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ORIGINAL PAPER

Feedback Spin Exciton Formation in Unconventional Superconductors

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Abstract The superconducting feedback resonance in inelastic neutron scattering (INS) has now been found in numerous unconventional superconductors of the cuprate, ferropnictide, and heavy fermion classes. The collective spin excitation appears below T_c at an energy less than the quasiparticle threshold with momentum $\mathbf{Q}$ provided the gap changes sign under translation by $\mathbf{Q}$. The resonance has been found in the heavy fermion (HF) superconductors $CeCu_2Si_2$, $CeCoIn_5$, and UPd_2Al_3, and recently in Fe-pnictide $Ba_{1-x}K_xFe_2As_2$, $BaFe_{2-x}Co_xAs_2$, $BaFe_{2-x}Ni_xAs_2$, and $FeSe_{1-x}Te_x$ compounds and may be a more general phenomenon. Of particular interest is the interaction of the 3d spin exciton with the 4f crystalline electric field (CEF) excitations in rare earth based unconventional superconductors like $CeFeAsO_{1-x}F_x$ pnictide and $Nd_{2-x}Ce_xCuO_4$ cuprate where a coupling between 3d spin resonance and 4f CEF excitations leads to intriguing interaction effects observed experimentally by INS.

Keywords Feedback effect · Unconventional superconductors · Inelastic neutron scattering

1 Introduction

The relation between magnetism, its excitation modes, and the unconventional superconductivity in 4f/5f heavy fermion compounds and 3d cuprates, and recently discovered Fe pnictides is a central topic of condensed matter research. Although the nature of the magnetism in these compounds may be much different, it is generally believed that spin fluctuations play the important role in the formation of Cooper pairs. The on-site Coulomb correlations of electrons are very strong in HF systems and cuprates and only moderate in the pnictides. In all cases, they presumably lead to unconventional order parameters which change sign under translation by the wave vector $\mathbf{Q}$ that characterizes the predominant AF spin fluctuations. While the unconventional order parameter symmetry is a direct consequence of the pair forming due to spin fluctuations, in reverse, the latter are severely modified in the superconducting phase by a "feedback-effect" in the case of an unconventional gap function $\Delta(\mathbf{k})$. The sign change according to $\Delta(\mathbf{k}+\mathbf{Q}) = -\Delta(\mathbf{k})$ leads to a singular behavior of the electronic spin response function $\chi_0(\mathbf{q}, \omega)$ at the threshold energy $2\Delta_0$ for quasiparticle pair creation which in turn leads to a resonance (spin exciton) formation due to quasiparticle interaction. It is usually centered around the wave vector $\mathbf{Q}$ with a typical resonance energy $\omega_r < 2\Delta_0$ below the threshold and a dispersion around $\mathbf{Q}$ which depends on the details of the momentum dependence of the gap function $\Delta(\mathbf{k})$ and the nesting behavior of normal state quasiparticle bands $\epsilon_{\mathbf{k}}$. The absolute value of the observed resonance energy for the various compounds varies by two orders of magnitude according to the T_c variation (Table 1). However, the above resonance condition must always be fulfilled. In addition, it was proposed that for cuprates there is a universal relation between the resonance energy and the critical temperature given by $\omega_r/T_c \simeq 5.8$ independent of the details of the pairing mechanism [1]. Aside from being an interesting many-body effect, the appearance or absence of the spin exciton below T_c provides a powerful criterion for the determination of the symmetry of the

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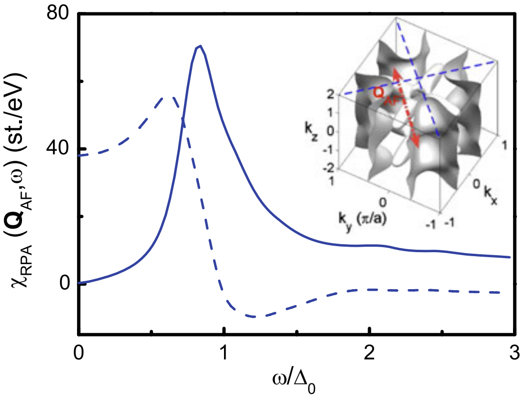

Fig. 1 Calculated real (*dashed*) and imaginary (*full*) part of RPA spin response for the superconducting B_{1g} order parameter in $CeCoIn_5$ showing the resonance peak at $\omega_r/2\Delta_0 \simeq 0.5$. The *inset* shows the corrugated Fermi surface columns of $CeCoIn_5$ due to hybridized heavy electron bands [5]. Here, $\mathbf{Q} = (\pi/a, \pi/a, \pi/c)$ is the AF nesting vector

gap function. It has been successfully applied in a number of cases discussed below.

