SURFACE BOUND STATES IN ANISOTROPIC SUPERCONDUCTORS

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Abstract. The Bogolubov-de Gennes equations for a non-homogenous superconductor are derived. Equilibrium transport properties through an S-I-N junction are calculated. A resonance condition for the Andreev reflection is found and it is shown that the resonances can be understood from quasi-classical bound states localized at the S-I-N interface.

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1. Mean field Hamiltonian

We start from the following field theory describing a non-relativistic, non-locally interacting electron gas in n dimensions[2]:

(1)
$$H = \sum_{\sigma} \int drdr' \{ \psi_\sigma(r)^\dagger H_e(r,r') \psi_\sigma(r') + \frac{1}{2} V(r,r') \left|\psi_\sigma(r)\right|^2 \left|\psi_{\bar{\sigma}}(r')\right|^2 \}$$

The fermionic field operators satisfy the usual commutation relations:

$$\{\psi_\sigma^\dagger(r), \psi_\mu(r')\} = \delta_{\sigma\mu}\delta(r-r') \tag{2a}$$

$$\{\psi_\sigma(r), \psi_\mu(r')\} = 0 \tag{2b}$$

The kinetic energy $H_e(r,r')$ is taken with respect to the Fermi energy. It is a symmetric function and typically of the form

$$H_e(r,r') = H_e(r-r') = \delta(r-r')(\frac{(p-eA)^2}{2m} + U(r) - \epsilon_F) \tag{3}$$

The 2-body interaction potential $V(r,r')$ is symmetric and real.

We are interested in the ground state and low-lying excitations of this Hamiltonian. We do a mean mean-field decoupling of the interaction term, supposing that the ground state is non-magnetic ($H_e = H_e^*$), so that $\langle \psi_\sigma^\dagger \psi_{\bar{\sigma}} \rangle = 0$. Terms of the form $\langle \psi_\sigma^\dagger \psi_\sigma \rangle$ are absorbed in the kinetic energy H_e. The resulting mean-field Hamiltonian is of a generalized BCS form:

(4)
$$H_{MF} = \int drdr' \{ \sum_\sigma \psi_\sigma(r)^\dagger H_e(r,r') \psi_\sigma(r') + \Delta(r,r') \psi_\uparrow^\dagger(r) \psi_\downarrow^\dagger(r') + h.c. \}$$

where $\Delta(r,r') = -V(r,r') \langle \psi_\uparrow(r) \psi_\downarrow(r') \rangle$. Spin-rotational symmetry of the ground state implies $\Delta(r,r') = \Delta(r',r)$.

2. Bogolubov-de Gennes equation

We want to diagonalize the mean field Hamiltonian (4). For this we do the following Bogolubov transformation:

$$\gamma_\sigma^{n\dagger} = \int dr \ \{ u_n(r) \psi_\sigma^\dagger(r) + \sigma v_n(r) \psi_{\bar{\sigma}}(r) \} \tag{5}$$

[2]We omit vector symbols here where it does not lead to confusion; the integrals are taken over a finite region of $\mathbf{R}^n$.

n labels the spectrum, $\sigma = \uparrow, \downarrow$ is the spin of the quasi-particle. We require the new operators γ_σ^n to be fermionic:

$$\{\gamma_\sigma^{n\dagger}, \gamma_\mu^m\} = \delta_{\sigma\mu}\delta^{nm} \tag{6a}$$

$$\{\gamma_\sigma^n, \gamma_\mu^m\} = 0 \tag{6b}$$

Equations (6a) and (6b) imply respectively that the u_n, v_n are orthogonal in the following sense

$$\int dr\ \{u_n(r)u_m^*(r) + v_n(r)v_m^*(r)\} = \delta_{nm} \tag{7a}$$

$$\int dr\ \{u_n(r)v_m(r) - u_m(r)v_n(r)\} = 0 \tag{7b}$$

Finally, from (5) and (6) it follows that

$$\psi_\sigma(r) = \sum_n \{u_n(r)\gamma_\sigma^n - \sigma v_n^*(r)\gamma_{\bar{\sigma}}^{n\dagger}\} \tag{8}$$

