Feedback Resonances in Unconventional Superconductors and Kondo Semiconductors

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The relation between unconventional superconductivity and magnetism in heavy-fermion (HF) systems [1], ferropnictides and cuprates is one of the most interesting research topics in condensed matter physics. Despite certain fundamental differences related to the orbital structure of conduction electrons and their correlation strengths, it is widely believed that in all cases short-range antiferromagnetic (AF) spin fluctuations are responsible for Cooper pairing with finite angular momentum, i,e., an unconventional gap function. Furthermore the latter has a pronounced resonant feedback below T_c on the spin excitations of the compound. One example is the famous resonance peak observed in high-T_c cuprates by means of inelastic neutron scattering (INS) whose nature is still actively investigated.

For some time this effect was considered as unique for the cuprates, however currently a number of other examples, namely UPd_2Al_3, $CeCu_2Si_2$, $CeCoIn_5$ in the HF systems and $Ba_{0.6}K_{0.4}Fe_2As_2$, $BaFe_{1.84}Co_{0.16}As_2$ for the ferropnictides are known. Therefore the resonant feedback is a universal phenomenon in unconventional superconductors. It is an interesting many-body effect and also a powerful tool to investigate the symmetry of the unconventional gap function $\Delta(\mathbf{k})$. In fact, it is not restricted to superconductors. In Kondo semiconductors such as YbB_{12}, which have no broken symmetry but show the gradual opening of a low energy hybridisation gap below the Kondo temperature a very similar resonance formation within the semiconducting gap was found by INS. The dispersion of these resonance excitations depends on the details of Fermi surface (FS) and gap anisotropy. It is commonly centered around the wave vector which has the dominating spin fluctuations for elevated temperatures. In most cases this is a commensurate AF zone boundary wave vector, except for $CeCu_2Si_2$.

In this report we will discuss the theory of spin resonance formation in the HF superconductors UPd_2Al_3, $CeCoIn_5$ and the Kondo semiconductor YbB_{12} in some detail, based on Refs. [2, 3, 4]. The first HF example found was UPd_2Al_3 [5]. This compound orders magnetically at $T_N = 14.3\,K$, much higher than $T_c = 1.8\,K$, with a commensurate AF ordering vector $\mathbf{Q} = (0,0,\frac{\pi}{c})$. The U $5f^3$ electrons have a 'dual' nature with localised $5f^2$ configurations and an additional $5f$ conduction electron. The former are split by the crystalline electric field (CEF) into two low-lying singlets an en-