2 Heavy Fermion Superconductors

The critical temperature of Ce- and U-based HF superconductors is limited to about 2 K. According to the above remarks, one then should expect $\omega_r \leq 1$ meV for the resonance energy which makes it difficult to observe in the HF compounds. In fact, in $CeCoIn_5$, which has the largest T_c among them the resonance was found only recently [2] at about the same time as the one in the oldest HF superconductor $CeCu_2Si_2$ [3]. Already before a spin resonance excitation was found in UPd_2Al_3, which appears as a satellite to a dispersive CEF excitation that exists already above T_c [4]. We focus here on the case of $CeCoIn_5$. In this compound, f-electron and conduction band states are hybridized in a complex way which may be described in an effective tight binding fit with a parameter set given in [5]. The resulting Fermi surface (FS) sheets are shown in the inset of Fig. 1. They exhibit a nesting property with the indicated wave vector $\mathbf{Q} = (\pi/a, \pi/a, \pi/c)$ leading to a pronounced maximum in the noninteracting static susceptibility $\chi_0(\mathbf{q})$ in the normal state. The spin resonance formation in the superconducting state is associated with the appearance of the complex poles in the dynamical RPA susceptibility $\chi_{\mathrm{RPA}}(\mathbf{q},\omega) = \chi_0(\mathbf{q},\omega)/(1 - U_{\mathbf{q}}\chi_0(\mathbf{q},\omega))$ around the nesting wave vector [5]. Here, $\chi_0(\mathbf{q},\omega)$ is the Lindhard function of $CeCoIn_5$ in the superconducting state. For $T \ll \Delta_0$, it has only one contribution coming from the creation of two quasiparticles out of the condensate. Furthermore, $U_{\mathbf{q}}$ is the effective quasiparticle interaction which peaks at the nesting vector $\mathbf{Q}$. For the appearance of the resonance pole, $Re\chi_0(\mathbf{q},\omega)$ must have a step like anomaly at the onset frequency $\Omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k+q}}|)$ of the quasiparticle continuum. It appears around the nesting vector $\mathbf{Q}$ at an energy $\omega_r < \Omega_c$ if the SC coherence factors (matrix elements for quasiparticle excitations) are large. This requires the condition $\Delta(\mathbf{k}+\mathbf{Q}) = -\Delta(\mathbf{k})$ for the SC gap function to be fulfilled. In reverse, the experimental observation of a resonance peak at $\mathbf{Q}$ demands that the true gap function must have this symmetry as necessary (but not sufficient) condition. In fact, in $CeCoIn_5$, the explicit calculation of $\chi_{\mathrm{RPA}}(\mathbf{q},\omega)$ shows that among all tetragonal representations only the $d_{x^2-y^2}$ or B_{1g} gap function $\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x a - \cos k_y a)$ leads to a pronounced resonance peak at a position $\omega_r/2\Delta_0 \simeq 0.5$ as shown in Fig. 1. This is in qualitative agreement with the experimental value 0.65 where $\omega_r = 0.6$ meV from INS [2] and $\Delta_0 \simeq 0.46$ meV from tunneling experiments. The calculation also predicts a slight downward dispersion of the spin exciton for wave vectors in the vicinity of $\mathbf{Q}$, experimentally this has not yet been investigated. It should be noted that the analysis in [5] resolved the controversial discussion of d_{xy} [6] vs. $d_{x^2-y^2}$ [7] pairing from specific heat and thermal conductivity measurements in favor of the latter.

