Critical voltage of a mesoscopic superconductor

R. S. Keizer\textsuperscript{1,†}, M. G. Flokstra\textsuperscript{2,†}, J. Aarts\textsuperscript{2} and T. M. Klapwijk\textsuperscript{1}

\textsuperscript{1}Kavli Institute of NanoScience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands

\textsuperscript{2}Kamerlingh Onnes Laboratory, Universiteit Leiden, 2300 RA Leiden, The Netherlands

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We study the role of the quasiparticle distribution function $f$ on the properties of a superconducting nanowire. We employ a numerical calculation based upon the Usadel equation. Going beyond linear response, we find a non-thermal distribution for $f$ caused by an applied bias voltage. We demonstrate that the even part of $f$ (the energy mode $f_{L}$) drives a first order transition from the superconducting state to the normal state irrespective of the current.

The energy distribution function of quasiparticles in a normal metal is under equilibrium conditions given by the Fermi-Dirac distribution $f_{0}$. In recent years it has been demonstrated that in a voltage ($V$)-based mesoscopic wire (length $L$) a two-step non-equilibrium distribution develops \cite{1} with additional rounding by quasiparticle scattering due to spin-flip and/or Coulomb interactions \cite{2}. Figure 1a shows the distribution, which resembles two shifted Fermi-Dirac functions:

$$f(x, \varepsilon) = (1-x)f_{0}(\varepsilon + eV/2) + xf_{0}(\varepsilon - eV/2)$$  \hspace{1cm} (1)

with $\varepsilon$ the quasiparticle energy and $x$ the coordinate along the wire. For strong enough relaxation ($L \gg L_{\phi}$) the distribution returns to a Fermi-Dirac distribution with a local effective temperature.

If the normal wire is replaced by a superconducting wire, the attractive interaction between electrons leads to the superconducting state. The questions we address here are how the distribution function is modified (for a typical result see Fig. 1b) and how this affects observable properties such as the current-voltage characteristics of the system and the breakdown of the superconducting state. To relate the distribution function to observable quantities, it is convenient to separate the symmetric part $f_{L}$ (energy mode) from the asymmetric part $f_{T}$ (charge mode) which each have a different spatial and spectral form (Fig. 1c and d). In particular we will show that the breakdown is characterized by a voltage rather than by a current; in other words, the system cannot be trivially treated as two resistors modelling the normal- to supercurrent conversion, with a superconducting element characterized by its depairing current in-between.

The transport and spectral properties of dirty superconducting systems ($\ell_{e} \ll \xi_{0}$, with $\ell_{e}$ the elastic mean free path and $\xi_{0}$ the superconducting phase coherence length) are described by the quasiclassical Green functions obeying the Usadel equation \cite{3}. For out of equilibrium systems we use the Keldysh technique in Nambu (particle-hole) space. We look at s-wave superconductors (singlet pairing) without any spin-dependent interactions. The Usadel equation then takes the form $hD\nabla(\hat{G}\nabla\hat{G}) = -i[\hat{H}, \hat{G}]$, where the check notation (\(\hat{G}\)) denotes a $4 \times 4$ matrix, $D$ is the diffusion constant, $\nabla$ is the spatial derivative $\hat{H}$ and we neglect any inelastic process. The elements of $\hat{G}$ and $\hat{H}$, when split up in Keldysh space, are $2 \times 2$ matrices in Nambu space, denoted by a hat:

$$\hat{G} = \left( \begin{array}{cc} \hat{G}^{R} & \hat{G}^{K} \\ 0 & \hat{G}^{A} \end{array} \right), \quad \hat{H} = \left( \begin{array}{cc} \hat{H} & 0 \\ 0 & \hat{H} \end{array} \right)$$ \hspace{1cm} (2)

Here, $\hat{G}^{R}$ and $\hat{G}^{A}$ are the retarded and advanced components describing equilibrium properties and $\hat{G}^{K}$ is the Keldysh component which describes the non-equilibrium properties. Their elements are the quasiclassical (energy-dependent) normal and anomalous Green functions and, for the Keldysh component only, the quasiparticle distribution functions (which take account of the non-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Quasiparticle distribution function $f(x, \varepsilon)$ as function of energy $\varepsilon$ and position $x$ for a normal wire (a) and a superconducting wire (b) between normal metallic reservoirs for $k_{B}T \ll eV < \Delta_{0}$, with (c) and (d) the decomposition of (b) into the charge mode $f_{T}$ and energy mode $f_{L}$.}
\end{figure}
equilibrium). For the Hamiltonian \( \hat{H} \) we write:

\[
\hat{H} = \begin{pmatrix}
\epsilon & -\Delta \\
\Delta^* & -\epsilon
\end{pmatrix}
\]

