On the observation of the spin resonance in superconducting CeCoIn$_5$

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Recent observation of a resonance spin excitation at (1/2,1/2,1/2) in the superconducting state of CeCoIn$_5$ [C. Stock et al., Phys. Rev. Lett. 100 087001 (2008)] was interpreted as an evidence for $d_{x^2-y^2}$ gap symmetry, by analogy with the cuprates. This is true if the resonance is a spin exciton. We argue that such description is undermined by the three-dimensionality of CeCoIn$_5$. We show that in 3D systems the excitonic resonance only emerges at strong coupling, and is weak. We argue in favor of the alternative, magnon scenario, which does not require a $d_{x^2-y^2}$ gap.

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Whether Heavy Fermion materials (HF) and high temperature superconductors (HTSC) are governed by the same physics has been repeatedly discussed in the past. Speculations about the similarities between the two classes of materials started immediately after Bednorz and Muller’s discovery of the high-temperature superconductivity in the cuprates. To a large extent, the discussion at that time centered around an observation that in both systems spin degrees of freedom are among low-energy excitations, and superconductivity should be unconventional if spins are involved in the pairing. It was later realized that, although electron-electron interactions and magnetism do play indispensable roles in both systems, the HTSC are different from HF in several important aspects. Among them: (i) the metallic state in the cuprates emerges as a result of a chemical doping into the antiferromagnetic (AFM) Mott insulator; (ii) the transport in the cuprates is very anisotropic, and the consensus is that the new physics is two-dimensional (2D) and uniquely related to $CuO_2$ planes; (iii) ARPES experiments in the optimally doped and underdoped cuprates do not see well-defined single particle excitations above $T_c$, except in the so-called nodal regions. On the contrary, in HF, like $U$Pt$_3$ or $CeAl_3$, the de Haas-van Alphen (dHvA)-type experiments clearly indicate that the physics is three-dimensional (3D), and that single-particle excitations remain metallic and well-defined, although electronic characteristics dramatically change upon lowering the temperature below an effective “Kondo temperature”, $T_K$, at which the local $f$-electron states “mix up” with the s-p-d bands.

The still unresolved issue is whether the difference in the effective dimensionality and the nature of normal state excitations gives rise to a different symmetry of the superconducting order parameter in the HF compared to HTSC. There is a consensus among researchers that the SC order parameter in HF is indeed non-$s$-wave, but there is no agreement about its symmetry (see Ref.2 for the summary of early results on HF ). The interest to this issue resurfaced recently after the discovery of the new class of HF with the chemical formula CeMI$n_5$ (labeled as $Ce115$), where $M = Co, Rh, Ir$ (Ref.3). These materials are much closer to the cuprates than other HF – they crystallize into the layered tetragonal structure and possess a considerable anisotropy in their electronic properties. The dHvA experiments have found that at least one FS (electron 15-band ) has a pronounced quasi two-dimensional (Q2D) character [2, 3] (see also Ref.4). The transport properties of $Ce115$s also display surprisingly similarities with Q2D cuprates [11].

Another remarkable feature of the $Ce115$ materials, also reminiscent of the cuprates, is the proximity between SC and AFM. The close interrelation between superconductivity and antiferromagnetism has been demonstrated by the experiments on different alloys of $Ce115$s (Ref.5). The transition from SC to AFM can be tuned by applied pressure or the magnetic field (see Ref.2 and references therein), or by substituting $Cd$ for $In$ [10].

Such closeness between HTSC and $Ce115$s stimulated anew speculations that the superconductivity in both families of materials may have the same (magnetic) origin, and the gap symmetry is the same [2]. However, unlike HTSC, where the $d_{x^2-y^2}$-symmetry of the SC gap is the well-established fact [2], less is known about the gap symmetry in HF $Ce115$s. In the absence of ARPES data, the positions of nodes in the SC gap for $Ce115$s are subject of debates, and there are only indirect arguments in favor of the $d_{x^2-y^2}$ symmetry in CeCoIn$_5$ [12]. Furthermore, CeCoIn$_5$ is the multi-band superconductor, in distinction to the cuprates, and experiments show that some of its Fermi surfaces (FS) are prominently three-dimensional (3D) [2, 3]. In 3D tetragonal materials, there are more choices for the symmetry of the SC gap [13].

