

Kondo screening in unconventional superconductors: The role of anomalous propagators

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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 pointlike impurities in d -wave superconductors. We comment on recent investigations [M. Matsumoto and M. Koga, J. Phys. Soc. Jpn. **70**, 2860 (2001); 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 the 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 shown¹ that this approximation is not justified: here the properties of a Kondo impurity are different from the ones of an impurity embedded in a nonsuperconducting system with the same DOS. More precisely, the superconducting bath turns out to be equivalent to a nonsuperconducting 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 pointlike 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 nontrivial “orbital effect of Cooper pairs” for pointlike 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:

$$S = \frac{1}{\beta N} \sum_{\omega_n} \sum_{k\sigma} \bar{c}_{k\sigma}(i\omega_n) [-i\omega_n + \epsilon_k] c_{k\sigma}(i\omega_n) + S_{\text{int}}(\bar{c}, c) + S_{\text{loc}}(f_\sigma) + \int_0^\beta d\tau \sum_{\{i\}\sigma} (V_i \bar{f}_\sigma c_{i\sigma} + \text{c.c.}), \quad (1)$$

where $\beta=1/T$ is the inverse temperature, c are the conduc-

tion electrons with dispersion ϵ_k on a regular lattice with \mathcal{N} sites, S_{int} are the interactions within the conduction band, and S_{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 pointlike impurity only a single V_i is nonzero. We can define a linear combination c_0 of conduction electron operators to which the impurity couples: $Vc_{0\sigma} = \sum_{\{i\}} V_i c_{i\sigma}$ with $[c_0, c_0^\dagger]_+ = 1$. After decoupling of S_{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 nonunitary 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

$$S = -\frac{1}{\beta} \sum_{\omega_n} \bar{\Psi}_0(i\omega_n) G_0^{-1}(i\omega_n) \Psi_0(i\omega_n) + S_{\text{loc}}(f_\sigma) + \int d\tau (V \bar{f}_\sigma c_{0\sigma} + \text{c.c.}). \quad (2)$$

Here, $G_0(i\omega_n)$ is the local conduction electron Green's function at the impurity location. In principle, a treatment of S_{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

$$G_0(i\omega_n) = \sum_k \begin{pmatrix} |h_k|^{-2}(i\omega_n - \epsilon_k) & h_k^{-2} \Delta_k \\ h_k^{*-2} \Delta_k^* & |h_k|^{-2}(i\omega_n + \epsilon_k) \end{pmatrix}^{-1}, \quad (3)$$

where Δ_k is the complex gap function, and the function h_k contains the geometry of the impurity coupling to the host:

$$h_k = \sum_{\{i\}} e^{ikR_i} V_i / V. \quad (4)$$

For a pointlike impurity $h_k=1$, and the anomalous (off-diagonal) part of G_0 is given by $G_0^a(i\omega_n) = \sum_k \Delta_k / D_k$ (with $D_k = \omega_n^2 + \epsilon_k^2 + |\Delta_k|^2$), which vanishes for unconventional su-

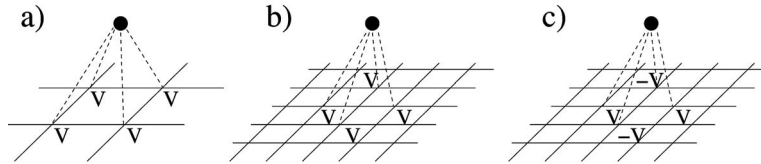


FIG. 1. Spatially extended impurities for which the anomalous propagator in G_0 drops out, i.e., $\sum_k h_k^2 \Delta_k / D_k = 0$, for a square-lattice d -wave superconductor. The dot represents the impurity orbital, the dashed lines show the nonzero hybridization paths (in the notation of an Anderson 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.

perconductors 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. 1(a)–1(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. Pointlike 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. 1(b) and 1(c) were used in Refs. 4 and 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^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 pointlike impurity in a s -wave superconductor. As explained in Refs. 1 and 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 and 13.

