Point-contact tunneling involving low-dimensional spin-triplet superconductors

C. J. Bolech and T. Giamarchi
Université de Genève, DPMC, 24 Quai Ernest Ansermet, CH-1211 Genève 4, Switzerland
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We modify and extend previous microscopic calculations of tunneling in superconducting junctions based on a non-equilibrium Green function formalism to include the case of spin-triplet pairing. We show that distinctive features are present in the I-V characteristics of different kinds of junctions, in particular when the effects of magnetic fields are taken into account, that permit to identify the type of pairing. We discuss the relevance of these results in the context of quasi one-dimensional organic superconductors like (TMTSF)$_2$PF$_6$ and layered compounds like Sr$_2$RuO$_4$.

Unconventional superconductivity is a generic classification for all those superconducting materials that do not fit into the s-wave spin-singlet pairing picture of standard BCS theory.[1] One of the possible extensions of that theory considers anisotropic pairing mechanisms accompanied by spin-triplet states. One such unconventional scenario is realized in the p-wave spin-triplet superfluid state of $^3$He. Among the superconductors the appearance of unconventional superconductivity, always accompanied by strong correlations, results in most cases in spin-singlet pairing. The search for triplet pairing superconductivity in strongly correlated electron systems becomes thus natural. It was proposed[2], for instance, in the case of Sr$_2$RuO$_4$ and has to date a considerable amount of experimental support.[3] This compound shows, in common with the high-$T_c$ cuprates, a layered structure. Other candidates for triplet pairing, though the evidence is less conclusive, are in the class of so called organic superconductors[4] like f.i. (TMTSF)$_2$X, with X a counter anion as PF$_6$, ClO$_4$, etc. Materials of this class are low-dimensional conductors in their normal state.

A distinctive feature of triplet superconductors is the possibility of large upper critical fields; this is contrary to BCS superconductors for which the paramagnetic response of the normal state puts a limit to the field up to which the superconducting phase is energetically favorable even in the absence of orbital effects (the Clogston or BCS Pauli paramagnetic limit, $H_p$). It was indeed observed during the last few years that at low temperatures the above mentioned organic compounds show upper critical fields that exceed $H_m$, usually depending on the angular orientation of the field with respect to the crystaline axes.[4] In general, for layered and chained compounds, superconductivity at high fields is attained when the field is oriented so that orbital effects are suppressed. Although high critical fields constitute an indication of triplet-pairing, unambiguous interpretation of this effect is difficult because one needs to rule out other possible phases able to accommodate large magnetic fields (e.g. the Larkin-Ovchinikov–Fulde-Ferrel phase).[5]

It would be highly desirable to have a direct indication of the nature of the pairing, as in the case of cuprates. A possible experimental determination of the symmetry of the pairing could come from tunneling experiments. In the past some of the most crucial experimental verifications of BCS theory came from tunneling experiments; and, after the discovery of the Josephson effect, some of the most important practical applications of superconductivity involve tunneling junctions. In addition, tunneling per se acquired renewed relevance with the development of scanning tunneling microscopy (STM), actively used nowadays in the study of superconductivity. The simplest theoretical models used to interpret tunneling experiments in superconductors are those that go under the name of semiconducting band models[6, 7]. A more systematic approach is that based on tunneling Hamiltonians[8, 9, 10]. Two limiting cases are usually considered in the calculations: planar interfaces and point contacts (the latter usually realized in experiments using break junctions, pressed crossed wires or close STM contacts).

In this letter we focus our attention on the point-contact case. We extend previous tunneling Hamiltonian calculations to include the case of triplet-pairing superconductors. As compared to previous calculations, we simplify considerably the formalism making it more versatile and easy to implement. Our aim is to explore the possible use of tunneling experiments as a way of characterizing the type of pairing in unconventional superconductors. Using non-equilibrium Keldysh Green functions we calculate the full current-voltage characteristics of different types of tunnel junctions mixing normal metals, singlet and triplet superconductors. We also study the effects of applied external magnetic fields on the transport properties of the different junctions.

Our starting point is the tunneling Hamiltonian,

$$H_{jun} = H_1 + H_2 + H_{tun}$$

$$H_{tun} = -t \sum_{\sigma} \left[ \psi_{2,\sigma}^\dagger (x = 0) \psi_{1,\sigma} (x = 0) + h.c. \right]$$

The first two terms describe the two leads (superconducting or otherwise) and the third one models the tunneling processes in which an electron with spin $\sigma$ hops from one lead into the other. The current is proportional to the rate of change in the relative particle number, $I = \frac{e}{2} \langle t \frac{\partial}{\partial t} (N_2 - N_1) \rangle = \frac{e}{2} \langle [H_{tun}, N_1 - N_2] \rangle$.