The subject of this paper is the analysis of recent neutron experiments on CeCoIn$_5$ (Ref.11), particularly their ability to resolve the issue of the gap symmetry. The experiments observed the spin resonance in CeCoIn$_5$ at the commensurate AFM vector $Q_{0}^{3D} = (1/2,1/2,1/2)$, and at temperatures below 1.35K (down to the lowest measured $T = 0.47K$). The resonance is very likely related to superconductivity, as measurements above $T_c = 2.3K$, show only a shallow feature around 0.6meV.
The authors of [14] used the analogy with the cuprates, where the spin resonance has been observed [15] at \( Q^{2D} = (1/2, 1/2) \), and argued that their data can be interpreted as the evidence that the superconducting gap in \( \text{CeCoIn}_5 \) is the same \( d^- \) wave gap with \( \Delta(p + Q^{2D}) = -\Delta(p) \), as in the cuprates. This is the case if the resonance is a spin exciton [16]. Below we demonstrate that three-dimensionality of \( Q_0 \), at which the resonance has been observed in [14], makes the analogy with the cuprates imprecise. We argue that the resonance unusually comes from 3D FS as we found that a 3D exciton is too weak. It may come from Q2D electron 15 band in \( \text{CeCoIn}_5 \), but then it should be visible only at \( (1/2, 1/2, 1/2) \), but also alone the line \( (1/2, 1/2, b) \) \( (0 < b < 1/2) \), which apparently is not the case experimentally. We argue that more likely explanation is that the resonance is a magnon-type excitation of \( f^- \)-electrons, cleared by a superconductivity.

To proceed, we first briefly review the situation in the 2D cuprates. Several candidates for the resonance have been proposed, including spin exciton, \( \pi \)-resonance, the mixture of the exciton and \( \pi \)-resonance, and a magnon, cleared up by a superconductivity [17]. We focus on the spin exciton scenario [16] because of its relation to \( d_{x^2-y^2} \) superconductivity.

The spin-exciton scenario associates the resonance with the feedback from the \( d_{x^2-y^2} \) pairing on the spin susceptibility of itinerant fermions near the AFM instability. The physics of this effect is not sensitive to the details of the model as long as the Fermi liquid concepts of the FS and the electron-hole excitations around it are preserved. The full dynamic spin susceptibility of itinerant fermions can be quite generally expressed as

\[
\chi(Q, \Omega) = \mu_B^2 \frac{\chi_0}{\xi^2 - \Pi(Q, \Omega)} \tag{1}
\]

where \( \mu_B \) is Bohr magneton, and dimensionless \( \xi \) is proportional to the magnetic correlation length \( (\xi^{-1} = 0 \) signals the onset of AFM order), and \( \Pi(Q, \Omega) \) is the polarization operator which has the form

\[
\Pi(Q, \Omega) = 16g^2 \chi_0 T \sum \int \frac{d^3p}{(2\pi)^3} \frac{G(p, \omega)G(p + Q, \omega + \Omega) + F(p, \omega)F^+(p + Q, \omega + \Omega)}{G(p, \omega)G(p + Q, \omega + \Omega) + F(p, \omega)F^+(p + Q, \omega + \Omega)} \tag{2}
\]

