Feedback Spin Resonance in Superconducting $CeCu_2Si_2$ and $CeCoIn_5$

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We show that the recently observed spin resonance modes in heavy-fermion superconductors $CeCoIn_5$ and $CeCu_2Si_2$ are magnetic excitons originating from superconducting quasiparticles. The wave vector $\mathbf{Q}$ of the resonance state leads to a powerful criterion for the symmetry and node positions of the unconventional gap function. The detailed analysis of the superconducting feedback on magnetic excitations reveals that the symmetry of the superconducting gap corresponds to a singlet $d_{x^2-y^2}$ state symmetry in both compounds. In particular this resolves the long-standing ambiguity of the gap symmetry in $CeCoIn_5$. We demonstrate that in both superconductors the resonance peak shows a significant dispersion away from $\mathbf{Q}$ which can be checked experimentally. Our analysis reveals the similar origin of the resonance peaks in the two heavy-fermion superconductors and in layered cuprates.

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The relation between unconventional superconductivity (SC) and magnetism in heavy-fermion systems and doped transition metal oxides is one of the most interesting research areas in condensed matter physics. Despite certain differences concerning the proximity to a Mott insulator in the transition metal oxides and the weak hybridization of the f electrons in the heavy-fermion systems, it is widely believed that in both cases short-range antiferromagnetic (AF) spin fluctuations are responsible for Cooper pairing with a d-wave order parameter. Furthermore, unconventional superconductivity itself has a strong feedback on the magnetic spin excitations in these systems below the superconducting transition temperature T_c. One example is the famous resonance peak observed in high-T_c cuprates by means of inelastic neutron scattering (INS) [1] whose nature is still actively debated [2].

For some time the cuprates were considered to be unique in displaying the resonance peak in the superconducting state. Then, remarkably INS revealed the formation of a new magnetic mode in the superconducting state of the $5f$-heavy-fermion compound UPd_2Al_3 with $T_c = 1.8$ K [3]. Its sharply peaked intensity, its temperature dependence and energy position well below $2\Delta_0$ (with Δ_0 being the maximum of the superconducting gap) strongly resembles the resonance peak seen in high-T_c cuprates. In distinction to the cuprates, the symmetry of the gap function was unclear for UPd_2Al_3. Thermal conductivity measurements in a rotating magnetic field showed that it has nodes in the hexagonal plane but could not determine the symmetry uniquely [4]. As already noticed in [3,5] and shown explicitly in [6] the observation of a resonance at the AF wave vector $\mathbf{Q}$ puts a stringent condition on the gap symmetry by requiring a sign change $\Delta_{\mathbf{k}+\mathbf{Q}} = -\Delta_{\mathbf{k}}$ under translation by $\mathbf{Q}$. Together with thermal conductivity results this determines unambiguously the gap function as $\Delta_{\mathbf{k}} = \Delta_0 \cos ck_z$ which has node lines at the boundaries of the antiferromagnetic Brillouin zone. The case of UPd_2Al_3 shows not only that the magnetic resonance due to a feedback effect of the SC state is a universal phenomenon in unconventional superconductors but also, that INS is a powerful technique to determine the superconducting gap symmetry.

Indeed, very recently the resonance peak has been also observed below the SC transition temperatures in Ce-based heavy-fermion compounds, namely, in $CeCu_2Si_2$ [7] at the (incommensurate) wave vector $\mathbf{Q}_{\rm SDW} \approx (0.22 \times 2\pi/a, 0.22 \times 2\pi/a, 0.52 \times 2\pi/c) = (0.22, 0.22, 0.52)$ reciprocal lattice units (r.l.u.) and in $CeCoIn_5$ [8] at the antiferromagnetic wave vector $\mathbf{Q}_{\rm AF} \approx (\pi/a, \pi/a, \pi/c) = (0.5, 0.5, 0.5)$ r.l.u. The latter system which has quasi-two-dimensional tetragonal crystal structure shows the highest SC transition temperature $T_c = 2.7$ K among heavy-fermion compounds [9]. Its gap symmetry has been long disputed because of conflicting results from angle resolved magnetothermal conductivity [10] ($d_{x^2-y^2}$-symmetry) and specific heat [11] (d_{xy}-symmetry) measurements [12]. The INS results [8] and the analysis presented here give a clear resolution of this puzzle in favor of the $d_{x^2-y^2}$ state which underlines again the importance of INS for determining the superconducting gap symmetry. Heavy quasiparticles in the Ce compounds [14,15] of predominantly $4f$ character are more strongly correlated than $5f$ quasiparticles of UPd_2Al_3 or quasiparticles in cuprates.

