Composite spin and orbital triplet superconductivity formed out of a Non-Fermi Liquid phase

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An unconventional superconducting phase is explored developing out of a non Fermi-liquid phase of the two-channel Anderson lattice model. It is characterized by a composite order parameter comprising of a local spin or orbital degree of freedom bound to triplet Cooper pairs with an isotropic and a nearest neighbour form factor. The superconducting transition temperature peaks in the moderate intermediate valence regime and vanishes at integral valence. The gap function is non analytic and odd in frequency, and a pseudo-gap develops in the conduction electron density of states which vanishes as $|\omega|$ close to $\omega = 0$.

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Introduction. Heavy Fermion (HF) superconductivity \cite{1} has drawn much attention since the discovery of superconductivity in CeCu$_2$Si$_2$ \cite{2} which is likely characterized by an anisotropic order parameter with symmetry yet to be determined. It became apparent over the last decade that almost all HF materials are unstable with respect to magnetic or superconducting phase transitions, which either compete with each other or can even coexist as found in uranium based materials. Non-Fermi liquid behaviour is often found in the vicinity of a so-called quantum critical point which is a point in parameter space where the ordering temperature is quenched to $T = 0$ by a control parameter like pressure or doping \cite{3}. Doped CeCu$_{6-x}$Ag$_x$ is one of the most prominent examples \cite{4}.

Two channel Anderson and Kondo lattice models, however, also exhibit non-Fermi liquid behaviour in the paramagnetic phase driven by unquenched and fluctuating local degrees of freedom \cite{5,6}. This phase is characterized by a large residual resistivity and entropy, and ill defined electronic quasi-particles. Fermi liquid physics is restored by cooperative ordering or applied magnetic field or stress \cite{7,8}. In particular, for a non Kramers doublet crystal field state in U$^{3+}$ or Pr$^{3+}$ ions, a two channel Kondo effect is possible \cite{9}. The magnetic “spin” of the electrons serves as channel index in this case. UBe$_{13}$ and PrFeP$_{12}$ are prominent candidates for a quadrupolar Kondo lattice description, as their enormous resistivity (> 100$\mu$Ohm) is removed only by phase transitions (superconductivity in UBe$_{13}$, antiferroquadrupolar order in PrFeP$_{12}$). Indeed, it has been shown that commensurate and incommensurate orbital ordering, as well as ferromagnetism are possible in this model depending upon coupling strength and filling \cite{10}. Evidence of a first order transition to an odd frequency pairing state in the Kondo limit (near integral valence) has been adduced, which is a singlet in both spin and channel indices, and no $q$ value was preferred for the center of mass momentum (COMM) \cite{11}.

In this paper, the possibility and nature of a superconducting phase transition out of the NFL paramagnetic phase within dynamical mean field theory (DMFT) \cite{12,13} will be explored. We show that in a intermediate valence (IV), two channel Anderson lattice a 2nd order transition to a triplet spin, triplet channel spin (StCt) order parameter with zero COMM will develop. The gap function is odd in frequency and singular, leading to a quasi-particle density of states that vanishes linearly with energy, in agreement with specific heat and spin lattice relaxation data for many HF materials. The order may arise form either two channel quadrupolar or magnetic ground states, and the transition temperature peaks in the moderate IV regime and vanishes at integral valence. The order parameter can be viewed as a composite of a bound spin and an even frequency triplet Cooper pair. Moreover, our analysis shows that isotropic and spatially extended states contribute to the superconducting phase, whereas the latter dominate in the IV regime. The binding of the fluctuating local degrees of freedom to the itinerant Cooper pair in the superconducting state is a natural consequence of the tendency to remove their residual entropy similar to a magnetic phase transition, a concept which was introduced first by Abrahams et. al. \cite{14}.

Composite order parameter. The two-channel periodic Anderson model \cite{15}

$$\hat{H} = \sum_{k\alpha,\sigma} \epsilon_k c_{k\alpha\sigma}^\dagger c_{k\alpha\sigma} + \sum_{i\sigma} E_{\sigma} X_{\sigma,\sigma}^{(i)} + \sum_{i\alpha} E_{\alpha} X_{\alpha,\alpha}^{(i)} + \sum_{i\sigma\alpha} (-1)^{1+\alpha} V \left( \epsilon_{i\sigma\alpha}^{\dagger} X_{-\sigma,\alpha}^{(i)} + h.c. \right)$$