where \( G, F, \) and \( F^+ \) are the normal and anomalous Gor’kov Green functions, correspondingly, and \( g \) is the exchange constant for the interaction between conduction electrons and their collective spin excitations. Spin-exciton scenario assumes that the FS crosses the magnetic Brillouin zone boundary at eight points (hot spots) separated by \( Q = Q_0^{2D} \) [the prefactor 16 in (2) is \( 2 \times 8 \), where extra 2 is the spin factor] [20]. It further assumes that spin excitations with momenta near \( Q_0^{2D} \) are completely overdamped in the normal state due to strong Landau damping into particle-hole fermionic pairs, such that \( Im\Pi_n(Q, \Omega) \approx \gamma\Omega \), where \( \gamma \) is proportional to \( g^2\chi_0(\nu(\nu)) \) is the density of states at the FS (note that \( g^2\chi_0(\nu) \) is dimensionless) The real part of \( \Pi_n(Q, \Omega) \) in the normal state can be safely approximated by its static value \( \Pi_n(Q, 0) \) which we absorb into \( \xi^{-2} \). In the superconducting state, fermions at hot spots become gapped, and the behavior of \( \Pi(Q, \Omega) \) changes. Expanding near the FS and integrating in Eq. (2) over the transverse momentum component, we obtain [16]

\[
\Pi_{sc}(Q, \Omega) = \frac{i\gamma}{2} \int d\omega \left[ \frac{1 - \omega_+\omega_- + \Delta_1\Delta_2}{\sqrt{\omega_+^2 - \Delta_1^2}\sqrt{\omega_-^2 - \Delta_2^2}} \right] \tag{3}
\]

where \( \omega_\pm = \omega \pm \Omega/2 + i\text{sign}(\omega \pm \Omega/2) \), and \( \Delta_1 \) and \( \Delta_2 \) are the gaps at the two hot spots separated by \( Q \).

The remarkable feature in 2D that distinguishes between \( s^- \)-wave, \( d_{xy} \) and \( d_{x^2-y^2} \) pairings comes about from the factor \( \Delta_1\Delta_2 \) in (3): if this factor is negative, which is the case for the \( d_{x^2-y^2} \) symmetry, but not the other two symmetries, then (i) \( \Pi(Q, 0) = 0 \), i.e., the value of \( \xi \) is unaffected by superconductivity, and (ii) \( Re\Pi_{sc}(Q, \Omega) \) diverges logarithmically at \( 2\Delta_1 \), as \( \gamma_1(\Omega_{1/2} - \Omega) \), and \( Im\Pi_{sc}(Q, \omega) \) jumps discontinuously at \( \Omega = 2\Delta_1 \) from zero to \( \pi\gamma\Delta_1 \). At \( \Omega < 2\Delta_1 \), \( Im\Pi_{sc}(Q, \Omega) = 0 \) while \( Re\Pi_{sc}(Q, \Omega) \) gradually decreases and behaves as \( \pi\gamma\Omega^2/(8\Delta_1) \) at small \( \Omega \). This behavior of \( \Pi_{sc}(Q, \Omega) \) guarantees that \( \chi(Q, \Omega) \) from (1) has a pole somewhere below \( 2\Delta_1 \) (a spin exciton) [21]. The exciton frequency is close to \( 2\Delta_1 \) at small \( \xi \), but progressively shifts down as \( \xi \) increases. At large \( \xi \), the pole is at \( \Omega = (8\Delta_1/(\pi\gamma))^{1/2} \xi^{-1} \). An important fingerprint of the 2D spin exciton scenario is a negative momentum dispersion of the peak, which originates from the fact that the energy of the exciton must vanish at the momentum which connects nodal points on the Fermi surface.

For \( s^- \)-wave gap symmetry, \( Re\Pi_{sc}(Q, 0) \) is negative, \( Re\Pi_{sc}(Q, 2\Delta_1) \) does not diverge, and the calculations show [13] that \( Re\Pi_{sc}(Q, \Omega) \) remains negative for all \( \Omega \) in which case spin exciton does not emerge.