Here, we analyze the magnetic susceptibility in $CeCu_2Si_2$ and $CeCoIn_5$ in the SC state. We show that in both cases the resonance feature evolves at the magnetic instability wave vector. We discuss the dispersion of the resonant excitations as a function of the momentum and demonstrate that in both compounds the $d_{x^2-y^2}$-wave symmetry of the superconducting order parameter is consistent with the INS experiments.

Starting our analysis by considering the $CeCu_2Si_2$ system, we note that a good starting point for calculating the magnetic susceptibility is the band structure obtained within the renormalized band theory [16–18]. This method is essentially a one-parameter theory which reproduces the Fermi surfaces and the highly anisotropic masses of the heavy-fermion compounds quite well. The ansatz starts from an *ab initio* local-density approximation (LDA) calculation for the weakly correlated conduction electrons. The strong correlations are introduced by choosing resonance-type $4f$ phase shifts. Both the width and the position of the resonance are closely related to a characteristic (Kondo) temperature which is determined from the linear slope of the low-temperature specific heat. Crystalline electric field splitting strongly affects the quasiparticle dispersion and has to be properly accounted for [19]. Note that the formation of a resonance in the spin response is determined mainly by the unconventional symmetry of the superconducting order parameter. Therefore it is reasonable to use a tight-binding fit to the main heavy-quasiparticle band that crosses the Fermi level. In particular, we assume an energy dispersion of the form $\varepsilon_{\mathbf{k}} = 2t_1(\cos k_x a + \cos k_y a) + 4t_2 \cos k_x a \cos k_y a + 8t_3 \cos\frac{k_x a}{2} \times \cos\frac{k_y a}{2} \cos\frac{k_z c}{2} - \mu$, where $t_1 = 17.5$, $t_2 = -5.2$, $t_3 = -11.2$, and $\mu = -57.4$ (in K) are the hopping integrals and the chemical potential, respectively. The corresponding Fermi surface (FS) consisting of stacked columns along c direction is shown in Fig. 1(a) in the first few Brillouin zones. The obtained FS shows a flat part connected by the nesting wave vector $\mathbf{Q}_{\mathrm{SDW}} = (0.22, 0.22, 0.52)$ r.l.u. as indicated by the arrow. As discussed in earlier work [20] the $\mathbf{Q}_{\mathrm{SDW}}$ agrees very well with the experimentally observed SDW in the so-called A phase of that compound.

In Fig. 1(b) we show the static Lindhard susceptibility $\chi_0(\mathbf{q})$ calculated with the parameterized heavy quasiparticles. One finds that $\chi_0(\mathbf{q})$ is peaked at $\mathbf{Q}_{\mathrm{SDW}}$. When compared with a fully renormalized band structure calculation [16] we observe that the tight-binding bands result in a somewhat more pronounced nesting and yield a whole contour of the nesting wave vectors around $\mathbf{Q}_{\mathrm{SDW}}$. This is due to the relatively simple band structure that contains few nearest neighbors hopping integrals only. However, this does not influence our results concerning the resonance feature below T_c, since the latter is determined mainly by the special nature of the superconducting gap.

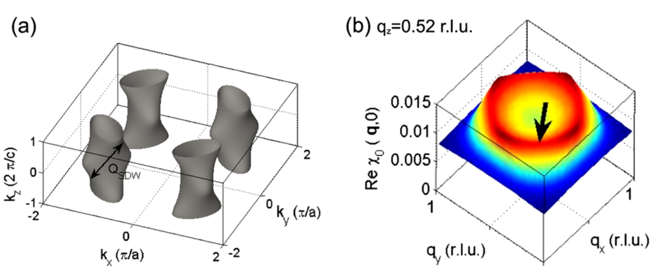

FIG. 1 (color online). (a) Calculated FS for the main heavy-quasiparticle band in $CeCu_2Si_2$ using the tight-binding parametrization as described in the text. Note that the values are strongly renormalized due to the coupling of the conducting electrons with $4f$ orbitals. Here, $a = 4.1$ Å and $c = 9.92$ Å are the lattice constants. The arrow indicates the SDW scattering wave vector. (b) Calculated static spin susceptibility on two-dimensional mesh for $q_z = 0.52$ r.l.u. The arrow indicates the SDW ordering wave vector, $\mathbf{Q}_{\mathrm{SDW}}$, as observed in experiment [16].