A similar resonance feature has possibly been found in the oldest HF superconductor $CeCu_2Si_2$ [3] which has a lower $T_c \simeq 0.60$ K and, therefore, smaller resonance energy $\omega_r = 0.2$ meV. In distinction to all other examples, the resonance in $CeCu_2Si_2$ occurs at an incommensurate wave vector therefore the condition $\Delta(\mathbf{k}+\mathbf{Q}) = -\Delta(\mathbf{k})$ is not fulfilled for all states on the Fermi surface. However, a detailed calculation using the corrugated Fermi surface columns [5] shows again that the B_{1g} state is the only one that leads to a sizeable resonance peak. Therefore, the experimental observation of this peak [3] provides evidence that the gap function in this compound is also of $d_{x^2-y^2}$ type. The first feedback resonance excitation in a HF compound has been found in hexagonal UPd_2Al_3 [4] where it occurs at the AF wave vector $\mathbf{Q} = (0, 0, \pi/c)$ at an energy $\omega_r \simeq 0.35$ meV. However, its physical origin is somewhat different since already above T_c a propagating CEF exciton mode with an energy $\omega_E(\mathbf{Q}) \simeq 1$ meV exists. The resonance appears as a pronounced satellite to this mode and its upward dispersion follows that of the CEF excitation. As explained in [8, 9] and references cited therein, a gap function of the A_{1g} type $\Delta(\mathbf{k}) = \Delta_0 \cos ck_z$ follows from the presence of the resonance and also from thermal conductivity. The known experimental characteristics of the feedback resonances in the HF superconductors are summarized in Table 1 together with the recent one from the Fe pnictide superconductors.

Table 1 Heavy fermion and Fe pnictide compounds which exhibit the superconducting feedback resonance in INS. Here, ω_r is the resonance energy and **Q** the momentum obtained as from INS. Δ_0 is the maximum of the gap from NMR, tunneling or photoemission results. The values (∗) are obtained by scaling of T_c

Compound	T_c (K)	Δ_0 (meV)	ω_r (meV)	**Q** (r.l.u.)	$\frac{\omega_r}{2\Delta_0}$	$\frac{\omega_r}{k_BT_c}$	$\frac{2\Delta_0}{k_BT_c}$	Ref.
$CeCu_2Si_2$	0.60	0.13	0.20	(0.226, 0.226, 1.467)	0.78	3.87	4.97	[3]
$CeCoIn_5$	2.30	0.46	0.60	(0.5, 0.5, 0.5)	0.65	3.03	4.66	[2]
UPd_2Al_3	1.80	0.43	0.35	(0., 0., 0.5)	0.40	2.26	5.60	[4]
$Ba_{1-x}K_xFe_2As_2$	38	12	14	(polycr.) $\lvert\mathbf{Q}\rvert = 0.5$	0.58	4.28	7.38	[11]
$BaFe_{2-x}Co_xAs_2$	22	6.25	8.6	(0.5, 0.5, L)	0.69	4.54	6.58	[12]
$BaFe_{2-x}Ni_xAs_2$	20	5.68*	9.1	(0.5, 0.5, L)	0.80*	5.28	6.58*	[13]
$FeSe_{1-x}Te_x$	14	3.75	6.5	(0.5, 0.5, L)	0.86	5.30	6.10	[14]

3 Iron Pnictide Superconductors

Soon after the discovery of superconductivity in Fe-pnictides, it was realized that the extended s-wave ($s_\pm$) state with a gap function $\Delta_\mathbf{k} = \frac{\Delta_0}{2}(\cos k_x a + \cos k_y a)$ provides an attractive model for these compounds. It leads to basically isotropic gaps on the electron and hole FS sheets around the Γ-point and M-point of the folded Brillouin zone and a sign change between them. This order parameter can take advantage of the repulsive interband-quasiparticle interactions at the wave vector $\mathbf{Q} = (\pi/a, \pi/a)$. It was then predicted theoretically [10] that this mechanism should also lead to a feedback resonance around this wave vector. This has now been found in $Ba_{1-x}K_xFe_2As_2$ [11], $BaFe_{2-x}Co_xAs_2$ [12], $BaFe_{2-x}Ni_xAs_2$ [13], and $FeSe_{1-x}Te_x$ [14] by INS experiments. A peculiar nonresonant feedback effect has recently been observed in the rare-earth based pnictide $CeFeAsO_{1-x}F_x$ [15] which was investigated in [16]. In this compound, the CEF split 4f (Ce) atoms reside in layers adjacent to the superconducting FeAs layers. Due to a small exchange coupling between the localized 4f and itinerant 3d moments, the former may be used as a probe for the superconductivity in the 3d FeAs layers. Although a direct feedback resonance in the 3d spin response has not been found (yet) in this compound, a definite signature of enhanced 3d spin susceptibility was identified through its influence on the 4f-CEF excitations at $\omega_\mathbf{q}(T = T_c) = 18.6$ meV. This may be described by the coupled mode equation [16]