(3)

where \( \epsilon \) is the (eigen)energy and the chosen gauge is such that the pair potential \( \Delta \) is in equilibrium a real quantity, \( \Delta = \Delta^* \). The matrix Green function \( \hat{G} \) satisfies the normalization condition \( \hat{G}\hat{1} = 1 \), leading to \( \hat{G}^R\hat{G}^R = \hat{A}^A\hat{A} = 1 \) and \( \hat{G}^R\hat{G}^K + \hat{G}^K\hat{G}^A = 0. \) If superconducting reservoirs in the system are kept at zero voltage (avoiding AC Josephson effects), \( \hat{G}^K \) can be written as \( \hat{G}^K = \hat{G}^R \hat{f} - \hat{f}\hat{G}^A \). Here \( \hat{f} \) is the diagonal generalized distribution number matrix of the quasiparticles in Nambu space. To relate \( \hat{f} \) to observable quantities we decompose it into an even part (or energy/longitudinal mode) and an odd part (or charge/transverse mode) in particle-hole space:

\[
\hat{f} = \hat{f}_L\tau_0 + \hat{f}_T\tau_2,
\]

where \( \tau_i \) are the Pauli matrices in particle-hole space \( \hat{f}_i \). The full distribution function is retained by: \( 2\hat{f}(x, \epsilon) = 1 - \hat{f}_L(x, \epsilon) - \hat{f}_T(x, \epsilon) \).

The retarded matrix Green function in terms of the position and energy dependent normal \( g(\epsilon, x) \) and anomalous \( f_i(\epsilon, x) \) Green functions is:

\[
\hat{G}^R = \begin{pmatrix}
g(\epsilon, x) & f_1(\epsilon, x) \\
f_2(\epsilon, x) & -g(\epsilon, x)
\end{pmatrix}
\]

(4)

Substituting this in the retarded part of the Usadel equation: \( hD\nabla(\hat{G}^R\nabla\hat{G}^R) = -i[\hat{H}, \hat{G}^R] \) and using the normalization condition (\( g^2 + f_1^2 + f_2^2 = 1 \)), we find the retarded Usadel equations:

\[
\begin{align*}
hD[g\nabla^2 f_1 - f_1\nabla^2 g] &= -2i\Delta g - 2\epsilon f_1 \\
hD[f_2\nabla^2 f_2 - f_2\nabla^2 f_1] &= 2i\Delta f_2 + 2i\Delta^* f_1
\end{align*}
\]

(5)

The second equation is essential when calculating the non-equilibrium properties of superconductors. Its left-hand-side is proportional to the divergence of the spectral (energy-dependent) supercurrent, which is (compared to the equilibrium case) no longer a conserved quantity.

A general relation between the advanced matrix Green function and the retarded matrix Green function is given by:

\[
\hat{G}^R = -\tau_0(\hat{G}^A)\tau_1.
\]

Using this, the Keldysh matrix Green function \( \hat{G}^K \) can be written entirely in terms of \( g, f_1, f_2, f_L \) and \( f_T \):

\[
\hat{G}^K = \begin{pmatrix}
g(\epsilon + \hat{g}) f_+ & \hat{f}_1 f_- - \hat{f}_2 f_+ \\
\hat{f}_2 f_- - \hat{f}_1 f_- & -(g(\epsilon + \hat{g})) f_-
\end{pmatrix}
\]

(6)

where \( \hat{f}_\pm = f_L \pm f_T \). Working out the kinetic part of the Usadel equation:

\[
\begin{align*}
hD\nabla j_{\text{energy}} &= 0 \\
hD\nabla j_{\text{charge}} &= 2R_L f_L + 2R_T f_T
\end{align*}
\]

(7)