Now we comment on recent papers by Matsumoto and Koga^{7,8} about a nontrivial “orbital effect of Cooper pairs” on the dynamics of pointlike impurities in $p+ip$ and $d+id$ superconductors. They argue that, although the impurity only

couple 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 $p+ip$ and $d+id$ pairing, where the problem reduces to two angular-momentum channels, they provided a numerical solution utilizing a two-band numerical renormalization group (NRG) method. Their findings show the absence of screening even for large *Kondo* coupling, in contrast to the s -wave situation. We believe that their mapping and results are likely to be correct, but allow for a much simpler interpretation. Specifically, (i) our above arguments, which are rigorous for a pointlike impurity in a d -wave or unitary p -wave BCS superconductor, show that only the local DOS enters the impurity problem. (ii) The two-band model of Ref. 8 [their Eq. (2.21)]

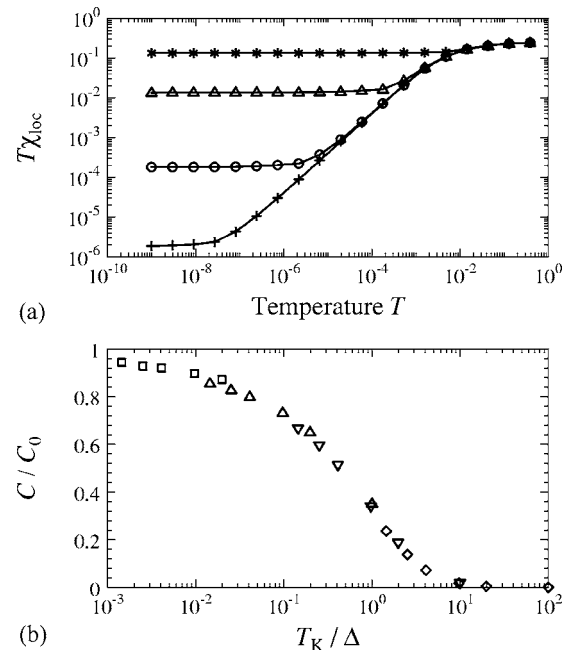


FIG. 2. Numerical results for the local susceptibility, obtained from a single-band NRG for a (semiconducting) bath with the hard-gap DOS of a $d+id$ (or $p+ip$) superconductor. The host bandwidth is unity, the NRG parameters are $\Lambda = 3$ and $N_s = 1000$. (a) $T\chi_{\text{loc}}$ for different 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 3×10^{-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 / Δ . Different symbols correspond to different values of Δ . (Deviations from a single universal curve are primarily due to NRG discretization effects.) The results can be compared with Fig. 4 of Ref. 8.

is in fact equivalent to a one-band model of the form (2) (in that it yields the same partition function and the same observables related to the impurity degrees of freedom). A first indication is that the impurity term in Eq. (2.21) of Ref. 8 mixes the two bands, i.e., contains channel-flip terms (in contrast to true two-band models). Formally, a one-band model can be obtained by integrating out the $a_{k,l=1}$ band in Eq. (2.4) of Ref. 8 exactly—this will generate a *normal* self-energy for the $a_{k,l=0}$ fermions and induce the quasiparticle gap.¹⁰ (iii) The local DOS of a $p+ip$ or $d+id$ superconductor displays a hard gap, thus we expect the qualitative impurity properties to be those of a hard-gap system.¹¹ In particular, for a $p-h$ symmetric band there is no screening even at large Kondo coupling, consistent with the results of Ref. 11. However, in the presence of $p-h$ asymmetry there will be a first-order transition to a screened phase as the Kondo coupling is increased.¹¹ This transition was not found in Refs. 7 and 8, instead the authors claim that their findings persist in the presence of $p-h$ asymmetry (but numerical results are not shown). We believe this claim to be incorrect. (iv) We have performed one-band NRG calculations using the local quasiparticle DOS of a $d+id$ (or $p+ip$) superconductor, and have essentially reproduced the results for the local susceptibility of Ref. 8, see Fig. 2.¹⁴ Taken together, the physics of point-

like impurities described in Refs. 7 and 8 is completely contained in a Kondo model where the impurity is coupled to a single band with a (fully gapped) local DOS of a nonsuperconducting host,¹⁰ and the “orbital effect of the Cooper pairs” does not exist. (This is different for spatially extended Kondo impurities where true multiband effects are obtained.⁹) The discussion in Sec. III B of Ref. 8 is formally correct, but misses that the mechanism leading to the doublet ground state of a strongly coupled Kondo impurity is identical for any $p-h$ symmetric hard-gap system.¹¹

In summary, we have argued that in unconventional BCS superconductors the properties of a Kondo impurity are not influenced by the presence of anomalous propagators, provided that $\sum_k h_k^2 \Delta_k / D_k = 0$ (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 and 5, is exact.

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¹⁰As our arguments are based on (exactly) integrating out certain conduction electrons, certain observables involving the conduction band cannot be obtained directly from Eq. (2). From the solution of the local impurity problem (2) one obtains the T matrix, which then allows one to directly calculate all conduction electron observables.

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¹⁴Due to the different truncation schemes in the one-band and two-band NRG codes *identical* results cannot be obtained.