The resonance peak in the SC state of $CeCu_2Si_2$ as well as of $CeCoIn_5$ can be understood by considering the dynamical spin susceptibility within the random phase approximation (RPA), i.e.,

$$\chi_{\mathrm{RPA}}(\mathbf{q}, \omega) = \frac{\chi_0(\mathbf{q}, \omega)}{1 - U_{\mathbf{q}}\chi_0(\mathbf{q}, \omega)}, \tag{1}$$

where $U_{\mathbf{q}}$ is the fermionic four-point vertex and $\chi_0(\mathbf{q}, \omega)$ is the heavy-quasiparticle susceptibility. The latter is given by the sum of the well-known bubble diagram consisting of either normal or anomalous ($T < T_c$) Green functions. For large momenta $\mathbf{q}$, $\mathrm{Im}\chi_0(\mathbf{q}, \omega)$ is zero at low frequencies and can exhibit a discontinuous jump at the onset frequency of the particle-hole (p-h) continuum $\Omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{q}}|)$, where both $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ lie on the Fermi surface [21]. Note, however, that the discontinuity in $\mathrm{Im}\chi_0$ occurs only if $\mathrm{sgn}(\Delta_{\mathbf{k}}) = -\mathrm{sgn}(\Delta_{\mathbf{k}+\mathbf{q}})$ which is not possible for isotropic s-wave order parameter. A discontinuity in $\mathrm{Im}\chi_0$ leads to a logarithmic singularity in $\mathrm{Re}\chi_0$. As a result, the resonance conditions (i) $U_{\mathbf{q}}\mathrm{Re}\chi_0(\mathbf{q}, \omega_{\mathrm{res}}) = 1$ and (ii) $\mathrm{Im}\chi_0(\mathbf{q}, \omega_{\mathrm{res}}) = 0$ can be both fulfilled at $\omega_{\mathrm{res}} < \Omega_c$ for any $U_{\mathbf{q}} > 0$, leading to the occurrence of a resonance peak in form of a spin exciton below T_c. For finite quasiparticle damping Γ, condition (i) can only be satisfied if $U_{\mathbf{q}} > 0$ exceeds a critical value, while condition (ii) is replaced by $\mathrm{Im}\chi_0(\mathbf{q}, \omega_{\mathrm{res}}) \ll 1$.

Since the symmetry of the superconducting gap has not yet been determined unambiguously in $CeCu_2Si_2$, we have analyzed all the spin singlet s- and d-wave functions allowed by the crystal-group symmetry of the lattice [16,22,23]. We have found that the resonancelike feature, i.e., the discontinuous jump in $\mathrm{Im}\chi_0$ and the corresponding logarithmic singularity in $\mathrm{Re}\chi_0$ occur at $\mathbf{Q}_{\mathrm{SDW}}$ for three types of the order parameters: two-dimensional $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x a - \cos k_y a)$ belonging to the B_{1g} irreducible representation, and also for each of the two components of the E_{1g} representation, $\Delta_{\mathbf{k}} = \Delta_0 \sin k_x a \sin k_z c$ and $\Delta_{\mathbf{k}} = \Delta_0 \sin\frac{(k_x+k_y)a}{2} \sin\frac{k_z c}{2}$. At the same time no resonance exists for the two-dimensional $\Delta_{\mathbf{k}} = \Delta_0 \sin k_x a \sin k_y a$ symmetry of the order parameter which belongs to the B_{2g} irreducible representation. An important finding is that for our dispersion the resonance in the B_{1g} channel is by far the strongest. In Fig. 2(a) we show the RPA susceptibility in the normal and the SC state for the B_{1g} ($\Delta_{\mathbf{k}} = \Delta_0(\cos k_x a - \cos k_y a)$) and for the B_{2g} ($\Delta_{\mathbf{k}} = \Delta_0 \sin k_x a \sin k_y a$) channels, respectively. One finds that the susceptibility for the B_{1g} symmetry is larger in the SC state than it is in the normal state, while in the B_{2g} channel there is no enhancement of the normal state spin susceptibility. This definitely points towards a $d_{x^2-y^2}$-wave symmetry of the SC gap in $CeCu_2Si_2$ since a very sharp resonance was found at $\mathbf{Q}_{\mathrm{SDW}}$ in INS [7]. We note, however, that the magnitude of the resonance for each symmetry is a result of a competition of various features, i.e., the curvature of the Fermi surface at the points connected by $\mathbf{Q}_{\mathrm{SDW}}$, the absolute value of the SC gap and also the velocity at the node of the gap. A modification of the electronic dispersion, and the actual angular dependence of the superconducting gap can modify the results for the absolute intensity of the resonance peak [24].

