Vol. 34 (2003) ACTA PHYSICA POLONICA B No 2

COMPOSITE SPIN AND ORBITAL TRIPLET SUPERCONDUCTIVITY*

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(Received July 10, 2002)

We show that the two-channel Anderson lattice model develops unconventional superconductivity out of a metallic non-Fermi liquid phase. 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 neighbor form factor. 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 $\omega = 0$.

PACS numbers: 75.20.Hr, 75.30.Mb, 71.27.+a

1. Introduction

Heavy Fermion [1] (HF) Superconductivity (SC) has drawn much attention since the discovery of superconductivity in $CeCu_2Si_2$ [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. Moreover, superconductivity in UBe_{13} develops out of a incoherent metallic phase with a high resistance at T_c of $\approx 100\mu\,\Omega\,$cm. The two-channel Anderson lattice model,

$$\hat{H} = \sum_{\vec{k}\alpha\sigma} \varepsilon_{\vec{k}}\, c^\dagger_{\vec{k}\alpha\sigma} c_{\vec{k}\alpha\sigma} + \sum_{i\sigma} E_\sigma X^{(i)}_{\sigma,\sigma} + \sum_{i\alpha} E_\alpha X^{(i)}_{\alpha,\alpha} + \sum_{i\sigma\alpha=\pm 1} \alpha V \left\{ c^\dagger_{i\alpha\sigma} X^{(i)}_{-\alpha,\sigma} + \text{h.c.} \right\} , \quad (1)$$

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

is believed to serve as a possible descriptions of the electronic properties of UBe_{13} or Pr^{3+} compounds with cubic symmetry. $\varepsilon_{\vec{k}}$ is the band dispersion of the two conduction bands α coupling to the localized doublets via hybridization V. $X^{(i)}_{\alpha,\beta}$ are the usual Hubbard operators describing local f-states at each lattice side i. One doublet is associated with a quadrupolar charge distribution $(X_{\alpha,\alpha})$ and one carried a spin $(X_{\sigma,\sigma})$. Its paramagnetic 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 [3].

2. Composite order parameter

It was observed that the local two-particle–particle irreducible vertex has a $1/\omega$ singularity and is odd with respect to the incoming and outgoing frequencies [4]. This is related to the fact that correlations are induced through consecutive hybridization processes on the f-shell due to the strong on-site Coulomb repulsion. Therefore, odd-frequency superconductivity [5] is favored in this model. Assuming an order-parameter with Γ_1 symmetry, the order-parameter must have Spin singlet, Channel single (SsCs) symmetry or Spin triplet, Channel triplet (StCt) symmetry. Only for the latter case, a stable solution was found. The order-parameter in the StCt sector

$$O_{ij} \;=\; \mathrm{sign}(E_\sigma - E_\alpha)\left[\langle s_i P^{\mathrm{s,t}}_j\rangle - \langle \tau_j P^{\mathrm{t,s}}_i\rangle\right], \tag{2}$$

correlates a local f-spin (quadrupolar moment) $s_i(\tau_i)$ — $i,j = x,y,z$ — component with a itinerate Cooper pair $\vec{P}^{\mathrm{s,t}}(\vec{P}^{\mathrm{t,s}})$ in the SsCt (StCs) sector

$$\vec{P}^{\mathrm{s,t}} \;=\; \frac{1}{N}\sum_{\vec{k}} S(\vec{k})\;\vec{\psi}^T(\vec{k})\; i\underline{\underline{\sigma}}_y i\underline{\underline{\tau}}_y \underline{\underline{\vec{\tau}}}\;\vec{\psi}(-\vec{k})\,, \tag{3}$$

$$\vec{P}^{\mathrm{t,s}} \;=\; \frac{1}{N}\sum_{\vec{k}} S(\vec{k})\;\vec{\psi}^T(\vec{k}) i\underline{\underline{\tau}}_y\; i\underline{\underline{\sigma}}_y \underline{\underline{\vec{\sigma}}}\;\vec{\psi}(-\vec{k})\,. \tag{4}$$

The form factor $S(\vec{k})$ transforms as Γ_1, and $\vec{\psi}(\vec{k})$ is a bi-spinor in spin and channel space. $O_{i,j}$ is invariant with respect to exchanging the orbital and the magnetic doublet $|\alpha\rangle$ and $|\sigma\rangle$ and a simultaneous particle–hole transformation of the conduction electrons. Hence, the occurrence of superconductivity is independent of the character of the local ground state of the local ion. We investigate the superconducting phase within the Dynamical Mean Field Theory (DMFT) by self-consistently calculating the anomalous self-energy under the presents of a Cooper-pair field.