(1)

describes the coupling of two degenerate conduction bands, labelled by a spin $\sigma$ and a channel index $\alpha = \pm 1$, to two localized doublets at each lattice site via hybridization matrix elements $(-1)^{1+\alpha} V$. $X$ are Hubbard operators, and $\epsilon_{k\sigma\alpha}$ the band dispersion. All energies will be given in units of $\Delta = V^2 \pi N_f$, the hybridization width. Since the model \cite{16} conserves spin and orbital quantum numbers, the symmetry of the conduction electron pair operator is classified in four sectors, comprising of the product space of spin and channel singlets or triplets. Introducing the transposed bi-spinor

\[\text{transposed bi-spinor}\]
The solution breaks spin-rotational invariance. From the definitions of the tensor pair operator in the triplet/triplet (StCt) sector are given by

\[ P_{ij}^{tt} = \frac{1}{N} \sum_{\vec{k}} S(\vec{k}) \tilde{\psi}^{\dagger}(\vec{k}) i\sigma_y \sigma_i \tau_j \tilde{\psi}(-\vec{k}), \]

where \( \vec{\sigma} \) acts in the spin sector and \( \vec{\tau} \) in the channel sector. The local nature of the DMFT permits only the Cooper pairs whose \( \vec{k} \)-dependent form factor \( S(\vec{k}) \) transforms according to \( \Gamma_1 \), the trivial irreducible representation. The pair expectation values \( \langle P_{ij}^{tt} \rangle \), however, always must vanish due to Pauli's principle. As a consequence, the anomalous Green functions in this sector have to be odd in frequency. This peculiar kind of pairing was first noticed that the time derivative \( \dot{C}_{\gamma'\gamma} = (\partial_t c_{\gamma}(\tau) c_{\gamma'}(\tau))_{\tau=0} \) is non-vanishing in the odd frequency superconducting phase and may possibly furnish an order parameter \[ \mathcal{O}_{ij} \] \( (\partial_t c_{\gamma}(\tau) c_{\gamma'}(\tau)) \) is equivalent to the commutator \([H, c_{\gamma}(\tau)] \) and consists of a product of two operators in the case of the two-channel periodic Anderson model \[ \mathcal{O}_{ij} \]: a conduction electron pair operator and a local magnetic or channel spin operator. Thus, one arrives at a composite order parameter, which correlates local and itinerant degrees of freedom: formation of band Cooper pairs is stimulated in the presence of a local pair resonating between definite spin and channel states with proper symmetry. Using equation of motion techniques on \[ \mathcal{O}_{ij} \], we derive \[ \mathcal{O}_{ij} \] with the definitions

\[ D_{\alpha\alpha'}^{\sigma\sigma'}(\vec{k}) = \frac{1}{\beta} \sum_{\vec{q}} e^{i\vec{q}\vec{k}} \chi_{\sigma\sigma'}^{\alpha\alpha'}(\vec{q}) = \frac{1}{N} \sum_{\vec{k}} G_{\vec{k} \sigma \sigma'} (\vec{k}) \chi_{\sigma\sigma'}^{\alpha\alpha'}(\vec{k}) \]

and \( G_{\vec{k} \alpha \sigma \sigma'} (\omega_n) \) is the Fourier transform of the anomalous Green function \( -\langle T(\bar{c}_{\vec{k} \alpha \sigma}(\tau) \bar{c}_{\vec{k} \alpha \sigma'}(\tau)) \rangle \).

The exact relations for the symmetrized order parameter components for the StCt sector

\[ O_{ij} = \frac{1}{\beta} \Gamma^{tt} = \text{sign}(\Delta E) \left[ \langle s_i \bar{P}^{tt} \rangle - \langle \bar{P}^{tt} \rangle \right] \]

by well established procedures within the DMFT. The local two particle band GF matrix \[ \chi^{pp}_{\sigma}(\vec{q}) = \sum q \chi^{pp}(\vec{q}) / N \] is given by \[ \chi^{pp}(\vec{q} = \vec{q}(\vec{k})) = \delta_{\vec{k},0} \delta_{\vec{q},0} \delta_{\vec{q},0} \delta_{\vec{k},0} G_c(\vec{q}), \] where \( G_c(\vec{q}) \) denotes the local conduction electron Green function and \( \Pi^{pp}_{\sigma} \) is the local conduction electron Green function. The composite order parameter \( \mathcal{O}_{ij} \) is invariant under exchange of the local doublets, and therefore superconductivity can arise from either a magnetic or quadrupolar ground state.
direct pp GF. Then, the pair susceptibility reads
\[ \chi_{PP}(q) = \frac{1}{\beta} |\lambda_m|^2 \frac{1}{1 - \lambda_m} + \text{regular terms} \quad (8) \]
where \( \lambda_m \) is the largest eigenvalue of the matrix \( M = \sqrt{\chi_{PP}(q)} \gamma \Gamma(0) \sqrt{\chi_{PP}(q)} \) in the odd frequency sector. \( c_{\lambda_m} = \sum_n i \omega_n [\chi(q, 0)(i \omega_n)] |\lambda\rangle_m \). This DMFT-analog to the Eliashberg equation was first used by Jarrell and co-workers \cite{11, 12}.