The resonance condition is also satisfied for momenta $\mathbf{q}_i$ slightly away from $\mathbf{Q}_{\mathrm{SDW}}$ as long as $\mathrm{sgn}(\Delta_{\mathbf{k}}) = -\mathrm{sgn}(\Delta_{\mathbf{k}+\mathbf{q}_i})$. We find that the resonance is readily suppressed by variation of the in-plane (q_x, q_y)-momentum and exists only in the close vicinity to $\mathbf{Q}_{\mathrm{SDW}}$. This is because for an incommensurate momentum there are always scattering processes which involve parts of the Fermi surface with $\mathrm{sgn}(\Delta_{\mathbf{k}}) = +\mathrm{sgn}(\Delta_{\mathbf{k}+\mathbf{Q}_i})$ thus suppressing the resonance. In addition, varying $\mathbf{Q}_i$ away from $\mathbf{Q}_{\mathrm{SDW}}$ along the in-plane $(q_x, q_y, q_z^{\mathrm{SDW}})$ direction the nesting condition is also lost which overall yields a decrease of $\mathrm{Re}\chi_0$ [see also Fig. 1(b)]. Since the suppression of the resonance occurs for all symmetries of the above mentioned superconducting order parameters the resonance peak is confined to momentum $(q_x, q_y, q_z^{\mathrm{SDW}})$ in the plane around $\mathbf{Q}_{\mathrm{SDW}}$. At the same time the situation is less dramatic with respect to the q_z momentum dependence. In Fig. 2(b) we show the dispersion of the resonance along the q_z direction. One finds that it remains nearly flat as one departs from $\mathbf{Q}_{\mathrm{SDW}}$. As a matter of fact, for a constant interaction $U_{\mathbf{q}}$, the resonance shows a weak dispersion resulting from the slight change of the $\mathrm{Re}\chi_0$ away from $\mathbf{Q}_{\mathrm{SDW}}$.

Let us now turn to the resonance peak formation in $CeCoIn_5$ [8]. According to the band structure calculations [25], $CeCoIn_5$ comprises several f- and conduction bands which are hybridized in a complex manner. Therefore, it is quite difficult to reproduce a resulting structure by using a single band model. Introducing a two-band model is much more appropriate. In fact, this has been done previously for $CeCoIn_5$ [25] and the resulting energy dispersion crossing the Fermi level can be written as:

$$E_{2\mathbf{k}} = \tfrac{1}{2}[(\varepsilon_{\mathbf{k}}^c + E_{\mathbf{k}}^f) - \sqrt{(E_{\mathbf{k}}^f - \varepsilon_{\mathbf{k}}^c)^2 + 4V_{\mathbf{k}}^2}], \qquad (2)$$

where $E_{\mathbf{k}}^f$ and $\varepsilon_{\mathbf{k}}^c$ is the effective f-band and the conduction band dispersions, respectively, and $V_{\mathbf{k}}$ is the effective hybridization strength, renormalized by the on-site $f-f$-Coulomb repulsion. The resulting FS is shown in Fig. 3(a). Like for $CeCu_2Si_2$ the present FS has again nesting properties. However, here it occurs for the the commensurate antiferromagnetic wave vector $\mathbf{Q}_{\mathrm{AF}} = (\pi/a, \pi/a, \pi/c)$. This agrees with recent INS data on the normal state [8]. In Fig. 3(b) we show the static Lindhard spin susceptibility for the normal state calculated on a two-

