Kondo screening in unconventional superconductors: The role of anomalous propagators

Lars Fritz and Matthias Vojta
Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany
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The Kondo effect in superconductors is frequently investigated using the local quasiparticle density of states as sole bath characteristics, i.e., the presence of anomalous propagators is ignored. Here we point out that this treatment is exact for a number of situations, including point-like impurities in d-wave superconductors. We comment on recent investigations [M. Matsumoto and M. Koga, J. Phys. Soc. Jpn. 70, 2860 (2001) and Phys. Rev. B 65, 024508 (2002)] which reached different conclusions: while their numerical results are likely correct, their interpretation in terms of two-channel Kondo physics and an “orbital effect of Cooper pairs” is incorrect.

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The physics of quantum impurity moments in superconductors, associated with the Kondo effect, has been subject of numerous investigations in recent years. Diverse theoretical techniques have been employed to study Kondo or Anderson models in a superconducting environment [1–9]. Most of these studies effectively neglect the presence of superconducting (sc) fluctuations in the host, i.e., they use the local fermionic density of states (DOS) as the only input quantity characterizing the environment of the Kondo impurity. For s-wave superconductors it has been shown [1] that this approximation is not justified: here the properties of a Kondo impurity are different from the ones of an impurity embedded in a non-superconducting system with the same DOS. More precisely, the superconducting bath turns out to be equivalent to a non-superconducting bath with additional particle-hole (p-h) asymmetry [1]. As a result, for a p-h symmetric conduction band a screened singlet state is realized at large Kondo coupling, in contrast to the non-sc case with a hard gap in the local DOS [11]. This difference can be understood as caused by the anomalous bath propagators.

In this Brief Report, we address the role of anomalous propagators in unconventional superconductors. We argue below that neglecting sc propagators is exact in many, potentially experimentally relevant, cases, e.g., for point-like impurities in d-wave and unitary p-wave superconductors. In these situations, the dynamics of the impurity degrees of freedom can be calculated using the normal bath propagators only. We also comment on recent papers by Matsumoto and Koga who argued in favor of a non-trivial “orbital effect of Cooper pairs” for point-like impurities in both p + ip and d + id superconductors [7, 8]. While we believe that their numerical results are correct, we point out that such an orbital effect does not exist: in their situation the impurity properties are exclusively determined by the local DOS.

We start from the action of an Anderson impurity in a general interacting host.

\[ S = \frac{1}{\beta N} \sum_{\omega_n} \sum_{k \sigma} \bar{c}_{k \sigma}(i \omega_n) \left[ -i \omega_n + \epsilon_k \right] c_{k \sigma}(i \omega_n) \]

(1)

\[ + S_{\text{int}}(\bar{c}, c) + S_{\text{loc}}(f_\sigma) + \int_0^\beta d\tau \sum_{\{i\} \sigma} \left( V_i \bar{f}_\sigma c_{i \sigma} + c.c. \right) \]

where \( \beta = 1/T \) is the inverse temperature, \( c \) are the conduction electrons with dispersion \( \epsilon_k \) on a regular lattice with \( N \) sites, \( S_{\text{int}} \) are the interactions within the conduction band, and \( S_{\text{loc}} \) describes the \( f \) electron impurity orbital with on-site energy and repulsion. The sum \( \sum_{\{i\}} \) runs over a set of lattice sites in the vicinity of the impurity, and \( V_i \) is the hybridization matrix element; for a point-like impurity only a single \( V_i \) is non-zero. We can define a linear combination \( c_0 \) of conduction electron operators to which the impurity couples: \( V_{0 \sigma} = \sum_{\{i\}} V_i c_{i \sigma} \) with \( |c_0, c_0\rangle = 1 \). After decoupling of \( S_{\text{int}} \) and a suitable saddle-point approximation of BCS type, all conduction electrons except \( c_0 \) can be integrated out. (After the BCS approximation, the remaining integral is Gaussian and can be performed exactly.) To simplify notation we will restrict ourselves to BCS singlet pairing; the arguments apply similarly to unitary triplet states, whereas non-unitary triplet states require an additional coupling between the impurity and the condensate spin moment. Introducing a Nambu spinor \( \Psi_0 = (c_{0 \uparrow}, c_{0 \downarrow}^\dagger) \) we obtain an action of the form:

\[ S = -\frac{1}{\beta} \sum_{\omega_n} \bar{\Psi}_0(i \omega_n) G_0^{-1}(i \omega_n) \Psi_0(i \omega_n) \]

(2)

\[ + S_{\text{loc}}(f_\sigma) + \int d\tau (\bar{V} \bar{f}_\sigma c_{0 \sigma} + c.c.) \]

Here, \( G_0(i \omega_n) \) is the local conduction electron Green’s function at the impurity location. In principle, a treatment of \( S_{\text{int}} \) beyond mean-field also generates a retarded self-interaction for the \( c_0 \). As we are mainly interested in a BCS-type host we will neglect this here. Then, the
properties of the bath are completely contained in \( G_0 \).