Consider now whether one can pass this consideration to a three-dimensional \( \text{CeCoIn}_5 \). The dHvA experiments on \( \text{Ce115} \) have found several small 3D FS and a large 3D hole FS, whose size is large enough such that this FS contains hot lines – contours of FS points connected by a 3D diagonal \( Q_0^{3D} \). To verify whether such FS may be responsible for the spin resonance, we now re-evaluate the staggered spin susceptibility, Eq. (1), for a model system with a spherical FS with a diameter \( r_0 > \sqrt{3}/4 \). The hot lines on this FS are specified by \( \cos \theta + \sqrt{3} \sin \theta \sin(\phi + \pi/4) = 3/(4r_0) \), where \( \theta \) and \( \phi \) are azimuthal and polar angles for a point on a hot line. We considered various symmetries of the pairing gap originating from different representations of the tetragonal
group, $D_4$: (i) one-dimensional representations $A_g$ ($\Delta_k \propto k_x^2 + k_y^2$), $B_{1g}$ ($\Delta_k \propto k_z^2 - k_y^2$), $B_{2g}$ ($\Delta_k \propto k_x k_y$), $A_{2g}$ ($\Delta_k \propto k_x k_y (k_z^2 - k_y^2)$) (the $A_{2g}$ gap would have too many nodes), and (ii) two-dimensional representation $E_g$ ($\Delta \propto k_z (k_x + ik_y)$, $\Delta \propto k_x k_z$, and $\Delta \propto k_z (k_x + k_y)$). We found that the 3D resonance in $\chi(Q, \Omega)$ is still possible only if the pairing gap retains the same $d$-wave, $k_x^2 - k_y^2$ symmetry as in the cuprates, i.e., at the spherical FS $\Delta_k = \Delta \sin^2 \theta \cos 2\phi$ (in 3D notations, $\Delta \propto Y_{2,2} + Y_{2,-2}$, where $Y_{1,m}(\theta, \phi)$ are spherical harmonics).

Compared to 2D case, the calculation of $\Pi(Q, \Omega)$ using 3D version of Eq. (3) involves a summation along the whole hot line. In the normal state, this does not lead to a new physics – we still have Landau overdamped excitations with $\Pi(Q, \Omega) = i\gamma_{3D} \Omega$. In a superconducting state, however, the integration along hot lines leads to three essential differences with the 2D case:

- 1. by symmetry, hot lines necessary cross the directions $\phi = (3\pi/4)(2n + 1)$, $n = 0, 1, 2, 3$, where the $d$-wave gap vanishes. This implies that $\text{Im} \Pi(Q, \Omega)$ is finite at any non-zero frequency

- 2. for an arbitrary point $k_F$ along a hot line, the gaps $\Delta_k$ and $\Delta_{k+Q}$ are not simply related, the condition $\Delta_k = -\Delta_{k+Q}$ is satisfied only for special symmetry points along a hot line. As a consequence, $\text{Re} \Pi(Q, 0) \propto \oint d\mathbf{k} (\Delta_k + \Delta_{k+Q})^2$ at $Q = Q_0^{(a)}$ is finite, negative, and of the order of $\gamma_{3D} \Delta$

- 3. the logarithmic divergence of $\text{Re} \Pi(q, \Omega)$ at a 3D analog of $2\Delta_1$ is removed due to gap variation along a hot line. A simple calculation shows that $\text{Re} \Pi(q, \Omega)$ only has a cusp at $\Omega \sim 1.55 \Delta$.

In Fig. 1 we plot real and imaginary parts of the polarization operator, and the full $\text{Im} \chi(Q, \Omega)$, Eq. (1) for two different $\xi$. We see that the resonance is still there, but it is rather broad, and the intensity is not enhanced compared to that of the normal state. This is in contrast to the sharp peak observed in the neutron experiment. Likely then, the observed peak does not come from 3D Fermi surfaces.

