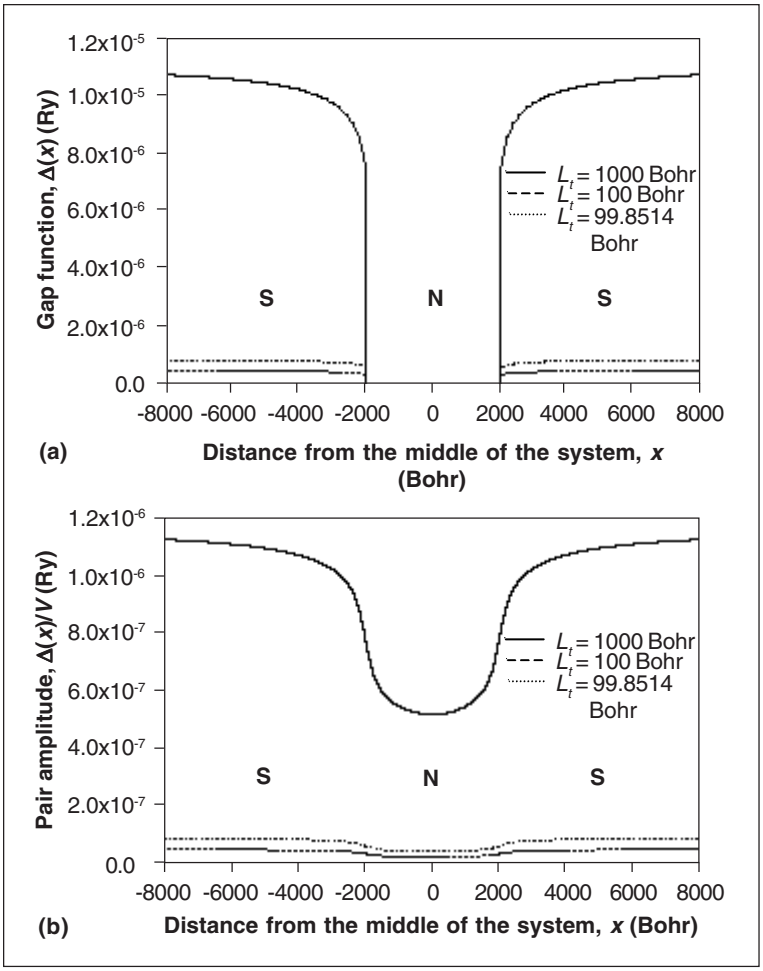

Fig. 5. (a) The gap function and (b) the pair amplitude of an SNS system against the distance from the middle of the system chosen at $x = 0$. The interfaces are located at $x = \pm 2000$.

Self-consistent gap function

We first present the results of the self-consistent gap calculation for a bar-shaped superconductor. In about 80 iterations, the gap values stabilize. In Fig. 4, we show the self-consistent gap values plotted against L_t for a bar-shaped superconductor. It can be seen that there are oscillations of the gap whose amplitudes decrease as L_t increases. These oscillations can be attributed to the discreteness of the transverse wave vectors. As L_t increases, the transverse wave vector approaches the continuous regime, which can be gauged from the gap becoming closer to its bulk value obtained by integrating, instead of summing over, the transverse wave vectors. Another interesting thing which can be seen in the figure is the suppression of superconductivity for narrower transverse widths. We notice that as the temperature increases, the onset of the suppression of the superconductivity occurs at higher values of L_t.

For the SNS system, our initial gap profile is the step-like gap shown in Fig. 1. By following the algorithm outlined in the theory, we obtain the results shown in Fig. 5. In Fig. 5a, the gap is depressed near the interface. This occurs because of the proximity of the superconductor to the normal metal. This phenomenon is known as the "proximity effect". In Fig. 5b, we show the pair amplitude or density of Cooper pairs. It is evident that even in the normal metal, Cooper pairs still exist. This is another manifestation of the proximity effect.

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