To model the leads in calculations of point-contact transport on conventional superconductors, simple mod-
els suffice to achieve quantitative agreement with the experiment. Since dimensionality plays no role in the tunneling, contrary to the case in some planar junction experiments, all the standard calculations can be formulated using one-dimensional leads. The situation is more complex for unconventional superconductors, for which, the anisotropic nature of the pairing has to be taken into account. However, the ruthenates and organic superconductors are deemed to have $p$-wave symmetry, and since both $s$-wave and $p$-wave symmetries can be modeled in a one dimensional chain, we can set up a formalism that comprises both cases. We consider a one dimensional band with two Fermi points and expand the fermion fields around them defining left ($L$) and right ($R$) moving fields. Using these fields, and in the spirit of BCS theory, we introduce the four gap functions:

$$
\Delta_n(x) \propto \left\langle \alpha \psi_{L,\alpha}^\dagger(x) \sigma}_{\alpha,\beta}^n \psi_{R,\beta}^\dagger(x) \right\rangle
$$

(2)

where $\alpha, \beta \in \{\uparrow, \downarrow\}$ ($\uparrow \equiv (-1, +1)$ are summed over ($\uparrow \equiv -\alpha$); $a = 0, \ldots, 3$; $\alpha^0_{\alpha,\beta}$ is the identity matrix while the other three are the usual Pauli matrices. With this definition $\Delta_0(x)$ is the conventional spin-singlet order parameter and the other three gap functions form a vector of spin-triplet order parameters $\Delta = \Delta(x) \mathbf{d}(x)$. Approximating the order parameter to have no spatial dependence, we write in Fourier space

$$
K_n = \xi_{ck\alpha}^n \psi_{ck\alpha}^\dagger \psi_{ck\alpha} - \left[ \Delta_0 \left( \psi_{R,\beta}^\dagger \sigma_{\beta,\alpha}^2 \alpha \psi_{L,\alpha}^\dagger \right) + \mathrm{h.c.} \right]
$$

where $K_n = H_n - \mu_n N_n$ with $\mu_n$ the chemical potential of lead $n$. All the indexes are summed over, in particular $c \in \{L, R\}$ ($\equiv (-1, +1)$ sums over the two possible chiralities and $\xi_{ck\alpha}^n = ck - \mu_n - ah$ are the corresponding linear dispersions, shifted by the inclusion of chemical potential and magnetic field along the $\hat{z}$-axis. We take the quantization axis ($\hat{z}$) along the field direction and consider the cases of triplet order parameters parallel or perpendicular to it.

Since we are dealing with an out of equilibrium phenomenon, we use Keldysh formalism to treat the tunneling term to all orders, calculating the full I-V line and giving a quantitative account of its subgap structure. One past implementation of such an approach, for the $s$-wave case, reduced the problem to the solution of a set of linear recursion relations. Here, instead, we notice that in this formalism the current becomes

$$
I = \frac{e \ell}{2i} \sum_\sigma \int \frac{d\omega}{2\pi} \left\langle \psi_{2,\sigma}^\dagger \psi_{1,\sigma} - \psi_{1,\sigma}^\dagger \psi_{2,\sigma} \right\rangle_{\mathrm{kel}}
$$

(3)

where ‘kel’ denotes the Keldysh component of the correlation function and the $\psi$ stand for $\psi(\omega, x = 0)$. Since the current depends only on the fields at $x = 0$ one can analytically integrate the $x$ dependence in the leads to obtain from Eq. a local and quadratic Keldysh action for the fields at $x = 0$: $S_{\text{full}} = S_1 + S_2 + S_{\text{tun}}$. Here $S_{\text{full}}$ is obtained from $H_{\text{full}}$ and $S_n$ is the local action of lead $n$, of the form $S_n = \int \frac{d\omega}{2\pi} \sum_{\alpha} \Psi_n^\dagger(\omega) \tilde{g}^{-1} \Psi_n(\omega)$. Where $\Psi_n$ is an $8$ component spinor (a Keldysh extended Nambu-Eliashberg spinor), and $\tilde{g}^{-1}$ is a matrix whose components can be computed from $K_n$. Its inverse ($\tilde{g}$) is given by the standard advanced, retarded and Keldysh components of the local Green functions of the lead. As an example we give the expressions for the case when $\Delta_1 = \Delta_2 = 0$,

$$
\text{g}_{\sigma,\sigma'}^{\text{ret,adv}} = \frac{-(\omega - \mu_n + c\sigma h \pm i0^+)}{2\sqrt{\Delta_0 + c\sigma \Delta_3}|_{\mu_n = L}^{|\mu_n = R|}^2} - (\omega - \mu_n + c\sigma h \pm i0^+)^2}
$$