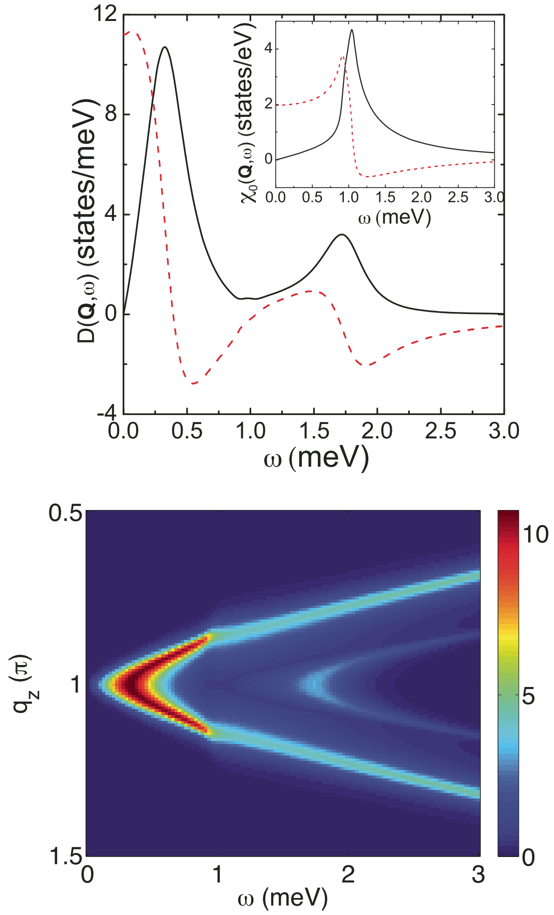

Fig. 1: Results for UPd_2Al_3. Top(a): Real (dashed lines) and imaginary (full lines) parts of susceptibility $\chi_0(\mathbf{Q},\omega)$ (inset) and CEF boson propagator $D(\mathbf{Q},\omega)$ (main figure). The INS intensity is proportional to $\mathrm{Im}\,D(\mathbf{Q},\omega)$ given by the full line of the main figure. Here we used $g = 10\,meV$. b: Contour plot of $\mathrm{Im}\,D(\mathbf{q},\omega)$ as function of ω and q_z. One clearly observes two distinct peaks at $\mathbf{Q}$. The one at low energies represents the resonance peak (ω_r) induced by the feedback of superconductivity and the one at higher ω is the shifted CEF boson $\tilde{\omega}_{\mathbf{q}}$. Away from $\mathbf{Q}$ both peaks disperse upward in energy following the behavior of the normal state CEF boson (from Ref. [2]).

ergy $\Delta \simeq 5.5\,\text{meV}$ apart. They disperse into a band of propagating bosonic modes $\omega_{\mathbf{q}}$ between 1.5 and 8 meV [6] due to RKKY interactions. The heavy 5f itinerant electrons form a corrugated cylinder FS along the hexagonal axis. There is considerable evidence that the bosonic modes lead to the quasiparticle mass enhancement in the normal state and to the Cooper pair formation [7, 8]. The gap function has the symmetry $\Delta^{sc}(\mathbf{k}) = \Delta_0^{sc} \cos k_z$ and has (equivalent) node lines at $k_z = \pm\frac{\pi}{2}$ which lie in the faces of the AF Brillouin zone (BZ) boundary where the gap function changes sign.

Below T_c INS experiments exhibit a sharp feedback resonance mode around $\mathbf{Q}$ with an energy $\omega_r \simeq 0.3\,\text{meV}$ which lies within the SC excitation 'gap' $2\Delta_0^{sc} \simeq 1\,\text{meV}$ and below the bosonic gap $\omega_{\mathbf{Q}} \simeq 1.5\,\text{meV}$ in the normal state. In this compound the feedback resonance appears as a satellite to an already existing dispersive CEF excitation above T_c. This is different to the other cases discussed here where only a broad continuum is observed above T_c. Although the SC feedback effect in UPd_2Al_3 may be described phenomenologically [5, 9], a complete microscopic explanation within the dual model of McHale et al [8] only appeared recently [2]. In this theory the conduction electrons couple to the magnetic bosons with one component of their spin density which renormalizes the bosonic propagator according to

$$D(\mathbf{q},\omega) = -\frac{2\omega_{\mathbf{q}}}{\omega^2 - [\omega_{\mathbf{q}}^2 - 2g^2\Delta\chi_0(\mathbf{q},\omega)]} \qquad (1)$$

Its spectral function $S(\mathbf{Q},\omega) = [1 - \exp(-\beta\omega)]^{-1}\,\mathrm{Im}\,D(\mathbf{Q}.\omega)$ is proportional to the INS cross section. The latter is therefore determined by the frequency dependence of the denominator in Eq. (1). In the normal state $D(\mathbf{q},\omega)$ only has a single pole at the bosonic CEF mode energy $\omega_{\mathbf{q}}$. When the electron-boson coupling g is sufficiently weak, only a frequency shift and change in line width ensues in the SC state. However if g is strong enough the propagator has two poles $\omega_\pm$ approximately given by

$$\omega_\pm^2 = \frac{1}{2}[\omega_{\mathbf{Q}}^2 + (2\Delta_0^{sc})^2] \pm\Big\{\frac{1}{4}[\omega_{\mathbf{Q}}^2 - (2\Delta_0^{sc})^2]^2 + 2g^2\Delta N(0)(2\Delta_0^{sc})^2\Big\}^{\frac{1}{2}} \qquad (2)$$

The lower one $\omega_r \equiv \omega_-$ is the resonance pole and ω_+ the up ward shifted bosonic frequency $\tilde{\omega}_{\mathbf{q}}$. Using the appropriate values $\Delta = 5.5\,\text{meV}$, $\omega_{\mathbf{Q}} = 1.54\,\text{meV}$, $g = 10\,\text{meV}$, $2\Delta_0^{sc} = 1\,\text{meV}$ and $N(0) =$