**StCt Sector.** The pair susceptibilities of all nine components of the tensor order parameter \( \langle \bar{\bar{I}} \rangle \) in the StCt sector are equal, as expected on symmetry grounds. No superconducting instability was previously found for the two-channel Kondo-lattice model \cite{6} since the model is restricted to integer \( n_f \) valence. In the StCt however, \( T_c \) is the largest for the IV regime, hence charge fluctuation driven rather than spin exchange induced. In Fig. 1a, \( T_c \) is shown in the stable magnetic phase and an infinitesimal odd-frequency anomalous Green function \( \Pi \) which is filling dependent for \( \Phi \sim 8 \cdot 10^{-3} \Delta \) which is an indicator for a second order phase transition in the triplet/triplet sector with an uniform order parameter.

We investigated the pair susceptibility \( \chi_{PP}^{\text{StCt}} \) in the IV, the Kondo and the stable moment regime for band-fillings between quarter and 3/4-filling and COMM of \( |q| = 0 \) and \( |q| = \pi \). A superconducting transition was always obtained, but only for \( q = 0 \). \( T_s \) is filling dependent for fixed coupling constant \( g = N_f J = \Delta / |\Delta E| \) as depicted for the IV regime in Fig. 1a. \( T_s \) is also compared to the characteristic temperature of the lattice, \( T^* \) as defined via a reduction of the effective moment \( \mu_{eff}^2(T) = T \chi(T) \) to 0.4 of its high temperature value. Hence, \( T^* \) serves as a phenomenological Kondo lattice temperature (see also \cite{7}). The pair susceptibility in the singlet/singlet sector (SsCs) agrees with the one reported for the Kondo lattice model \cite{13}. The instability, however, occurs always at lower temperatures compared to the one in the StCt sector.

**DMFT for the Superconducting Phase.** The Nambu Green function is an \( 8 \times 8 \) matrix in spin and orbital space. Assuming no directional coupling between spin and orbital degrees of freedom, the anomalous 4 \( \times \) 4 self-energy matrix may be written as \( g(i \omega_n, \vec{k}) \mathbf{\sigma}_s \mathbf{\sigma}_t [\vec{n}_s, \vec{n}_t, \tau] \) similar to He\(^3\) \cite{14}. \( \vec{n}_s \) and \( \vec{n}_t \) are constant unity vectors in spin and channel space, and the amplitude function \( g(i \omega_n, \vec{k}) \) has to be odd in frequency. This reduces the full problem to a standard 2 \( \times \) 2 size for \( g(z, \vec{k}) \) and the diagonal self-energy \( \Sigma \). In order to derive DMFT equations with a purely local self-energy matrix \( \Sigma(z) \), the anomalous self-energy is restricted to isotropic pairs, e. g. \( g(z, \vec{k}) = \tilde{g}(z) \). \( \tilde{G}(z) \) denotes the medium matrix in which the effective impurity is embedded. It is related to a generalized Anderson width matrix through \( \Delta(z) = V^2 \mathbf{\sigma}_2 \tilde{G}(z) \mathbf{\sigma}_2 \) and has normal and anomalous components describing quasi-particle propagation and pair-creation and annihilation, respectively.

The band electron self-energy \( \Sigma(z) = T \left[ 1 + G_T \right]^{-1} \) is determined by the local \( T \)-matrix \( T \). The diagonal elements of the \( T \)-matrix are given by the local quasi-particle scattering matrices \( T_{11}(z) = V^2 G_f(z) \), and its anomalous contribution is calculated from
\[ T_{12}(i \omega_n) = -V^4 \frac{1}{\beta} \sum_n i \omega_m \Pi_{PP}(i \omega_n, i \omega_m; 0) \tilde{f}(i \omega_m) \quad (9) \]
The negative sign takes into account that \( \Delta_{12}(z) = -V^2 \tilde{f}(z) \) where \( \tilde{f}(z) = \left[ \tilde{G}(z) \right]_{12} \) and \( \tilde{e}(z) = \left[ \tilde{G}(z) \right]_{11} \). We obtained a solution for the superconducting phase close to \( T_c \), using the normal state self-energy \( \Sigma(z) = T_c(z)/(1 + \tilde{e}(z) T_c(z)) \), iterating only the anomalous \( T \)-matrix \( T_s \) and medium \( \tilde{f} \). The spectra of the quasi-particle and the anomalous Green functions are shown in Fig. 2. Since the quasi-particle (qp) scattering rate \( \Gamma_{qp} = 3 m \Sigma(-i \delta) \) tends to become strongly reduced close to \( \omega = 0 \) as expected, the full DMFT(NCA) turns out to be unstable in the SC phase which is related to the well known convergence problems in the Fermi liquid regime \cite{15}. The resulting qp density of states \( \rho_{qp}(\omega) \) below \( T_c \) is proportional to \( |\omega| \) for small \( \omega \) as depicted in the inset of Fig. 2, as can also be analytically shown using a temperature broadened Lorentzian as an ansatz for \( g(z) \) which reflects the \( 1/z \) singularity of \( \Pi_{PP}^z \) \cite{13}.