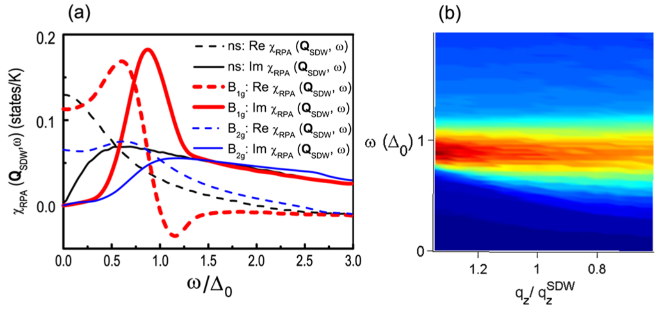

FIG. 2 (color online). (a) Calculated real and imaginary parts of the RPA spin susceptibility for the normal (black) and superconducting state for the B_{1g} (red) and B_{2g} (blue) symmetry of the superconducting gap. Here, we assume $U_{\mathbf{Q}_{\mathrm{SDW}}} \approx 4t_1$ to satisfy the resonance condition in the superconducting state. For numerical purposes we also set the damping $\Gamma = 2$ K. (b) Calculated dispersion of the resonance peak in $CeCu_2Si_2$ for $(0.22, 0.22, q_z)$ direction. The dispersion is nearly flat around $\mathbf{Q}_{\mathrm{SDW}}$ due to the two-dimensional structure of the superconducting gap. Here, we have introduced an interaction peaked at $\mathbf{Q}_{\mathrm{SDW}}$ in the form $U_{\mathbf{q}} \approx U_{\mathbf{Q}_{\mathrm{SDW}}}[1 - B \cdot \frac{(\mathbf{q}-\mathbf{Q}_{\mathrm{SDW}})^2}{\mathbf{Q}_{\mathrm{SDW}}^2}]$ with $B = 0.5$. This phenomenological form of the vertex yields the total RPA susceptibility in the normal state to be peaked at $\mathbf{Q}_{\mathrm{SDW}}$.

dimensional mesh. In accordance with the FS topology we find that the spin susceptibility is peaked at the antiferromagnetic wave vector, $\mathbf{Q}_{\mathrm{AF}}$.

To address the issue of the resonance peak formation, we show in Fig. 4(a) the calculated real and imaginary part of the RPA susceptibility at the AF wave vector in the normal and the SC states. Among possible superconducting symmetries in $CeCoIn_5$ a resonance peak forms only for the B_{1g} $(\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x a - \cos k_y a))$ symmetry. As in the case of $CeCu_2Si_2$ the antiferromagnetic wave vector connects states with opposite sign of the superconducting gap. As is clearly visible from Fig. 3(a) this results in the formation of

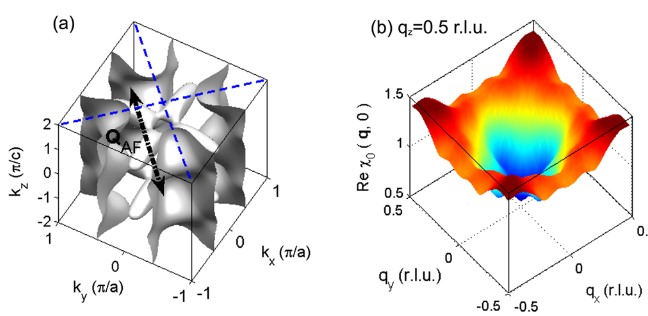

FIG. 3 (color online). (a) Calculated Fermi surface for $CeCoIn_5$ using the band structure parameters adopted previously [25]. The dash-dotted arrow points at states at the Fermi surface scattered by the antiferromagnetic wave vector, $\mathbf{Q}_{\mathrm{AF}}$. The dashed lines depict the position of nodes in the first BZ for a superconducting order parameter of $d_{x^2-y^2}$-wave symmetry. Following Ref. [25] we set the energy unit 0.26 eV. (b) Calculated static spin susceptibility of Kondo-hybridized bands in $CeCoIn_5$ for $q_z = 0.5$ r.l.u. on a two-dimensional mesh.