Still, the observed resonance could potentially be a spin exciton. As we said, dHvA experiments have found, that Ce115 has at least one Q2D FS (a FS for the electron 15-band). The last FS is a slightly corrugated parallelepiped with the base close to a square. If this FS was strictly cylindrical along the $z$-axis, the hot lines would be parallel to $z$, and for $d_{y^2-x^2}$ symmetry of the gap, $\Delta_{k+Q} = -\Delta_k$ for any $k$-point along a hot line. The integration over $z$ then would be harmless, and the excitonic resonance would be identical to the one in a purely 2D system, where it is sharp. There are two requirements: one is that the resonance frequency must be smaller than twice the gap maximum. The resonance in CeCoIn$_5$ is observed at $\Omega_{res} = 0.6meV$, below $T_c = 2.3K$. If we use a conservative estimate $2\Delta_{max} \sim 4T_c$, we do find that $\Omega_{res}$ is indeed smaller than $2\Delta_{max}$. The other requirement is that such Q2D FS must be large enough to contain hot spots in the $xy$ plane. For this, the area encircled by the extreme dHvA orbits, $S_{ext}$, (marked as $\alpha_{1,2,3}$ in Refs. [3, 4]) must exceed a quarter of the area of the Brillouin Zone: $S_{BZ} = (2\pi/a)^2$ ($a = 4.61410^{-8}cm$ in CeCoIn$_5$). One has:

$$S_{ext} = \mathcal{F} \left( \frac{2e\pi}{cb} \right),$$  (4)

where $\mathcal{F}$ is the experimental dHvA frequency. According to Refs. [3, 4, 7], the experimental ratio $4S_{ext}/S_{BZ}$ for $\alpha_1$ orbit is $1.15 > 1$. This implies that the area of a Q2D FS is indeed large enough to contain hot spots.

Such explanation of the resonance in CeCoIn$_5$, however, disagrees with the experiments in one important aspect. If the resonance is an effective 2D exciton, it should be present not only for $(1/2, 1/2, 1/2)$, but also for the whole set of momenta $Q = (1/2, 1/2, b)$, where $0 < b < 1/2$. In $\Delta$ the resonance intensity is clearly peaked at $b = 1/2$. The absence of strong resonances at other momenta may be the consequence of the facts that the Q2D FS is not a perfect cylinder as evidenced by the existence of 3 different dHvA orbits, that $\Delta$ generally varies along $z$ axis, and that 3D FS also contribute to $\Pi(Q, \Omega)$

Still, the constraints on the excitonic description call
for another possible explanations for the resonance in CeCoIn$_5$. A potential candidate is the “magnon” scenario, originally suggested for the cuprates [18]. In application to CeCoIn$_5$, this scenario assumes that this system is close to a AFM state, and contains quasi-localized spins of $f-$electrons coupled to each other and to conduction electrons. To account for the localized spins, one should include into the denominator of Eq. (1) an additional term $(\Omega/\omega_0)^2$ which in the hypothetical absence of the damping would give rise to a magnon mode with $\Omega = \omega_0 e^{-1}$. For itinerant fermions, $\omega_0$ is of order Fermi energy, and such term is negligible for $\omega \sim \Delta$. For HF materials, $\omega_0$ is much smaller, and a magnon mode well may have energy comparable to $\Delta$.

This mode should in principle be present both above and below $T_c$, but in the normal state it is washed out by Landau damping. In a superconductor, Landau damping is strongly reduced and below $\omega_c \sim \Delta$, and may have energy comparable to $\Delta$. If the Hamiltonian above $T_c$ is such that, in the hypothetical absence of damping would give rise to a magnon mode with $\Omega = \omega_0 e^{-1}$. For itinerant fermions, $\omega_0$ is of order Fermi energy, and such term is negligible for $\omega \sim \Delta$. For HF materials, $\omega_0$ is much smaller, and a magnon mode well may have energy comparable to $\Delta$.