The Hamiltonian H_{MF} is diagonal if

$$[\gamma_\sigma^n, H_{MF}] = E_n\gamma_\sigma^n \tag{9}$$

This requirement fixes the Bogolubov functions (u_n, v_n). We calculate the commutator $[\psi_\sigma(r), H_{MF}]$ using (9) and replacing ψ with help of relation (8). On the other hand, the same quantity is calculated using the original expression for H_{MF} (4). The resulting expressions must be equal for all n. They are given by:

$$\begin{aligned} [\psi_\sigma(r), H_{MF}] &= \sum_n [u_n(r)\gamma_\sigma^n - \sigma v_n^*\gamma_{\bar{\sigma}}^{n\dagger}, H_{MF}] \\ &= \sum_n E_n(u_n(r)\gamma_\sigma^n + \sigma v_n^*\gamma_{\bar{\sigma}}^{n\dagger}) \end{aligned} \tag{10a}$$

$$\begin{aligned} [\psi_\sigma(r), H_{MF}] &= \int dr'\ \{H_e(r,r')\psi_\sigma(r') + \sigma\Delta(r,r')\psi_{\bar{\sigma}}^\dagger(r')\} \\ &= \sum_n \int dr'\ [H_e(r,r')u_n(r') + \Delta(r,r')v_n(r')]\gamma_\sigma^n \\ &\quad + \sigma[-H_e(r,r')v_n^*(r') + \Delta(r,r')u_n^*(r')]\gamma_{\bar{\sigma}}^{n\dagger} \end{aligned} \tag{10b}$$

Equating coefficients of γ_σ^n and $\gamma_{\bar{\sigma}}^{n\dagger}$ in (10) results in the space dependent Bogolubov-de Gennes equations:

$$\int dr' \begin{pmatrix} H_e(r,r') & \Delta(r,r') \\ \Delta^*(r',r) & -H_e^*(r',r) \end{pmatrix} \mathbf{\Psi}_n(r') = E_n\mathbf{\Psi}_n(r) \tag{11}$$

where we have used the notation $\mathbf{\Psi}_n = (u_n, v_n)^T$. Time reversal symmetry can be broken in presence of an external magnetic field, in this case $H_e \neq H_e^*$. Since we assume a non-magnetic ground-state, we will set $H_e(r,r') = \delta(r-r')\xi(-i\hbar\nabla)$, $\xi = \xi^*$ in the following. We will also set $\hbar = 1$ from now on.

3. Bulk spectrum, Andreev and Local approximation

In the bulk of a homogenous superconductor, we have

$$\Delta(r,r') = \Delta(r-r') \tag{12}$$

In this case, the Bogloubov-de Gennes equations are diagonalized by plain waves:

$$\mathbf{\Psi}_n(r) = \bar{\mathbf{\Psi}}_{k_n} \exp(ik_n r) \tag{13}$$

Equation (11) is now

$$\begin{pmatrix} \xi(k) & \Delta_k \\ \Delta_k^* & -\xi(k) \end{pmatrix} \bar{\mathbf{\Psi}}_k = E_k \bar{\mathbf{\Psi}}_k \tag{14}$$

where $\Delta_k = \int dr \Delta(r) \exp(-ikr)$. The spectrum is given by:

$$E = E_k \ , \qquad \bar{\mathbf{\Psi}}_k^p = (W_k^+, \eta_k^* W_k^-)^T \tag{15a}$$

$$E = -E_k \ , \qquad \bar{\mathbf{\Psi}}_k^h = (-\eta_k W_k^{-*}, W_k^{+*})^T \tag{15b}$$

where

$$\begin{aligned} E_k &= \sqrt{\xi(k)^2 + |\Delta_k|^2} \\ W_k^\pm &= \sqrt{\frac{1}{2}(1 \pm \frac{\xi(k)}{E_k})} \\ \eta_k &= \frac{\Delta_k}{|\Delta_k|} \end{aligned} \tag{16}$$

In the Andreev approximation[1] we suppose that excitations very close to the Fermi energy are nearly plain waves. In other terms, their fourier expansion is highly peaked around a wave vector lying on the Fermi surface.

$$\mathbf{\Psi}_n(r) \simeq \bar{\mathbf{\Psi}}_{\vec{k}_F}(r) e^{i\vec{k}_F \cdot \vec{r}} \tag{17}$$

where $\bar{\mathbf{\Psi}}_{\vec{k}_F}(r)$ is a slowly varying function on the length scale $1/k_F$.