**Discussion and Conclusion.** There is a controversial debate (see \cite{14} and reference therein) as to whether an odd-frequency solution with a COMM \( Q = 0 \) is connected to a minimum or a maximum of the free energy for a second order phase transition and, hence, may be thermodynamically unstable. Assuming a Fermi-liquid normal phase and an infinitesimal odd-frequency anomalous
self-energy $g(z)$ at $T_c$, Heid showed that one indeed obtains an increase of the free energy in the superconducting phase for $Q = 0$ [19]. This also holds for a non-Fermi liquid normal phase.

Based on the self-consistent solution for the anomalous Green function, $g(z)$ converges to a finite value such that always a gap is generated in the lattice Green functions. $g(z)$ might be approximated in leading order by a Lorentzian with a finite weight $A = \sqrt{T_{qp} \alpha T}$. The assumption of an infinitesimal value of $g(z)$ for all frequencies is violated and hence Heid’s theorem is not applicable in our case. Additionally, in the presence of an anomalous medium, the quasi-particle self-energy is also modified and, therefore, the feedback onto the effective site must be calculated self-consistently. We expect that the self-consistent solution for the one-particle Green function in the superconducting phase exhibits $\lim_{\omega \to 0} \Gamma_{qp} = 0$. In this case, a non-analytic self-energy $\Sigma_g$ with a finite weight $A$, will be always produce a gap. Even though the DMFT(NCA) equations for the superconducting phase are numerically unstable, they indeed indicate a reduction of the local free energy in the presence of a finite anomalous Green function and a tendency to reduce the scattering rate for the quasi-particles. Therefore, even though we cannot derive conclusively the type of the phase transition, we believe that these arguments support a second-order transition in the StCt sector. This phase transition is associated with a minimum of the free energy in the presence of a finite $g(z)$. An instability in the $T_{m}(AF)$ symmetry. An instability in the SsCs reported in the two-channel Kondo lattice could be reproduced but occurs at much lower temperatures. Spin-density wave phase transitions take over in the Kondo-regime at $g \approx 1.3$ corresponding to $\Delta E = -2.4\Delta$. The SDW wave-vector is continuously shifted towards nearest-neighbour antiferromagnetism, which is suppressed for $g \to 0$. Since all calculations were performed in the paramagnetic phase of the model, the highest transition temperature defines the nature of the incipient order. One cannot rule out, however, that an SDW or orbital ordering phase is replaced by, or even coexists with, a superconducting phase as found in some Uranium based HF compounds. We also would expect that the antiferroquadrupolar ordered PrFe$_2$P$_{12}$ might become superconducting when pressure is applied.

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The phase diagram shown for $n_c = 2.2$ in Fig. 3 summarizes our investigation of superconductivity and magnetism in the two-channel Anderson model. Superconductivity dominates the IV regime and the corresponding order parameter has spin and channel spin triplet symmetry. An instability in the SsCs reported in the two-channel Kondo lattice could be reproduced but occurs at much lower temperatures. Spin-density wave phase transitions take over in the Kondo-regime at $g \approx 1.3$ corresponding to $\Delta E = -2.4\Delta$. The SDW wave-vector is continuously shifted towards nearest-neighbour antiferromagnetism, which is suppressed for $g \to 0$. Since all calculations were performed in the paramagnetic phase of the model, the highest transition temperature defines the nature of the incipient order. One cannot rule out, however, that an SDW or orbital ordering phase is replaced by, or even coexists with, a superconducting phase as found in some Uranium based HF compounds. We also would expect that the antiferroquadrupolar ordered PrFe$_2$P$_{12}$ might become superconducting when pressure is applied.

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