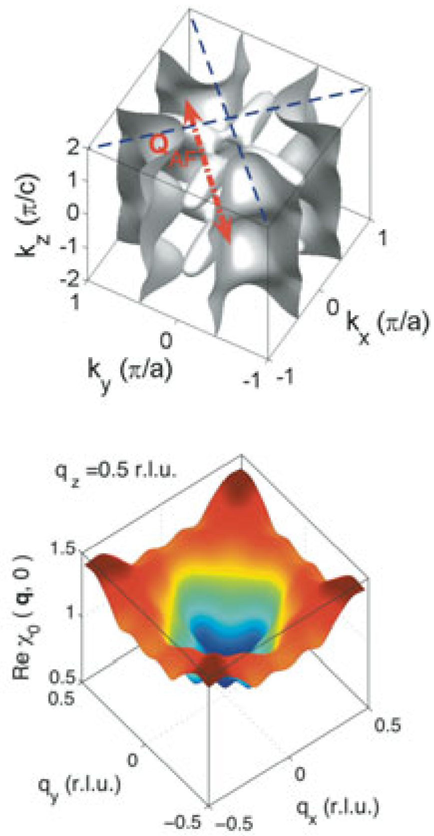

Fig. 2: Top(a): Calculated Fermi surface of $CeCoIn_5$ from hybridisation model in Eq. (3). Nesting vector $\mathbf{Q}_{AF}$ is indicated, dashed lines are node positions of B_{1g} gap function. Bottom(b): Calculated static spin susceptibility exhibits maximum at nesting vector (from Ref. [3]).

2 states/eV for conduction electron DOS we obtain the upward shifted boson frequency $\tilde{\omega}_{\mathbf{Q}} = 1.89\,\text{meV}$ and resonance position $\omega_r = 0.23\,\text{meV} < 2\Delta_0^{sc}$, in reasonable agreement with the peak positons of the fully numerical calculation of the spectral function in Fig. 1. An essential signature of a sharp resonance is the inequality $\omega_r < 2\Delta_0^{sc}$, i.e. that it appears below the quasiparticle continuum threshold. The reason for the existence of ω_r is the strong frequency dependence of the conduction electron spin susceptibility $\chi_0(\mathbf{q},\omega)$ for $\omega \simeq 2\Delta_0^{sc}$ in the superconducting state (see inset of Fig. 1a). This is true only if the quasiparticle matrix elements or 'coherence factors' in $\chi_0(\mathbf{q},\omega)$ are large. For $\mathbf{q}$ close to the AF $\mathbf{Q}$ vector this requires that the gap function satisfies the condition $\Delta_{\mathbf{k}+\mathbf{Q}}^{sc} = -\Delta_{\mathbf{k}}^{sc}$ (sign change under translation). Reversing the argument an observation of a well formed resonance at $\mathbf{Q}$ with energy $\omega_r < 2\Delta_0$ excludes any gap function model which does