We expand the kinetic term in (11) around the Fermi wave vector:

$$
\begin{aligned}
e^{-i\vec{k}_F\cdot\vec{r}}\xi(-i\vec{\nabla})\Psi(\vec{r}) &\simeq e^{-i\vec{k}_F\cdot\vec{r}}\xi(-i\,\vec{\nabla})\bar{\Psi}_{\vec{k}_F}(r)e^{i\vec{k}_F\cdot\vec{r}} \\
&\simeq \xi(\,\vec{k}_F - i\vec{\nabla})\bar{\Psi}_{\vec{k}_F}(\vec{r}) \\
&\simeq (\xi(\vec{k}_F) - i\vec{v}_{k_F}\cdot\vec{\nabla} + \ldots)\bar{\Psi}_{\vec{k}_F}(\vec{r}) \\
&\simeq -i\vec{v}_{k_F}\cdot\vec{\nabla}\bar{\Psi}_{\vec{k}_F}(r)
\end{aligned}
\tag{18}
$$

To approximate the integration over the pair potential, we use in addition the local approximation[1]. The local approximation consists in saying that $\bar{\Psi}(r)$ varies negligibly on the coherence length scale $\frac{v_F}{\Delta}$. This allows us to write

$$
\begin{aligned}
&\int dr'\Delta(r,r')\Psi(r')e^{-ik_F r} \\
&\simeq \int dr'\Delta(R-x,R+x)\bar{\Psi}_{k_F}(r-x)e^{ik_F x} \simeq \bar{\Psi}(r)\Delta_{k_F}(R)
\end{aligned}
\tag{19}
$$

where

$$
\begin{aligned}
x &= \frac{r'-r}{2} \\
R &= \frac{r+r'}{2} \\
\Delta_{k_F}(\vec{R}) &= \int d^n x\, \Delta(\vec{R}-\vec{x},\vec{R}+\vec{x})e^{2i\,\vec{k_F}\cdot\vec{x}}
\end{aligned}
\tag{20}
$$

Using these approximations, the BdG equations (11) reduce to

$$
\begin{pmatrix} -i\,\vec{v}_{k_F}\cdot\vec{\nabla} & \Delta_{k_F}(r) \\ \Delta^*_{k_F}(r) & i\,\vec{v}_{k_F}\cdot\vec{\nabla} \end{pmatrix} \bar{\mathbf{\Psi}}_{k_F}(r) = E\bar{\mathbf{\Psi}}_{k_F}(r)
\tag{21}
$$

In the bulk, we recover the exact equations (14). The solutions are of course the same, expanded for small excitations around the Fermi energy.

4. Transport through an N-I-S junction

We consider now an normal metal covered by a thin insulating layer in contact with a superconductor. The interface is perpendicular to the x-axis. The pairing interaction Δ vanishes in the normal metal and takes a constant value in the superconductor. The insulator is modeled by a sharp delta potential.

$$
\Delta_{\vec{k}_F}(\vec{r}) = \Delta_{\vec{k}_F}\Theta(x) \tag{22a}
$$

$$
U(\vec{r}) = V\delta(x) \tag{22b}
$$

The S an N bulk solutions are matched at the interface by the following continuity condition:

$$\bar{\mathbf{\Psi}}_S(0) - \bar{\mathbf{\Psi}}_N(0) = 0 \tag{23a}$$

$$i\, v^x_{\vec{k}_F} (\bar{\mathbf{\Psi}}_S(0) - \bar{\mathbf{\Psi}}_N(0)) = 2V\, \bar{\mathbf{\Psi}}_N(0) \tag{23b}$$

Matching condition (23b) is obtained by integrating the BdG equation (21) along the x axis from $-\epsilon$ to ϵ and letting $\epsilon \to 0$. We must be careful to use the correct sign for the Fermi velocity around which we approximate the different N and S excitations.