The notation in the numerator of the anomalous functions means that complex conjugation is in order when $c = L$. The Keldysh component is obtained immediately as $g^{\text{kel}}_{\sigma,\sigma'} = (g^{\text{ret}} - g^{\text{adv}}) \tanh (\omega - \mu_n)/2T$.

Since the action is quadratic, it can be diagonalized which allows to compute the current from $\Psi$. For normal leads this can be done analytically. However, for superconducting leads, special attention must be paid to the fact that frequencies have different reference Fermi levels in each lead when there is a bias applied. Within each lead, frequencies with equal positive and negative shifts from the Fermi level form part of the same spinor element and the corresponding states are related by the coherent pairing processes in the superconductors; across leads, same frequency states are related by the tunneling matrix elements of the action. As a result, the full action for the junction is no longer frequency diagonal. However, since it is quadratic it can still be written explicitly as a matrix. To each value ($\omega$) in the frequency window (of size $eV = \mu_1 - \mu_2$) defined by the chemical potentials in the two leads, one infinite set of related frequencies can thus be assigned ($p > 0$):

$$
\begin{align*}
\omega_p &= 2\mu_2 - p \mod 2 - \omega_{p-1} \\
\omega_{-p} &= 2\mu_1 + p \mod 2 - \omega_{1-p}
\end{align*}
$$

(4)

These sets are all independent and the action is block diagonal between different ones. Discretizing the frequencies in this window, automatically defines a discretization of the whole frequency axis. This allows for a numerical solution of the problem: we deal with one set of frequencies at a time, and since the sets are infinite, we truncate their hierarchy at some distance from the central frequency window. This is equivalent to introducing a soft limit in the number of allowed Andreev reflections ($N_A$). We can then numerically invert the corresponding block-diagonal action, written as a matrix in frequency space. The off-diagonal Green function matrix elements thus obtained allow to compute the current using Eq. $\Psi$.

The practical implementation of this approach is quite simple and allows to consider the (combined) effects of
finite temperature, applied magnetic fields, contact potentials in the junction, spin-flip tunneling or spin-flip scattering processes in the leads. It is also possible to compute the a.c. response. Our interest is in comparing singlet and triplet superconductor junctions and how they respond differently in the presence of an external field; we will ignore other additional complications.

In order to illustrate the different I-V characteristics for different types of junctions, we fix a set of parameters. We take $t = 0.2$ for the tunneling overlap integral, and when there is a magnetic field we fix its value to $h = 0.2$ in units of $\Delta$ (the magnitude of the singlet gap, $\Delta_0$, or of the triplet vector order parameter depending on the case). All the curves we show are for the d.c. response in the limit of vanishing temperatures. For the truncation procedure we take $N_A = 3$ (and verify that larger values produce identical curves). Let us use the notation, N: normal-metal, S: singlet-superconductor and T: triplet-superconductor. We show in Fig. 1-(a) typical curves for an N-S junction. The effect of the field (for any orientation) is to produce what would be seen as a Zeeman splitting in the differential conductance peak. Notice the sub-gap shoulder on the I-V curve when $eV < \Delta$ (for $h = 0$); its origin is in the coherent Andreev processes that take place in the junction contact.

We show in Fig. 1-(b) typical curves for an N-T junction. The solid line corresponds to zero field and the dashed line is for that same junction but in the presence of a field that is aligned with the vector order parameter. If one considers a field perpendicular to the order parameter ($\vec{h} \perp \hat{d}$), the I-V characteristic remains unaffected, i.e. identical to the one for zero field. Notice the absence of a sub-gap shoulder on the I-V curve, a result of the odd real-space symmetry of the superconductor probed locally by an ideal point-contact junction. Given the model we consider, these results would be relevant for tunneling experiments into a sample edge parallel to the chains, when a zero-bias peak is not expected [12][29].