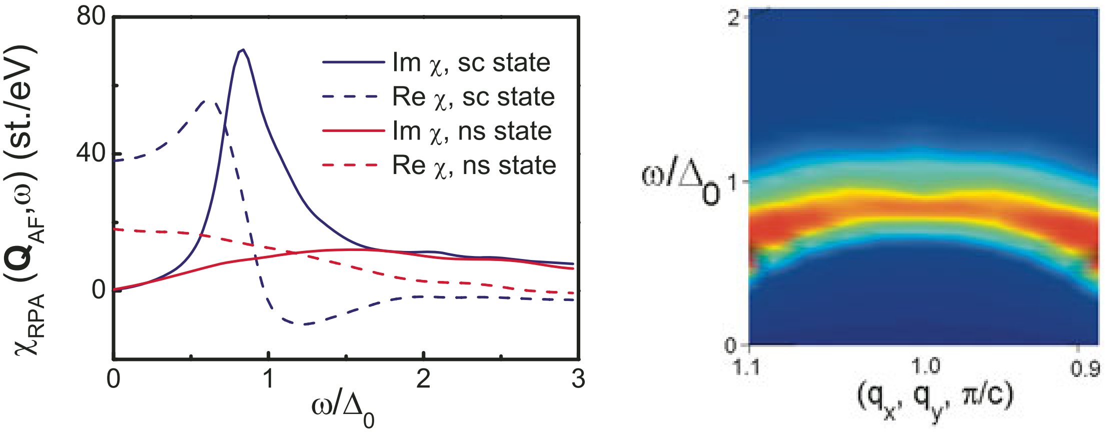

Fig. 3: Left(a): Calculated real (dashed) and imaginary (full) part of the RPA susceptibility at $\mathbf{Q}$ *for* $CeCoIn_5$ *as function of frequency in the normal and superconducting state of* $B_{1g}(d_{x^2-y^2})$ *symmetry. Imaginary part shows the spin exciton peak. Right(b): Dispersion of the resonance peak along (q,q,* $\frac{\pi}{c}$*) direction using a Lorentzian shape of* $J_\mathbf{q}$ *around* $\mathbf{Q}$ *(from Ref. [3]).*

not satisfy this condition, specifically those without sign change transforming like $\Delta^{sc}_{\mathbf{k}+\mathbf{Q}} = \Delta^{sc}_{\mathbf{k}}$. Combined with Knight shift experiments which point to singlet pairing the resonance formation in UPd_2Al_3 is therefore a strong argument for a gap function $\Delta^{sc}_0 \cos k_z$ [2]. Indeed this is also fully compatible with angle resolved magnetothermal conductivity results [10, 11]. Finally Fig. 1a shows the dispersion of the (lower and most intense) resonance branch and the upper magnetic boson branch $\tilde{\omega}_\mathbf{q}$. The resonance dispersion simply follows the latter which steeply increases away from $\mathbf{Q}$ as a satellite excitation.

The resonant SC feedback effect has subsequently been found in other HF compounds, namely, in $CeCoIn_5$ at $\omega_r = 0.6\,\mathrm{meV}$ and $\mathbf{Q} = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{c})$ [12] and in $CeCu_2Si_2$ at $\omega_r = 0.2\,\mathrm{meV}$ with an incommensurate $\mathbf{Q} = (0.22\frac{\pi}{a}, 0.22\frac{\pi}{a}, 0.51\frac{\pi}{c})$ [13]. Here we discuss only the former because for commensurate $\mathbf{Q}$ theoretical arguments for the resonance appearance are more clearcut.

In $CeCoIn_5$ the hybridsation of $4f^1$ electrons with conduction electrons leads to a multisheeted FS of heavy electrons which may be approximately described by an f-band ($E^f_\mathbf{k}$) and conduction band ($\varepsilon_\mathbf{k}$) model with (effective) hybridization ($V_\mathbf{k}$) [14] of the type

$$E_{2\mathbf{k}} = \frac{1}{2}\left[(\varepsilon_\mathbf{k} + E^f_\mathbf{k}) - \sqrt{(\varepsilon_\mathbf{k} - E^f_\mathbf{k})^2 + 4V^2_\mathbf{k}}\right] \qquad (3)$$

Where the lower band given here is partly occupied and leads to main FS sheets consisting of strongly corrugated collumns along the tetragonal axis (Fig. 2a). As indicated this FS has a nesting property with a commensurate wave vector $\mathbf{Q} = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{c})$. Therefore the noninteracting (Lindhard) spin susceptibility has a pronounced maximum at the nesting vector in the normal state which has been confirmed by INS results [12]. The magnetic response of the interacting HF quasiparticles is given by the RPA expression

$$\chi_{RPA}(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 - J_\mathbf{q}\chi_0(\mathbf{q},\omega)} \qquad (4)$$

where $J_\mathbf{q}$ is the four point interaction of quasiparticles and χ_0 their noninteracting susceptibilty, both in the normal or superconducting state. This expression is related but not identical to the boson propagator in Eq. (1). In the case of $CeCoIn_5$ there are no low energy propagating CEF bosons in the normal state. Therefore this equation leads to a featureless magnetic spectrum above T_c. However for $T < T_c$ a pronounced frequency dependence of $\chi_0(\mathbf{q},\omega)$ evolves due to the gap opening. For large momentum $\mathbf{q} \simeq \mathbf{Q}$, $\mathrm{Im}\,\chi_0(\mathbf{q},\omega)$ exhibits discontinuous jump at the threshold energy $\Omega_c = \min_\mathbf{k}(|\varepsilon_\mathbf{k}| + |\varepsilon_{\mathbf{k}+\mathbf{Q}}|)$ with an associated logarithmic peak in the real part of the susceptibility. Therefore a resonance or spin exciton pole appears in the RPA response function at an energy $\omega_r < \Omega_c$. Note that in contrast to UPd_2Al_3 only the lower resonance pole exists since there is no propagating CEF boson present. As before the discontinuity and the pole appear when the coherence factors in $\chi_0(\mathbf{q},\omega)$ are large which means that $\Delta^{sc}_{\mathbf{k}+\mathbf{Q}} = -\Delta^{sc}_\mathbf{k}$ must be fulfilled. Indeed, it turns out that among the possible candidate gap function with tetragonal symmetry only the B_{1g} gap functions ('$d_{x^2-y^2}$