We use the following superposition of excitations at a given energy E. In the normal metal we have:

$$\mathbf{\Psi}_N = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i\,(\vec{r}\cdot\vec{k}_{F+} + x\, q_+)} + \begin{pmatrix} 0 \\ a \end{pmatrix} e^{i\,(\vec{r}\cdot\vec{k}_{F+} + x\, q_-)} + \begin{pmatrix} b \\ 0 \end{pmatrix} e^{i\,(\vec{r}\cdot\vec{k}_{F-} + x\, q_-)} \tag{24}$$

$\vec{k}_{F+}$ is an arbitrary (incident) vector on the Fermi surface and $\vec{k}_{F-} = \vec{k}_{F+} - 2\hat{x} \cdot \vec{k}_{F+}$ is the normally reflected wave vector. An electron is incident at a wave vector $\vec{k}_{F+} + \vec{q}_+$, while there is an Andreev reflected hole with wave vector $\vec{k}_{F+} + \vec{q}_-$ and an ordinarily reflected electron with $\vec{k}_{F-} + \vec{q}_-$. We suppose that there is no incident hole in the normal metal.

We only take particle-like excitations with positive group velocity in the superconductor (only transmitted, no incident particles):

$$\mathbf{\Psi}_S = c \begin{pmatrix} W^+_+ \\ \eta^*_+ W^-_+ \end{pmatrix} e^{i\,(\vec{r}\cdot\vec{k}_{F+} + x\, k_+)} + d \begin{pmatrix} \eta_- W^-_- \\ W^+_- \end{pmatrix} e^{i\,(\vec{r}\cdot\vec{k}_{F-} + x\, k_+)} \tag{25}$$

The coefficients W and η are the positive energy solutions to the Bogolubov equations given in (16). The subscript denotes the Fermi vector around which we develop the BdG equations, $\pm$ meaning $\vec{k}_{F\pm}$.

The excitations are small with respect to k_F. They are given by:

$$\begin{aligned} q_\pm &= \pm \frac{E}{|v^x_{k_F}|} \\ k_\pm &= \pm \frac{\sqrt{E^2 - |\Delta_{k_{F\pm}}|^2}}{|v^x_{k_F}|} \end{aligned} \tag{26}$$

Their direction is along the x-axis.

These excitations represent are all possible processes at given energy E respecting the translational invariance parallel to the interface.[3]

[3] In fact, I don't quite understand why we don't take transmitted anti-cooper pairs. Probably because we suppose that a large fraction of electrons is still in the Fermi sea and we cannot create Bogolubov particles there.

The matching conditions (23) produce the following 4 equations which we can solve for the transmission and reflection coefficients a, b, c and d.

$$\begin{aligned} 1+b &= c\,W_+^+ + d\,\eta_- W_-^- \\ a &= c\,\eta_+^* W_+^- + d\,W_-^+ \\ 1-b &= c\,W_+^+ - d\,\eta_- W_-^- + 2iZ\,(1+b) \\ a &= c\,\eta_+^* W_+^- - d\,W_-^+ + 2iZ\,a \end{aligned} \tag{27}$$

Where the barrier strength Z is given by:

$$Z = \frac{V}{|v_{k_F}^x|}$$

The solution for the scattering coefficients is:

$$\begin{aligned} a(E) &= \frac{\eta_+^* W_+^- W_-^+}{W_+^+ W_-^+ + Z^2\,\Gamma} \\ b(E) &= \frac{-Z(Z+i)\,\Gamma}{W_+^+ W_-^+ + Z^2\,\Gamma} \\ c(E) &= \frac{W_-^+(1-iZ)}{W_+^+ W_-^+ + Z^2\,\Gamma} \\ d(E) &= \frac{iZ\,\eta_+^* W_+^-}{W_+^+ W_-^+ + Z^2\,\Gamma} \end{aligned} \tag{28}$$

where

$$\Gamma = W_+^+ W_-^+ - \eta_+^* \eta_- W_+^- W_-^-$$

4.1. **Quasi-particle current conservation.** The current conservation is slightly subtle and often wrongly stated in the literature. A good review discussing the currents in detail was given by Kashiwaya [6].

On one hand, the global phase invariance of the original Hamiltonian (1) implies a conserved electric current[4]. On the other hand, the diagonalized mean field Hamiltonian (4) implies the conservation of the quasi-particle excitation number. The latter is considered in the following. The single particle excitation $\mathbf{\Psi} = (u(r), v(r))^T$ carries the QP-current [6]:

$$J_q^x(r) = \mathrm{Im}(u^*(r)\partial_x u(r) - v^*(r)\partial_x v(r)) \tag{29}$$

[4]The conventional electric current conservation is of course broken in the superconductor. It is only conserved up to a source term coming from QP supercurrent.