This mode should in principle be present both above and below $T_c$, but in the normal state it is washed out by Landau damping. In a superconductor, Landau damping is strongly reduced at $\Omega \leq 2\Delta$, and the magnon may “clear up”. Furthermore, in 3D, $\text{Re} \Pi(Q, \Omega)$ is negative at $\Omega = Q^2 \Delta^2 D_1$, what effectively reduces $\xi$ and hence increases the stability of SC state against the onset of AFM.

Parameterwise, a magnon is overdamped above $T_c$ if $\gamma_{3D} \geq \xi^{-1}/\omega_0 \sim \xi^{-2}/\Delta$. Using $\gamma_{3D} \sim g^2\chi_0\nu(E_F)/E_F$, $g^2\chi_0\nu(E_F) \sim 1$, and taking $E_F \sim T_K$ for HF materials ($T_K$ is a Kondo temperature), we find that the inequality amounts to $(\Delta/T_K) \geq \xi^{-2}$, which can well be satisfied in Ce115 due to its proximity to AFM. Below $T_c$, the damping is reduced and $\text{Re} \Pi(Q, \Omega)$ changes sign. This $\text{Re} \Pi$ scales with frequency as $\gamma_{3D} \Omega^2/\Delta$, such that the denominator of Eq. (1) contains two $\Omega^2$ terms, and becomes (roughly)

$$\xi_{eff}^{-2} - \Omega^2 \left( \frac{1}{\omega_0^2} + \frac{\gamma_{3D}}{\Delta} \right),$$

where $\xi_{eff} = \xi - \text{Re} \Pi(0,0)$. Using $\omega_0 \sim \Delta$ and $\gamma_{3D} \geq \xi^{-2}/\Delta$, we see that the two $\Omega^2$ contributions are of comparable magnitude, i.e., the, restored resonance is partly a magnon, partly an exciton. We also note that, for the model considered above, $\text{Re} \Pi(Q, \Omega)$ changes sign and is quite small at $\Omega \sim \Delta$ (see Fig. 1b). If the magnon energy is in this range, the feedback electronic contribution is negligible, and the resonance below $T_c$ is simply a magnon, restored by superconductivity.

Quite obviously, the magnon scenario is not peculiar to $d_{x^2-y^2}$ gap symmetry, and holds also if the superconducting gap has an $s-$wave symmetry. The only difference is that, in the $s-$wave case, $\text{Re} \Pi(Q, 0)$ does not change sign for $Q = Q_{SD}^2$, and remains negative for all frequencies [19].

A possible way to distinguish between magnon and spin-exciton scenario is to study the dispersion of the resonance peak, $\Omega(Q \neq Q_{SD}^2)$. In the spin- exciton scenario, the dispersion must be negative, at least in some range of $Q$, because once $Q$ becomes equal to the diameter of the FS (modulo $2\pi$), it must, by symmetry, connect the points on the FS for which $d_{x^2-y^2}$ gap vanishes. For such $Q$, the frequency of the exciton must vanish. On the other hand, if the resonance is a magnon, its frequency should monotonically increase with deviations from $Q_{SD}^2$.

To summarize, in this paper we addressed the issue whether the resonance neutron peak observed in the superconducting state of CeCoIn$_5$ may be a spin exciton peculiar to $d_{x^2-y^2}$ symmetry of the pairing gap. We argued that the peak is unlikely a 3D exciton originating from 3D FS of CeCoIn$_5$, as such peak is too weak and does not raise above the normal state result. The sharp excitonic resonance still might come from Q2D FS of CeCoIn$_5$, but such resonance should be observed not only at $Q^2_{SD} = (1/2, 1/2, 1/2)$ but along the whole line of $(1/2, 1/2, b)$. We argued that the experimental data [14] do not immediately support this scenario. We presented another, more plausible explanation of the neutron data, namely, that the resonance is a magnon-type excitation of localized $f-$electrons, restored and modified by superconductivity. If the resonance is a magnon, its observation is not an argument for $d_{x^2-y^2}$ gap symmetry. We suggest to study the dispersion of the resonance to distinguish between the two scenarios.

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