Unconventional Cooper pairing in the superconducting state of UPd_2Al_3

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A possible type of Cooper pairing in an anisotropic superconducting state of UPd_2Al_3 is discussed on the basis of the recent measurement of magnetic exciton modes which are expected to mediate the pairing interaction. The most likely gap is one with A_g symmetry with the line node on the plane very close to the zone boundary of the folded Brillouin zone in the antiferromagnetically ordered state.

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Recent neutron-scattering experiments regarding UPd_2Al_3, following the paper by Sato *et al.*,[1] have provided us crucial information regarding the type of Cooper pairing of its unconventional superconducting state. In particular, Bernhoeft suggested, in regard to the effect of the coherence factor on neutron-scattering intensity, that the following anisotropic gap with A_g symmetry may be realized in its superconducting state:[2]

$$\Delta_{\vec{k}} \propto \cos(k_z c) - \frac{1}{5}\cos(3k_z c) + \frac{1}{30}\cos(5k_z c), \tag{1}$$

where c is the lattice constant in the c direction of the paramagnetic state. We have also shown independently using a more explicit model of this system's magnetic excitations that the pairing may be mediated by the magentic excitons associated with crystal-field singlet ground state and that its symmetry may be also be that of A_g.[3,4] Recently, Huth *et al.* showed, on the basis of a phenomenological form of spin-fluctuation spectrum, that the type of gap proposed by Bernhoeft can be realized.[5]

In this paper, we supplement the discussions on the type of Cooper pairing expected in Ref. 3 in which the origin of pairing interaction $V_{\vec{k},\vec{k}'}$ is attributed to the exchange of magnetic excitons which have an excitation threshold at $\vec{Q}_0 = (0,0,\pi/c)$, c being the lattice constant in the c direction in the paramagnetic phase, and which have considerable dispersion $\omega(\vec{Q}_0+\vec{q})$ along $\vec{q}\parallel c$. Our discussion is based on a more explicit picture of heavy electrons in the antiferromagnetically ordered state, relative to that described in Ref. 4.

In the itinerant-localized duality model of heavy fermions,[6] the itinerant quasiparticles interact with the localized component of spin degrees of freedom via exchange coupling $\lambda \sim \mathcal{O}(T_0)$, T_0 being the characteristic energy scale of quasiparticles, although the basic physics behind this picture in U-based heavy fermions,[7] containing plural f electrons per U ion, is rather different from that in Ce-based ones which contain nearly one f electron per Ce ion.[6] In this model, the dynamical susceptibility $\chi(\vec{Q}_0,\omega)$ is given by

$$\chi^{-1}(\vec{q},\omega) = \chi_0^{-1}(\omega) - J(\vec{q}) - \lambda^2 \Pi(\vec{q},\omega), \tag{2}$$

where $\chi_0(\omega)$ is the local susceptibility, $J(\vec{q})$ is the exchange interaction between the local component of spins, λ is the exchange coupling between the spins of quasiparticles and the local component of spins, and $\Pi(\vec{q},\omega)$ is the polarization function of quasiparticles.[6,8]

Thus, the pairing interaction $H_{\rm pair}$ mediated by ''spin fluctuations'' is given by, in the weak-coupling limit,

$$H_{\rm pair} = \sum_{\vec{k},\vec{k}'} \sum_{\alpha\beta,\gamma\delta} V_{\vec{k},\vec{k}'} (\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta}) a^\dagger_{\vec{k}\alpha} a^\dagger_{-\vec{k}\gamma} a_{-\vec{k}'\delta} a_{\vec{k}'\beta}, \tag{3}$$

where the $V_{\vec{k},\vec{k}'}$ is given by

$$V_{\vec{k},\vec{k}'} = -\lambda^2 \chi(\vec{k}-\vec{k}',0), \tag{4}$$

and $\vec{\sigma}$ denotes a vector spanned by the Pauli matrices. It is noted here that $(\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta}) = -3$ for the even-parity (''spin-singlet'') pairings and $(\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta}) = 1$ for the odd-parity (''spin-triplet'') pairings. While we here discuss the problem in the weak-coupling language, it can be readily extended to the strong-coupling formalism on which we have analyzed in Ref. 3 the data of tunneling experiment.[9]

Since the zeros of $\chi^{-1}(\vec{q},\omega)$ in the ω plane gives the dispersion $\omega(\vec{q})$ of the magnetic excitons and $\omega(\vec{q})$ has a minimum at $\vec{q}=\vec{Q}_0 \equiv (0,0,\pi/c)$, $\chi(\vec{q},0)$ has a maximum at $\vec{q}=\vec{Q}$. Thus, $-V_{\vec{k},\vec{k}'}$ at $\vec{k}-\vec{k}'=\vec{Q}_0$. It is also noted that the Brillouin zone for magnetism is the same as that in the paramagnetic state while the Brillouin zone of the quasiparticles is folded so that the Γ point (0,0,0) and the point $(0,0,\pi/c)$ are equivalent with each other. This is due to the periodicity of J being $J(\vec{q}+2\vec{Q}_0)=J(\mathbf{q})$, while that of Π is $\Pi(\vec{q}+\vec{Q}_0)=\Pi(\vec{q})$, as shown schematically in Fig. 1. Therefore, due to the $\vec{q}$ dependence of exchange interaction J, $\chi(\vec{q},0)$ may have minimum at around $\vec{q}=(0,0,0)$, and thus $V_{\vec{k},\vec{k}'}$ at $\vec{k}-\vec{k}'=(0,0,0)$.