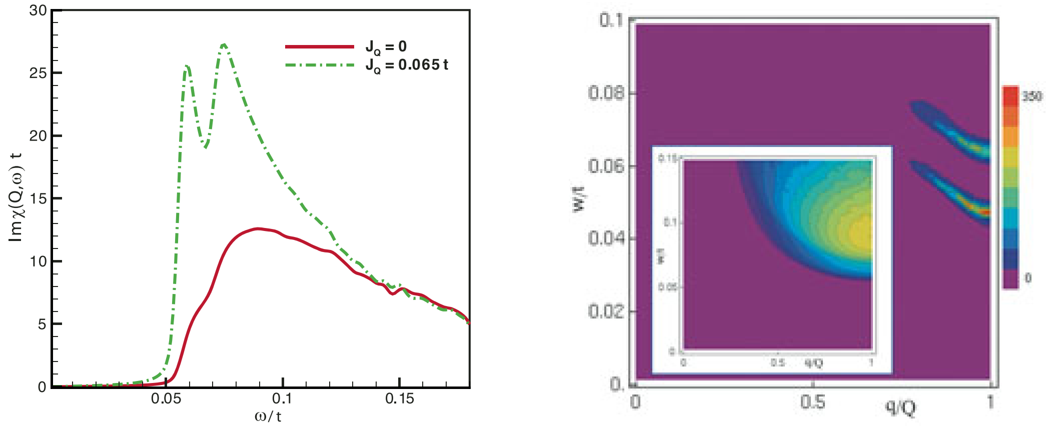

Fig. 4: Results for YbB_{12}. Left(a): Imaginary part of the susceptibility for the noninteracting ($J_{\mathbf{q}} = 0$) and interacting case (finite Lorentzian $J_{\mathbf{q}}$ peaked at $\mathbf{Q}$). Right(b): Contour plot of imaginary part of RPA dynamical susceptibility with Lorentzian interaction $J_\Gamma(q)$. Parameters are chosen to obtain spin exciton peaks at $\omega_1 = 15\,meV$ and $\omega_2 = 20\,meV$ at the $(1,1,1)$ zone boundary. These positions and shape and range of dispersion are comparable to experimental results. The inset shows the contour plot of imaginary part of dynamical susceptibility of noninteracting *degenerate bands in the direction $(1,1,1)$ for comparison, showing the indirect hybridisation gap. The color scale of the inset is reduced by a factor of 35. Energy scale $t = 0.32\,eV$ (from Ref. [4]).*

wave') $\Delta^{sc}(\mathbf{k}) = \frac{\Delta_0^{sc}(\mathbf{k})}{2}(\cos k_x a - \cos k_y a)$ which satisfies this condition leads to a spin resonance formation below T_c. This is shown in Fig. 3a. In $CeCoIn_5$ the symmetry of $\Delta(\mathbf{k})$ has been controversial and was predicted as d_{xy} from specific heat and $d_{x^2-y^2}$ from thermal conductivity measurements under rotating field geometry. Since the observation of a resonance peak requires $\Delta_{\mathbf{k}+\mathbf{Q}} = -\Delta_{\mathbf{k}}$ it is clear that INS results [12] decide in favor of $d_{x^2-y^2}$ gap symmetry because d_{xy} has no sign change under $\mathbf{k} \to \mathbf{k}+\mathbf{Q}$ contrary to $d_{x^2-y^2}$. Therefore INS is an additional powerful tool to investigate gap function symmetry of unconventional superconductors.