Let us now examine the case of S-T junctions, see Fig. 1-(c). One dotted line is the N-N characteristic as in the other cases; the other is the I-V curve of an S-S junction that shows all the features well known in the literature in particular a ‘sub-gap’ shoulder with Andreev steps at $eV = 2\Delta/n$ (with $n = 1, 2, \ldots$). This curve is, bar orbital effects, not sensitive to applied fields. The solid line is always the same regardless of the orientation of the vector order parameter on the triplet-pairing side and the current amplitude is systematically smaller than in the S-S case. Distinctively, the ‘sub-gap’ structure shows only the first two steps and the current becomes zero for $eV < \Delta$. Regarding the effect of an applied field, the curve remains unchanged if the field is parallel to the vector-order-parameter direction, but shows a Zeeman effect if the field is perpendicular to it (dashed line). This is to be confronted with the N-T case where the splitting accompanies a field $\vec{h} \parallel \hat{d}$.

Let us make contact with the experimental situation on the different compounds afore mentioned, and dwell first on the particularly interesting case of (TMTSF)$_2$PF$_6$. This quasi-one-dimensional organic compound shows the largest deviations from the $H_p$ limit among the different members of the Bechgaard salts family, and also as compared with other organic superconducting salts [13]. A recent series of experiments focused on measuring $H_{c2}(T)$ for this material [13][14][15][16][17]. The observed large deviations from the $H_p$ limit as well as the anisotropy and angular dependence of the upper critical field make the case for an equal-spin triplet-pairing superconducting phase with an order parameter oriented mainly along the chains [18]. Other evidences for spin-triplet pairing in (TMTSF)$_2$PF$_6$ also exist, but as with the $H_{c2}$ measurements, most of these experiments do not probe the spin parity directly and their conclusions are difficult to interpret due to the uncertainties regarding the orbital symmetry of the superconductor phase; however, recent NMR Knight Shift measurements add strong support to the spin-triplet scenario [13]. Here we argue that the magnetic field response in N-T point-contact tunneling experiments would also constitute a direct probe of the spin-pairing symmetry (in contrast with tunneling
across planar junctions that is sensitive to the orbital-pairing symmetry. $H_{c2}$ measurements show that for magnetic fields along the direction of the conducting chains (a-axis) the upper critical field is paramagnetically limited. This corresponds, in our convention, to a vector order parameter aligned with the field ($\hat{b} \parallel \hat{d}$). In this case a Zeeman splitting of the differential conductance peak, similar to that in conventional superconductors (N-S junctions), should be observed. As the field is rotated, the splitting would be suppressed and for a magnetic field oriented parallel to the b' axis there would be no Zeeman effect (accompanied by the possibility of applying large fields that are not paramagnetically limited). The disappearance of splitting even as the field is being increased would constitute a clear signature of spin-triplet superconductivity.

As in the case of N-T junctions, we can envisage using the Zeeman response of S-T junctions as a direct probe for spin-triplet order. If for instance, a field is applied along the b' axis of (TMTSF)$_2$PF$_6$, we predict a Zeeman splitting of the main differential conductance peak. This would constitute a clear sign of unconventional superconductivity since such an effect does not take place for standard BCS superconductors (S-S junctions). The b' direction is the one on which the upper critical field is not paramagnetically limited, so relatively large fields could be applied in order to obtain a clear signal.

Our considerations could be extended to the case of the layered compounds believed to be triplet superconductors. Among them, Sr$_2$RuO$_4$ is the best studied so far, but only few tunneling experiments were performed, and none so far with good resolution in the presence of an applied external magnetic field to observe Zeeman effects. One of the conspicuous features observed in some of these experiments is the presence of a zero-bias anomaly in the differential conductance. Its explanation is still a matter of debate, but seems to require extended contacts and sign changing order parameters. To include the effect of 'zero energy states' at the interfaces would require extensions to our scheme, possibly incorporating certain aspects of those calculations already done for planar junctions. Our general findings about the effect of magnetic fields should however apply, since they refer to features to be measured at voltages of the order of the superconducting gap.

Summarizing, the point-contact tunneling involving unconventional superconductors with spin-triplet pairing displays interesting characteristic features. In particular the Zeeman response to an external magnetic field is such that it may allow for the identification of triplet phases and might be relevant for future experiments. The prediction of a truncated sub-gap structure in S-T junctions is also very interesting. For future extensions of this work, different effects (finite temperature, contact potentials in the junction, spin-flip tunneling, etc.) can be easily incorporated to our calculations.

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