According to this argument, we can see that the strength of pairing interaction $-3V_{\vec{k},\vec{k}'} = 3\lambda^2\chi(\vec{k}-\vec{k}',0)$, in the singlet channel, has a maximum at $\vec{k}-\vec{k}'=(*,*,\pi/c)$ and a minimum at $\vec{k}-\vec{k}'=(*,*,0)$. Therefore, it may be expanded as

$$-3V_{\vec{k},\vec{k}'} = V_0 - \sum_{n=1} V_n \cos[(2n-1)(k_z-k_z')c], \tag{5}$$

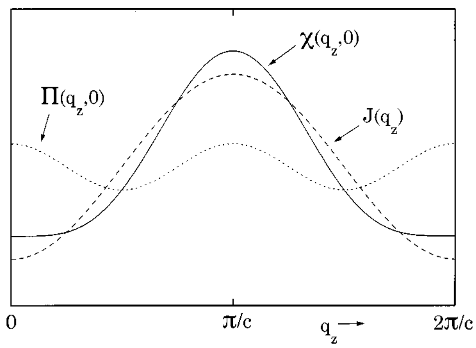

FIG. 1. Schematic q_z dependence of $J(q_z)$, $\Pi(q_z,0)$, and $\chi(q_z,0)$: Dashed line for J, dotted line for Π, and solid line for χ. While $q_z=\pi/c$ is the zone boundary of the 1st Brillouin zone in the paramagnetic state, it is equivalent to the Γ point in the antiferromagnetically ordered state as far as the quasiparticle dispersions are concerned. It is noted that $\Pi(q_z+\pi/c,0)=\Pi(q_z,0)$.

where V's are some positive constants with weak dependence on (k_x-k_x') and (k_y-k_y') in general which we denote a *'s above. This is a generalization of the form of pairing interaction discussed in Ref. 10.

With use of the addition theorem of trigonometric function, the terms of the right-hand side of Eq. (4) are expressed in the form

$$[\cos(mk_zc)\cos(mk_z'c)+\sin(mk_zc)\sin(mk_z'c)],$$

so that the superconducting gap in the ''spin-singlet'' channel can be expanded as

$$\Delta_k=\Delta_0+\sum_{n=1}\Delta_n\cos[(2n-1)k_zc], \tag{6}$$

with constants Δ's, because the gap is given by

$$\Delta_{\vec{k}}=-\sum_{\vec{k}'}(-3)V_{\vec{k},\vec{k}'}\frac{\Delta_{\vec{k}'}}{E_{\vec{k}'}}\tanh\frac{E_{\vec{k}'}}{2T}, \tag{7}$$

where $E_{\vec{k}}\equiv[\xi_{\vec{k}}^2+|\Delta_{\vec{k}}|^2]^{1/2}$, with the quasiparticle dispersion $\xi_{\vec{k}}$. It is noted that the ''spin-triplet'' pairing is difficult to form because the factor $(\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta})=1$ in Eq. (3) causes the dominant component of paring interaction $V_{\vec{k},\vec{k}'}$ given by Eq. (5) to be repulsive.[10] However, it is not completely excluded in principle that the triplet pairing is induced with use of salient variation of V_n's, which are all positive, as discussed in Ref. 11.

The constant component of gap Δ_0 is known to be small enough compared to the other component with $n\geqslant 1$ in general, as long as the paring interaction has strong on-site repulsion.[12] This type of gap has line nodes on the plane very near $k_z=\pi/2c$, while its symmetry belongs to A_g due to a speciality of the magnetic order of UPd_2Al_3. Namely, the counterpart of this pairing, in the system with a hypothetical isotropic band, does not correspond to the s-wave pairing, but say to the d-wave one with a basis function such as

$$Y_2^0(\hat{k})\equiv\sqrt{5/16\pi}(3\hat{k}_z^2-1), \tag{8}$$

with some admixtures of $Y_0^0(\hat{k})\equiv 1/\sqrt{2\pi}$.

The gap of the type (6) vanishes on the plane very near the zone boundary $k_z=\pi/2c$ of the magnetically ordered state. This type of gap is approximately the same as that proposed by Bernhoeft[2] so as to explain the wave-number dependence of the magnetic structure factor, and is also consistent with that proposed in Refs. 9 and 4.

In conclusion, we have discussed how the anisotropic superconducting gap with A_g symmetry in UPd_2Al_3 is induced by the pairing interaction through the exchanging magnetic excitons which have been observed in inelestic neutron scatterings.

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