Finally in Fig. 3b the dispersion of the resonance excitation away from $\mathbf{Q}$ is shown. It bends downward because one must have $\omega_r < \Omega_c$ and the latter is reduced for the wave vector $(q_x, q_y, \frac{\pi}{c})$ since it connects states in the BZ where the superconducting gap is smaller. This downward dispersion is quite similar to the main feature in the cuprates but opposite to the observation in UPd_2Al_3 where the upward dispersion is not an intrinsic property of the resonance pole, but is enforced by the dispersion of the normal state CEF boson. The dispersion in $CeCoIn_5$ is sensitive to the model parametes, experimentally it has not yet been investigated in detail.

The spin resonance type excitations have recently also been observed for the ferropnictide superconductor $Ba_{0.6}K_{0.4}Fe_2As_2$ and $BaFe_{1.84}Co_{0.16}As_2$. These compounds have small hole like FS sheets and electron sheets at the zone center and boundary, respectively, connected by a nesting vector $\mathbf{Q} = (\frac{\pi}{a}, \frac{\pi}{a}, 0)$ This means the gap function must change sign between the hole and electron sheet. Combined with ARPES results which show that the gap is nearly isotropic on the sheets this leaves little choice but the extended $s_\pm$-wave state which may be represented as $\Delta^{sc}(\mathbf{k}) = \frac{\Delta_0^{sc}(\mathbf{k})}{2}(\cos k_x a + \cos k_y a)$ [15].

The spin resonance phenomenon observed in unconventional superconductors is connected with a special symmetry property of the order parameter or gap function. However the broken symmetry is not a necessary condition. In fact a very similar phenomenon was observed in the small gap Kondo semiconductor YbB_{12}. There the gap opening is not due to spontaneous order but due to a gradual crossover from a metallic state at higher temperatures whereby a hybridisation gap is opened. The gap size of 15 meV is of the order of the Kondo temperature and may be observed in thermodynamic and transport properties but also directly by INS [17]. In addition the unpolarized [17] and polarized [18] INS has found an interesting dispersive fine structure around the semiconducting gap threshold. Three excitation branches have been identified with energies 15, 20 and 38 meV, respectively by analyzing the spectral function of the dynamical susceptibility. Since the lower two INS peaks are narrow and mostly centered at the zone boundary L-point with $\mathbf{Q} = (\pi/a, \pi/a, \pi/a)$ they may be associated with the formation of a collective quasiparticle spin resonance exciton appearing around the spin gap threshold [17, 18] which is driven by heavy quasiparticle interactions. The collective modes remain visible in the 20 meV region up to $T = 159$ K. The upper peak is much broader and shows little dispersion. It is also rapidly suppressed with increasing temperature. It has been associated with continuum excitations also visible in a broad maximum in the optical conductivity [19] around 38 meV.

The theoretical explanation of these intriguing experiments has been previously unclear and was recently given in Ref. [4]. The model assumes the stable Yb $4f^{13}$ configuration corresponding to a single hole in the $4f$-shell [20]. Therefore, the Anderson lattice model with a f-hole in a $j = 7/2$ state, including the CEF effect is used as a starting point. The latter leads to two quasi-quartets ($\Gamma = 1, 2$) split by an energy Δ and having a different hybridisation V_Γ. Using the mean field slave boson representation of the Anderson lattice Hamiltonian where only no hole ($4f^{14}$) and single hole ($4f^{13}$) configurations are included the CEF-split heavy quasiparticle bands may be derived [4]. From this one obtains the noninteracting spin response with the single particle spin gap of 15 meV (inset of Fig. 4b) and the interacting RPA susceptibility. The former, due to the gap threshold shows a pronounced enhancement in the real part which leads to the spin exciton pole in the latter. Here the role of coherence factors is played by the c-f mixing amplitudes of the heavy quasiparticle states. The spectrum of the noninteracting and RPA susceptibility are shown in Fig. 4a where one can clearly see a double resonance peak evolving from the one particle background. The double peak structure is due to the effect of CEF splitting and, more importantly different hybridisation strengths V_Γ ($\Gamma = 1, 2$) of the quasi-quartets. The model parameters have been chosen to reproduce the experimental peak positions and the dispersion (Fig. 4b). The latter extends about one third into the BZ which is due to the strong suppression of the real part of $\chi_0(\mathbf{q}, \omega)$ when one moves away from the AF $\mathbf{Q}$-vector where one has excitations with the small indirect hybridsation gap. The features of the theoretical spin exciton dispersions correspond very nicely to the experimentally observed ones [18]. We note that an increase in $J_\mathbf{Q}$ (or a decrease of the hybridsation gap) will lead to a decrease of the spin exciton mode frequencies at $\mathbf{Q}$. At a critical value $J^c_\mathbf{Q}$ the lowest mode would become soft which would signify the onset of AF order in a Kondo semiconductor. This is not observed in YbB_{12} at ambient pressure. An investigation of the pressure dependence of spin exciton mode frequencies at $\mathbf{Q}$ might therefore be interesting because it would offer important clues as to how close YbB_{12} is to a quantum phase transition to AF order.