The quasi-particle current is equal on both sides of the interface. This implies:

$$|a|^2 + |b|^2 + \mathrm{Re}(\frac{k^+}{q^+})(|c|^2 + |d|^2) = 1 \tag{30}$$

For sub-gap energies, k^+ is completely imaginary and the QP-current in the superconductor vanishes.[5]

5. Reflection resonances

We are interested in resonances in the Andreev reflected holes. It is clear from the current conservation relation (30) that $|a|$ is maximal in the sub-gap region ($E < |\Delta_{k_F}|$) where $k^\pm$ are purely imaginary. It is furthermore clear from (28) and (30) that the reflection peaks in the sub-gap region are given by $b = 0$ or equivalently $\Gamma = 0$. In this case $|a| = 1$ and all electrons are Andreev reflected. Thus, we get the resonance condition for complete Andreev reflection:

$$\Gamma(E) = 0 \tag{31}$$

This resonance condition can be written as:

$$W_+^+ W_-^+ = \eta_+^* \eta_- W_+^- W_-^- \tag{32}$$

The norm as well as the phase of the complex numbers on right and left hand side must be the equal. The condition on the norm is always fulfilled in the sub-gap region. The condition on the phase is:

$$-\phi_+ + \phi_- + \arg\left(\frac{W_+^-}{W_+^+}\right) + \arg\left(\frac{W_-^-}{W_-^+}\right) = 2\pi n \tag{33}$$

This equation may have several sub-gap resonance solutions E_n^{res}. We do not dwell on solving them here.

6. Surface bound states

We know from scattering theory that resonances in scattering states always indicate the existence of bound states. We will see in the following that this is indeed the case here: there exists bound states localized on the S-I-N interface which have exactly the resonance energies, at least at the semiclassical level.

Consider a thin layer of normal metal in contact with a superconductor. The layer has thickness d_N. It is covered by a "mirror" which specularly reflects incident electrons or holes.

[5]Not so the electric current, but this is out of scope of this work. See [6] for details.

Suppose an electron incident on the superconductor at a sub-gap energy with the wave vector $\vec{k}_{F+}$. The electron is fully Andreev reflected as a hole. The hole is then specularly reflected at an infinite potential step and again incident on the superconductor with a wave vector $\vec{k}_{F-}$, where it is Andreev reflected back as an electron. This process lies on a closed path and its spectrum can be found in the semiclassical approximation by the Bohr-Sommerfeld quantization rule:

$$\delta\Phi = (2n+1)\,\pi \tag{34}$$

where $\delta\Phi$ is the total phase the particle acquires during a closed trajectory and n is integer. The phase change during the Andreev $e \longrightarrow h$ reflection is given by the phase of coefficient $a(E)$ in (28):

$$\Phi_{e\rightarrow h} = -\phi_+ + \arg\left(\frac{W_+^-}{W_+^+}\right)$$

At the specular reflection, the wave acquires the phase π. To calculate the Andreev reflection coefficient for the $h \longrightarrow e$ process, we note that we first need to exchange $\vec{k}_{F+} \leftrightarrow \vec{k}_{F-}$ in the excitations (24) and (25). To have again the same expressions, we further need to replace $k^+ \leftrightarrow k^-$. This amounts in changing all sub- and superscripts $\pm \leftrightarrow \mp$ of W and η in the scattering coefficients (28). The phase of the Andreev reflected electron is given by a^{-1}:

$$\Phi_{h\rightarrow e} = \phi_- + \arg\left(\frac{W_-^-}{W_-^+}\right)$$

During the propagation in the normal metal, the wave acquires the phase

$$\Phi = 4d_N q^+$$

Finally, the total phase shift is given by

$$\delta\Phi = -\phi_+ + \arg\left(\frac{W_+^-}{W_+^+}\right) + \pi + \phi_- + \arg\left(\frac{W_-^-}{W_-^+}\right) + 4d_N q^+ \tag{35}$$

Setting the layer thickness d_N to zero, we see that the Bohr-Sommerfeld quantization condition for the surface bound states is the same as the resonance condition in the sub-gap region (33):

$$\delta\Phi = -\phi_+ + \phi_- + \arg\left(\frac{W_+^-}{W_+^+}\right) + \arg\left(\frac{W_-^-}{W_-^+}\right) = 2n\,\pi \tag{36}$$

We have thus shown that the Andreev resonances correspond to semiclassical bound states living on the S-I-N surface.

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