Explicitly we have

\[
G_0(i\omega_n) = \sum_k \begin{pmatrix} \frac{h_k^2}{\Delta_k} & h_k^2 \Delta_k \\ \frac{h_k^2}{\Delta_k} & \frac{h_k^2}{\Delta_k} \end{pmatrix}^{-1}
\]

(3)

where \( \Delta_k \) is the complex gap function, and the function \( h_k \) contains the geometry of the impurity coupling to the host:

\[
h_k = \sum_i \epsilon e^{i k R_i} V_i / V.
\]

(4)

For a point-like impurity \( h_k = 1 \), and the anomalous (off-diagonal) part of \( G_0 \) is given by \( G_0^\text{a}(i\omega_n) = \sum_k \Delta_k / D_k \) (with \( D_k = \omega_n^2 + \epsilon_k^2 + |\Delta_k|^2 \)), which vanishes for unconventional superconductors with inversion symmetry and Cooper pair angular momentum \( l > 0 \), i.e., \( p \)-wave, \( d \)-wave or higher symmetries. (This also applies to \( p_x + ip_y \) or \( d_{x^2-y^2} + id_{xy} \) pairing states, but not necessarily to \( d + is \) states.) Then, only the diagonal part of \( G_0 \) enters the impurity action (2), which is completely determined by the local DOS. For a spatially extended impurity hybridized with more than one site the anomalous piece of \( G_0 \) is given by \( \sum_k h_k^2 \Delta_k / D_k \) which still vanishes for some important situations: Consider a \( d \)-wave superconductor, \( \Delta_k = \Delta_0 (\cos k_x - \cos k_y) \), and an impurity hybridized e.g. with four sites as in Figs. 1a,b,c. In all cases the average over \( h_k^2 \Delta_k / D_k \) vanishes for symmetry reasons.

At this point a brief comment on the experimental situation is in order. Point-like impurities can be realized in layered superconductors with out-of-plane impurity moments coupling to a single conduction electron orbital only. In contrast, in-plane impurities will typically couple to a number of sites, see Fig. 1. The signs of the various hybridization matrix elements depend on the involved orbitals of both impurity and host atoms. We note that the situations in Figs. 1b,c,e were used in Refs. 4, 5 to model the magnetic moment induced by a Zn impurity in a high-temperature superconductor. (There, a Kondo model for a spatially extended impurity was employed, leading to multiple screening channels. In addition, the situation for Zn is complicated by the fact that Zn, having a filled d shell, acts as a vacancy, but induces a magnetic moment in its vicinity – for details see Ref. 5.)

Returning to the models discussion – what about the behavior of a spatially extended Anderson impurity, where \( G_0^\text{a} \) does not vanish? Formally, we still have a single-channel model (2), but now in the presence of both a normal and an anomalous bath – this is similar to a point-like impurity in a \( s \)-wave superconductor. As explained in Refs. 1, 12 the main effect of the anomalous bath can be understood as a transverse charge pseudospin field which induces an additional particle-hole asymmetry.

So far we have discussed Anderson impurity models. For a single-site impurity the above discussion applies identically to a Kondo model (via Schrieffer-Wolff transformation). Multichannel physics arises only in a spatially extended Kondo impurity model (independent of anomalous propagators), see Refs. 5, 13.

Now we comment on recent papers by Matsumoto and

FIG. 1: Spatially extended impurities for which the anomalous propagator in \( G_0 \) drops out, i.e., \( \sum_k h_k^2 \Delta_k / D_k = 0 \), for a square-lattice \( d \)-wave superconductor. The dot represents the impurity orbital, the dashed lines show the non-zero hybridization paths (in the notation of an Anderson model). The situations b) and c) correspond to the s-wave and d-wave linear combinations, i.e., screening channels, of the four host sites, which occur in a Kondo model for a spatially extended impurity, as discussed in Ref. 5.

FIG. 2: Numerical results for the local susceptibility, obtained from a single-band NRG for a (semiconducting) bath with the hard-gap DOS of a \( d + id \) (or \( p + ip \)) superconductor. The host bandwidth is unity, the NRG parameters are \( \Lambda = 3 \) and \( N_z = 1000 \). a) \( T_{\text{K,loc}} \) for different gap values \( \Delta = 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5} \) (from top to bottom) where the Kondo temperature \( T_K \) of the model at \( \Delta = 0 \) is \( 3 \times 10^{-3} \). b) The value of the local Curie constant \( C \), normalized to its free-spin value 1/4, as a function of the ratio \( T_K / \Delta \). Different symbols correspond to different values of \( \Delta \). (Deviations from a single universal curve are primarily due to NRG discretization effects.) The results can be compared with Fig. 4 of Ref. 8.
Koga [7, 8] about a non-trivial “orbital effect of Cooper pairs” on the dynamics of point-like impurities in \( p + i p \) and \( d + i d \) superconductors. They argue that, although the impurity only couples to the \( s \)-wave channel of the conduction band, the \( l \neq 0 \) Cooper pairs mediate an indirect coupling to higher angular momentum channels, leading eventually to a multichannel Kondo problem. For the cases of \( p + i p \) and \( d + i d \) pairing, in contrast to the

\[
\sum_k \hbar^2 \Delta_k / D_k = 0 \quad (4)
\]

– this is e.g. the case for point-like impurities and a vanishing local superconducting order parameter. Under these conditions, using only the local density of states as bath input quantity for impurity calculations, as done in Refs. 4, 5, is exact.

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