References

[1] *P. Thalmeier and G. Zwicknagl* in Handbook on the Phys. and Chem. of Rare Earths ed. by K. A. Gschneidner, Jr et al. (Elsevier, Amsterdam) **34** (2005) 135.

[2] *J. Chang, I. Eremin, P. Thalmeier, and P. Fulde*, Phys. Rev. B **75** (2007) 024503.

[3] *I. Eremin, G. Zwicknagl, P. Thalmeier, and P. Fulde*, Phys. Rev. Lett. **101** (2008) 187001.

[4] *A. Akbari, P. Thalmeier, and P. Fulde*, Phys. Rev. Lett. (2009, in press); arXiv:0901.3247.

[5] *N. Sato, N. Aso, K. Miyake, R. Shiina, P. Thalmeier, G. Varelogiannis, C. Geibel, F. Steglich, P. Fulde, and T. Komatsubara*, Nature **410** (2001) 340.

[6] *A. Hiess, N. Bernhoeft, N. Metoki, G. H. Lander, B. Roessli, N. K. Sato, N. Aso, Y. Haga, Y. Koike, T. Komatsubara, and Y. Onuki*, J. Phys.: Cond. Mat. **18** (2006) R437.

[7] *G. Zwicknagl, A. Yaresko, and P. Fulde*, Phys. Rev. B **68** (2003) 052508.

[8] *P. McHale, P. Fulde, and P. Thalmeier*, Phys. Rev. B **70** (2004) 014513.

[9] *N. Bernhoeft*, Eur. Phys. J. B **13** (2000) 685.

[10] *T. Watanabe, K. Izawa, Y. Kasahara, Y. Haga, Y. Onuki, P. Thalmeier, K. Maki, and Y. Matsuda*, Phys. Rev. B **70** (2004) 184502.

[11] *P. Thalmeier, T. Watanabe, K. Izawa, and Y. Matsuda*, Phys. Rev. B **72** (2005) 024539.

[12] *C. Stock, C. Broholm, J. Hudis, H.J. Kang, and C. Petrovic*, Phys. Rev. Lett. **100** (2008) 087001.

[13] *O. Stockert et al.*, Physica B **403** (2008) 973.

[14] *K. Tanaka, K. Ikeda, Y. Nishikawa, and K. Imada*, J. Phys. Soc. Jpn. **75** (2006) 024713.

[15] *M. M. Korshunov and I. Eremin*, Phys. Rev. B **78** (2008) 140509(R).

[16] *P. S. Riseborough*, Adv. Phys. **49** (2000) 257.

[17] *J.-M. Mignot, P. A. Alekseev, K. S. Nemkovski, L.-P. Regnault, F. Iga, and T. Takabatake*, Phys. Rev. Lett. **94** (2005) 247204.

[18] *K. S. Nemkovski, J.-M. Mignot, P. A. Alekseev, A. S. Ivanov, E.V. Nefeodova, A. V. Rybina, L. -P., F. Iga, and T. Takabatake*, Phys. Rev. Lett. **99** (2007) 137204.

[19] *H. Okamura, T. Michizawa, T. Nanba, S. Kimura, F. Iga, and T. Takabatake*, J. Phys. Soc. Jpn. **74** (2005) 1954.

[20] *P. A. Alekseev, E. V. Nefeodova, U. Staub, J.-M. Mignot, V. N. Lazukov, I. P. Sadikov, L. Soderholm, S. R. Wassermann, Yu. B. Paderno, N. Yu Shitsevalova, and A. Murani*, Phys. Rev. B **63** (2001) 064411.

[1] Max Planck Institute for the Physics of Complex Systems, Dresden, Germany