3. DMFT in the superconduction phase

The Nambu–Green function is an 8×8 matrix in spin and orbital space. Assuming no directional coupling between spin and orbital degrees of freedom, the anomalous 4×4 self-energy matrix may be written as $g(z,\vec{k})\,\underline{\underline{\sigma}}_2\,\underline{\underline{\tau}}_2\left[\vec{n_s}\underline{\underline{\vec{\sigma}}}\vec{n_c}\underline{\underline{\vec{\tau}}}\right]$ where $\vec{n_s}$ and $\vec{n_c}$ are constant unity vectors in spin and channel space, and the amplitude function $g(z,\vec{k})$ has to be odd in frequency. This reduces the full problem to a standard 2×2 size for $g(z,\vec{k})$ and the diagonal self-energy Σ. In order to derive DMFT equations with a purely local self-energy matrix $\underline{\underline{\Sigma}}_c(z)$, the anomalous self-energy is restricted to isotropic pairs, *e.g.* $g(z,\vec{k}) = g(z)$. $\underline{\underline{\tilde{G}}}_c(z)$ denotes the medium matrix in which the effective impurity is embedded. It is related to a generalized Anderson width matrix through $\Delta(z) = V^2\underline{\underline{\sigma}}_2\,\underline{\underline{\tilde{G}}}_c(z)\,\underline{\underline{\sigma}}_2$ and has normal and anomalous components describing quasi-particle propagation and pair-creation and annihilation, respectively. The band electron self-energy $\Sigma_c(z) = \underline{\underline{T}}\left[\underline{\underline{1}} + \underline{\underline{\tilde{G}T}}\right]^{-1}$ is determined by the local T-matrix $\underline{\underline{T}}$ whose diagonal elements are given by the local quasi-particle scattering matrices $\underline{\underline{T}}_{11}(z) = V^2 G_f(z)$, and its anomalous contribution stems from Cooper pairs scattered on the local shells.

As an impurity solver for effective site problem of the DMFT, the NCA [6] was extended to the superconducting phase. The additional terms $\Delta\Sigma_\gamma(z)$ to the self-consistency equation for the local ionic propagators are generated by the anomalous media in the SC phase.

$$\begin{aligned}\Delta\Sigma_\alpha(z) &= \sum_\sigma |V|^4 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\varepsilon\, d\varepsilon' \rho_f(\varepsilon)\rho_f(\varepsilon) f(-\varepsilon') \\ &\quad \times P_\sigma(z+\varepsilon)P_\alpha(z+\varepsilon-\varepsilon')P_\sigma(z-\varepsilon')\,, \qquad (5)\\ \Delta\Sigma_\sigma(z) &= \sum_\alpha |V|^4 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\varepsilon\, d\varepsilon' \rho_f(\varepsilon)\rho_f(\varepsilon) f(-\varepsilon') \\ &\quad \times P_\alpha(z-\varepsilon)P_\sigma(z+\varepsilon'-\varepsilon)P_\sigma(z+\varepsilon')\,, \qquad (6)\end{aligned}$$

where $\rho_f(\varepsilon) = \Im m[\underline{\underline{\tilde{G}}}]_{12}(\varepsilon - i\delta)/\pi$ is the spectral function of the anomalous media. The anomalous local T-matrix is also obtained by the same additional diagram of the generating functional and reads

$$\begin{aligned}T_{12}(i\omega_n) &= \int_{-\infty}^{\infty} d\varepsilon\, \rho_f(\varepsilon) f(-\varepsilon) \oint_{\mathcal{C}} \frac{e^{-\beta z}}{2\pi i Z_f} P_\alpha(z) \\ &\quad \times P_\sigma(z+i\omega_n)P_\alpha(z+i\omega_n-\varepsilon)P_\sigma(z-\varepsilon)\,, \qquad (7)\end{aligned}$$

where Z_f is the partition function of the effective site, and the contour $\mathcal{C}$ encircles all singularities of the integral kernel. These coupled double integral equations are numerically solved using similar techniques as developed for the Post-NCA equations [7].

We calculated the self-consistent DMFT solution of the spectral functions close to T_c which are displayed in Fig. 1. The linear frequency dependency of the quasi-particle and anomalous Green function very close to $\omega = 0$, similar to d-wave superconductivity, is clearly visible. The opening of a pseudo-gap indicates a decrease of the energy in the superconducting phase, and, hence, its thermodynamical stability. Details of the filling dependence and the phase diagram are beyond the scope of this paper and will be published elsewhere [4].

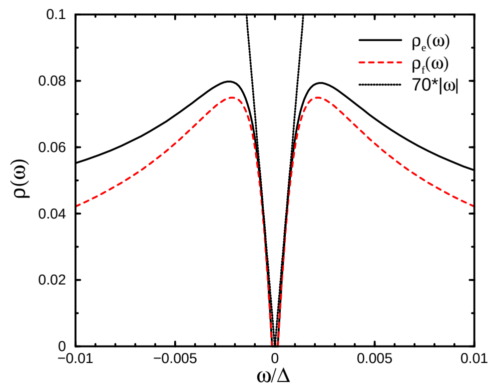

Fig. 1. Spectral functions of the quasi-particle and the anomalous Green function in DMFT (NCA) in the superconducting phase for $1 - T/T_c \ll 1$ in the vicinity of $\omega - \mu = 0$. The dotted curve shows a fit with $a * |\omega|$, Parameters are $\rho(\varepsilon) = \exp(-[(\varepsilon - \mu)/W]^2)/(\sqrt{\pi}W)$ conduction band DOS, band width $W = 10\Delta$, $E_\sigma - E_\alpha = -2\Delta$, $\Delta = V^2\pi\rho(\mu)$,

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