The various elements in Eq. (7) are given by:

\[
\begin{align*}
\Pi_L &= \frac{1}{2}(2 + 2|\epsilon|^2 - |F_1|^2 - |F_2|^2) \\
\Pi_T &= \frac{1}{2}(2 + 2|\epsilon|^2 + |F_1|^2 + |F_2|^2) \\
\Pi_X &= \frac{1}{2}(|F_1|^2 - |F_2|^2) \\
\Pi_\epsilon &= \frac{1}{2}\Re\{F_1^* F_2 - F_2^* F_1\} \\
R_L &= -\frac{1}{3}\Re\{\Delta F_2 + \Delta^* F_1\} \\
R_T &= -\frac{1}{3}\Re\{\Delta F_2 - \Delta^* F_1\}
\end{align*}
\]

(8)

Equations (7) are two coupled diffusion equations for \( f_L \) and \( f_T \), describing the divergences in the spectral energy current and the spectral charge current. The total charge current is given by \( J = \frac{1}{2e}\int \epsilon j_{\text{charge}} d\epsilon \) with \( \rho \) the resistivity. The terms \( \Pi_L \) and \( \Pi_T \) can be related to an effective diffusion constant for the energy and charge mode respectively and \( \Pi_X \) as a "cross-diffusion" between them. \( j_\epsilon \) is the spectral supercurrent and \( R_L \) and \( R_T \) describe the "leakage" of spectral current to different energies, where the total leakage-current \( \propto \int |[R_L f_L + R_T f_T]| d\epsilon \) is zero.

In the small signal limit the terms \( \Pi_\epsilon, j_\epsilon \) and \( R_L \) and \( R_T \) are small and can in many cases be neglected (linear approach), effectively decoupling \( f_L \) and \( f_T \). In this article we go beyond this limit.

The Usadel equation is supplemented by a self-consistency relation:

\[
\hat{H}(1,2) = \frac{N_0 V_{\text{eff}}}{4} \int_{\omega_D} d\epsilon \hat{G}_{(1,2)}^K d\epsilon
\]

(9)

Here, \( N_0 \) is the normal density of states around the Fermi energy, \( V_{\text{eff}} \) the effective attractive interaction and the integral limits are set by the Debye energy \( \omega_D \). The resulting equation for \( \Delta \) becomes:

\[
\Delta = -\frac{1}{2}N_0 V_{\text{eff}} \int_{-\omega_D}^{\omega_D} d\epsilon (|F_1 - F_2|^2) f_L - (F_1 + F_2^*) f_T d\epsilon.
\]

To calculate spectral and transport properties, one needs to know the self-consistent solution of \( \Delta \). In most practical cases, this has to be done numerically. A convenient solution scheme is to first find the Green functions of the system by solving the retarded equations for a certain \( \Delta \), next to determine the quasiparticle distribution functions by solving the kinetic equations and then calculate a new \( \Delta \) using the self-consistency relation. This process has to be repeated until \( \Delta \) converges.

As a starting value for \( \Delta \) we use the BCS form at zero temperature. To simplify the calculations a parameterization is used that automatically fulfills the normalization condition. It is convenient to take \( g = \cosh(\theta) \), \( F_1 = \sinh(\theta) e^{i\chi} \) and \( F_2 = -\sinh(\theta) e^{-i\chi} \), where \( \theta \) and \( \chi \) are position and energy dependent (complex) variables. At the interfaces between the superconducting wire and the normal metallic reservoirs we use the following boundary conditions:

\[
\theta = \nabla \chi = 0 \quad \text{(retarded equation)} \quad \text{and} \quad f_L, f_T = \frac{1}{2}(\tanh \frac{\epsilon + eV}{2k_B T} \pm \tanh \frac{\epsilon - eV}{2k_B T}) \quad \text{(kinetic)}
\]
The transport properties of the NSN system can now be calculated with the equations described above. In a previous analysis a finite differential conductance was found at zero bias employing a linear response calculation \cite{6}. With the approach introduced here, the full current-voltage relation can be obtained. The result at several temperatures (T = 0, 0.5 Tc, 0.75 Tc, T = 0 (1/Tc)) is shown in Fig. 2, which is controlled by the voltage and cannot be interpreted as a critical current density, and ∆ is the critical current density.