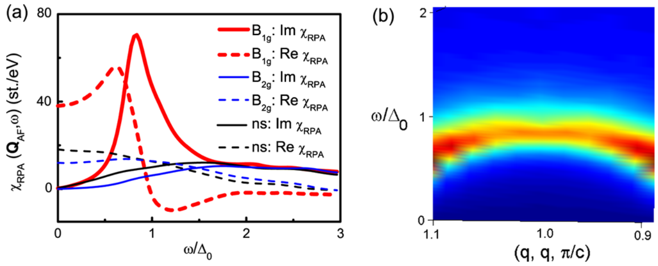

FIG. 4 (color online). (a) Calculated real and imaginary part of the RPA susceptibility at the $\mathbf{Q}_{\rm AF}$ for $CeCoIn_5$ as a function of frequency in the normal (black) and superconducting, B_{1g} (red) and B_{2g} (blue) states. We have assumed that $U_{\mathbf{Q}_{\rm AF}} = U_0 \approx 1.66t$. (b) Calculated dispersion of the resonance peak in $CeCoIn_5$ for the $d_{x^2-y^2}$-wave symmetry of the superconducting order parameter along the $(q, q, \pi/c)$ direction. Similar to $CeCu_2Si_2$ we use $U_{\mathbf{q}} \approx U_{\mathbf{Q}_{\rm AF}}[1 - B \cdot \frac{(\mathbf{q}-\mathbf{Q}_{\rm AF})^2}{\mathbf{Q}_{\rm AF}^2}]$ with $B = 0.8$.

a resonance peak similar to the one in $CeCu_2Si_2$. The resonance peak forms near the particle-hole continuum, i.e., close to $\Omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{q}}|)$ which is around Δ_0. This is because the points connected by $\mathbf{Q}_{\rm AF}$ are lying relatively far from the part of the Fermi surface where the gap function has maximum value. Note, if the Cooper-pairing itself arises due to an exchange of AF spin fluctuations, the maximum of the SC gap occurs at points of the Fermi surface which are connected by $\mathbf{Q}_{\rm AF}$. At the same time, the superconducting gap possesses still the $d_{x^2-y^2}$-wave symmetry though including higher harmonics. It is remarkable that like in $CeCu_2Si_2$ we find that only a gap function of $d_{x^2-y^2}$-wave (B_{1g}) type results in the formation of the resonance peak at $\mathbf{Q}_{\rm AF}$. This unambiguously confirms the bulk symmetry of the superconducting gap in $CeCoIn_5$. The d_{xy}-wave (B_{2g}) symmetry discussed in the literature is clearly ruled out.

Finally, in Fig. 4(b) we show the dispersion of the resonance excitations away from the $\mathbf{Q}_{\rm AF}$. We observe that the resonance disperses downwards as a function of frequency. This behavior is similar to that found in hole-doped high-T_c cuprates. In particular, the value of the critical frequency $\Omega_c = |\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{q}}|$ lowers for $\mathbf{q} < \mathbf{Q}_{\rm AF}$ for the in-plane momentum, since this wave vector connects states closer to the diagonal part of the BZ where the superconducting gap is smaller. As a result, the resonance condition shifts to lower energies.

In conclusion, we have analyzed the dynamical magnetic susceptibility in $CeCu_2Si_2$ and $CeCoIn_5$ below the SC transition temperature. We show that in both cases a resonance feature evolves at the wave vector of the magnetic instability. Our results show that the two heavy-fermion superconductors and the high-T_c cuprates possess the same symmetry of the superconducting order parameter suggesting that a similar mechanism for Cooper-pairing is probably involved. Furthermore, despite of the three-dimensional electronic structure, the two-dimensional $d_{x^2-y^2}$-wave superconducting gap in $CeCu_2Si_2$ and $CeCoIn_5$ may provide further hints on the microscopic mechanism of unconventional superconductivity in heavy-fermion systems and in layered cuprates.

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Note added in proof.—After submission of this work, we became aware of Ref. [26], where the similar problem has been addressed for the spherical Fermi surface.

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