$$\Delta_{\mathrm{CEF}}^2 - \omega_\mathbf{q}^2 - 2\Delta_{\mathrm{CEF}} I_0^2 |m_\perp|^2 \left[\chi_{\mathrm{RPA}}^{(d)}(\mathbf{q}, \omega_\mathbf{q})\right]' = 0$$

where I_0 is the 3d–4f exchange coupling and Δ_{CEF}, $m_\perp$ are bare CEF splitting and transition matrix element, respectively. In the case of weak 3d–4f coupling and $\Delta_{\mathrm{CEF}} > 2\Delta_0$, this leads to a small upward shift in the CEF excitation energy $\omega_\mathbf{q}$ below T_c which follows the order parameter increase. This is due to the negative sign of $\chi_{\mathrm{RPA}}^{(d)}$ for $\Delta_{\mathrm{CEF}} > \omega_r$ in the above equation. The theoretical calculation of this effect is shown in Fig. 2 together with the experimental results in the inset. In principle, this perturbative effect may become much more dramatic when the coupling increases leading to the evolution of a double peak structure in the f-electron spectral function below T_c. This is shown as a contour plot in Fig. 3 with bound at an antibound state of CEF excitation and 3d spin exciton at lower and higher energies, respectively. Whether such a structure can be found in the rare earth based pnictides remains to be seen. There are, however, some indications that it is present in rare earth-based cuprates like $Nd_{2-x}Ce_xCuO_4$ [16, 17].

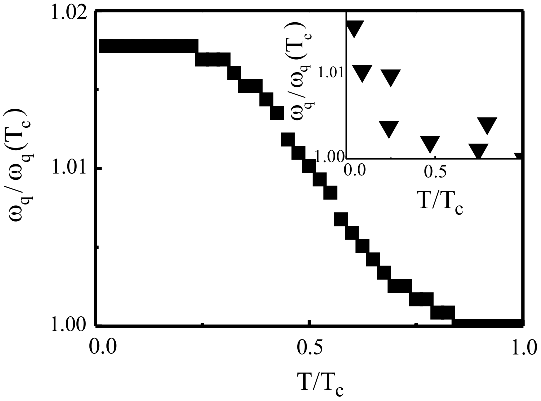

Fig. 2 Calculated frequency position ω_q of the 4f CEF excitation $\omega_\mathbf{q}$ ($\omega_\mathbf{q}(T_c) = 18.6$ meV) renormalized by coupling to the 3d spin response $\chi_{\mathrm{RPA}}^{(d)}(\mathbf{q}, \omega_\mathbf{q})$ [16]. *Inset* shows experimental results for $CeFeAsO_{1-x}F_x$ [15]

4 Conclusion

To summarize, we note that the spin resonance formation within the superconducting gap by the feedback effect below T_c has now been found in many unconventional superconductors. Its appearance demands large coherence factors

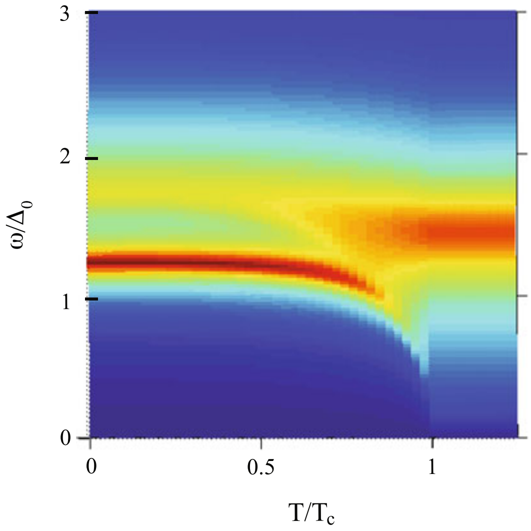

Fig. 3 Contour plot of the 4f spectral function for strongly coupled ($I_0 \simeq \Delta_0$) 4f-CEF excitation and 3d-spin exciton ($T < T_c$). The single CEF excitation above T_c evolves into bound and anti-bound state peaks below T_c

at nesting positions **Q** of the Fermi surface which dominate the spin fluctuations in the normal state. This requires a sign change of the gap function under translation by **Q**. This condition is very powerful in selecting the proper symmetry class of the unconventional superconductor, especially in the heavy fermion compounds where more conventional methods are difficult to apply.

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