In Fig. 3 the electrostatic potential φ = \int_0^\infty f_F \mathcal{R} \{ g \} dx along the wire is shown at zero temperature prior to (eV/\Delta_0 = 0.013, 0.646) and immediately after (eV/\Delta_0 = 0.651) the transition. The potential can be seen to drop to zero over a distance of the order of the coherence length due to the normal- to supercurrent conversion. This mechanism also gives rise to the finite zero bias resistance. The profile hardly changes over the full range of voltages, until the critical value is reached, after which the electrostatic potential drops in a linear fashion, indicating the system is in the normal state. The minimal changes emphasize the limited influence of f_T on the superconducting state (i.e. on ∆).

The current density at which the superconductor switches to the normal state (for T = 0) is much smaller than the critical current density in an infinitely long wire (J/J_c = 1). Neither is the transition triggered at the weaker superconducting edges as indicated by the shape of the electrostatic potential profile in Fig. 3. The parameter that determines whether or not the superconducting state exist is ∆, as follows from Eq. 9. The integral in this self-consistency equation sums all pair-states (either occupied by a Cooper pair, or empty). F_i gives the Cooper pair density-of-states and f_L and f_T determine which of those states are doubly occupied or doubly empty and which are singly occupied (broken) due to the presence of quasiparticles. In equilibrium at T = 0, a switch to the normal state can only be caused by reaching a critical phase gradient, entering ∆ via F_i. In the presence of quasiparticles, ∆ (and thus potentially the state of the system), is also influenced by the distribution functions. It was noticed above that the charge mode f_T has a very limited influence on ∆. The effect of the energy mode f_L is examined below.

By a small modification of our system to a T-shaped geometry as shown in Fig. 4, we can in a direct way disentangle the effects of f_L and f_T on ∆. This setup can be thought of as the connection of the superconducting wire to the center of a normal wire. In the middle of such a wire f_T is equal to zero, but f_L is not. The result for the pair potential at the edge of the superconducting wire as a function of the voltage of the reservoirs is shown in Fig. 4. Although there is no net current flowing through the superconductor, at a certain voltage the pair potential collapses. The voltage that is necessary to trigger this transition to the normal state is very close to the transition in Fig. 2 (where we used the two terminal setup). Apparently the influence of f_L is important, since it can cause the superconductor to switch to the normal state irrespective of the value of the supercurrent. Clearly the influence of f_L on the state of the supercon-
The superconductor is larger than the influence of the supercurrent on this same quantity.

The quantity that defines the possible states of the system is the free energy. Evidently the superconductor compares two states for the minimization of this free energy: the first state is the superconducting state in which the free energy remains constant as a function of voltage (and independent of the shape of $f_L$ provided this shape does not change for energies larger than the gap). The second possible state is the normal state. At zero temperature, in the absence of a bias voltage, the difference in free energy between the two states is the condensation energy of the superconductor. When the voltage is increased (but still $eV < \Delta$), the free energy of the superconducting state remains constant while the free energy of the normal state decreases since in that case electrons occupy higher energy states due to the applied voltage.

To illustrate the effect, we calculate explicitly the free energy difference between the superconducting state ($F_S$) and normal state ($F_N$) at zero temperature for a bulk superconductor (analytically) and the T-shaped structure (numerically), as a function of voltage (which appears in $f_L$) and $\Delta$. At zero temperature the free energy of the system reduces to the internal energy (kinetic plus potential) $E$. From the analytical calculation for the bulk following Bardeen [8] we find that $f_L$ changes the free energy in such a way that at $eV = \frac{1}{2}\sqrt{2}\Delta_0$ the superconductor undergoes a first order phase transition. For the voltage range $\frac{1}{2}\Delta_0 < eV < \Delta_0$ the state of the system has two solutions. The free energy difference for the bulk superconductor is shown in Fig. 5. Numerical results for the free energy of the T-shaped geometry are shown as well (both as function of position and as function of voltage). For long wires, the numerical results approach the analytical (bulk) calculation. This indicates that the effect of the bias voltage can indeed be related to the existence of a first order phase transition at zero temperature.

In conclusion, we have studied the role of the energy mode $f_L$ of the quasiparticle distribution on the properties of a superconducting nanowire. We employ a numerical simulation of the Usadel equation in full-response and find a non-thermal distribution for $f_L$ (caused by an applied bias voltage) which drives a first order transition from the superconducting state to the normal state irrespective of the current. A direct calculation on the free energy of a bulk superconductor confirms that the voltage indeed causes the phase transition. In general, the significant role played by $f_L$ found in these superconducting nanowires stresses the importance of treating $f_L$ and $f_T$ on equal footing.

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