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LETTER TO THE EDITOR

Unconventional superconductivity with a radial-node gap in quasi-one-dimensional metals

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Abstract
It is shown that a new type of superconductivity is possible in one-dimensional (1D) and quasi-one-dimensional (Q1D) metals where the pairing interaction is mediated by both spin and charge fluctuations. The gap function inevitably changes sign in the radial direction near the Fermi surface; it vanishes at the Fermi points for 1D, and for Q1D it has line nodes on the Fermi surface as in usual anisotropic pairings. The transition temperature T_c is generally higher for the singlet pairing than for the triplet, but only by a few times. This implies that T_c for the triplet pairing can exceed that of the singlet under a moderately large Zeeman magnetic field, i.e., field-induced triplet pairing. This feature seems to explain the anomalous behaviours of H_{c2} and the Knight shift observed in $(TMTSF)_2PF_6$.

1. Introduction

The systematics of the superconducting mechanism in strongly correlated electron systems may be one of the most important subjects in condensed matter physics. In superconductors adjacent to the antiferromagnetic states, it is generally believed that anisotropic spin-singlet pairing (SP) is realized due to the effects of antiferromagnetic spin fluctuations [1–3]. The superconducting phase of the quasi-one-dimensional (Q1D) conductor $(TMTSF)_2PF_6$ is located close to the spin density wave (SDW) phase [4], and it is naturally assumed that SP is realized also in $(TMTSF)_2PF_6$. However, recent experimental data on $(TMTSF)_2PF_6$, such as the unsaturated behaviour of H_{c2} in the low-temperature region [5] and the absence of the Knight shift suppression below the transition temperature T_c [6], suggest that spin-triplet pairing (TP) is realized in such Q1D metals under magnetic fields. Recently, Kuroki *et al* [7] tackled this system with the FLEX approximation and observed that SP is stabilized compared to

TP. They then proposed, on phenomenological grounds, that a coexistence of charge and spin fluctuations, not included in the FLEX approximation, may stabilize TP.

One of the characteristic features of the one-dimensional (1D) interacting fermion system is that the charge and spin fluctuations show the same power-law singularity at wavenumber $2k_{\rm F}$ ($k_{\rm F}$ being the Fermi wavenumber) [8]. Therefore, the two fluctuation types are expected to contribute to the pairing interaction with comparable weight [9].

The purpose of this letter is to explain the apparently puzzling behaviour of $(TMTSF)_2PF_6$ by taking into account these 1D characteristics of spin and charge fluctuations. As shown below, such pairing interaction leads to a novel type of superconducting gap, which changes sign in the radial direction. The TP can be competitive with the SP and will be stabilized under moderately large magnetic fields. This feature seems to simulate well the existing experimental data on $(TMTSF)_2PF_6$ [5, 6].

We first study the purely 1D system to gain a clear picture to the origin of this novel radial-node gap. It is known that in purely 1D metals the fluctuations destroy superconductivity. We shall implicitly assume that a interchain hopping $t_\perp$ necessary for the stabilization of the superconductivity which, however does not introduce large corrections to the main effect. Next, we introduce $t_\perp$ and discuss the competition between the SDW ordering and the present superconductivity ordering. The effects of the unitary impurities are also studied for Q1D systems.

2. Purely one-dimensional case

We consider 1D and Q1D systems described by the Hubbard Hamiltonian

$$H = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + U \sum_{i,\ell} n_{i\ell,\uparrow} n_{i\ell,\downarrow}, \tag{1}$$

where $c^\dagger_{\boldsymbol{k}\sigma}$ is the electron creation operator of wavevector $\boldsymbol{k} = (k, k_\perp)$ and spin σ, $n_{i\ell,\sigma}$ is the number of spin-σ electrons at site i on the ℓth chain, and $U > 0$. The kinetic energy is given by

$$\xi_{\boldsymbol{k}} = -2t \cos k - 2t_\perp \cos k_\perp - \mu \qquad (t \gg t_\perp), \tag{2}$$

where k ($k_\perp$) and t ($t_\perp$) are the wavenumber and the transfer integral, respectively, along (perpendicular to) the conducting chains. The lattice constants are taken as unity for both directions.

In purely 1D systems ($t_\perp = 0$), the charge ($\chi_{\rm c}$) and spin ($\chi_{\rm s}$) susceptibilities show power-law singularities $\sim |q \pm 2k_{\rm F}|^{-\alpha}$ with the same exponent α [8]. For convenience, we model their q-dependence by

$$\chi_{\rm 1D}(q) = \frac{\left(\tan\frac{k_{\rm F}}{2}\right)^\alpha}{4\pi t\alpha \sin\frac{q}{2}} \left\{ \left| \tan\frac{q - 2k_{\rm F}}{4} \right|^{-\alpha} - (q \to -q) \right\} \tag{3}$$

and write it as $\chi_{\rm c,s}(q) = (2v_{\rm F} K_{\rm c,s}/v_{\rm c,s})\chi_{\rm 1D}(q)$. Here $v_{\rm F} = 2t \sin k_{\rm F}$ is the Fermi velocity and $v_{\rm c}$ ($v_{\rm s}$) is the charge (spin) velocity. Equation (3) has the same singularity at $q = \pm 2k_{\rm F}$, has a fixed (α-independent) value of $1/\pi v_{\rm F}$ at $q = 0$, and reduces to the susceptibility of non-interacting electrons (with logarithmic singularity) in the limit $\alpha \to 0$. This form is not unique, but other choices do not affect the main results of this letter. The exponent α is known to lie in a range $0 < \alpha < 0.5$ for repulsive interaction $U > 0$.

The pairing interaction generally takes the form $V_{\boldsymbol{k},\boldsymbol{k}'} = I_{\boldsymbol{k},\boldsymbol{k}'} + (\vec{\sigma}\cdot\vec{\sigma}') J_{\boldsymbol{k},\boldsymbol{k}'}$, where I and J arise from processes exchanging charge and spin fluctuations, respectively, and $(\vec{\sigma}\cdot\vec{\sigma}') = -3$ for SP and 1 for TP [10, 11]. We adopt the model interactions $I_{\boldsymbol{k},\boldsymbol{k}'} = \tilde{U} - (I_{\rm c}^2/4)\chi_{\rm c}(|k - k'|)$ and $J_{\boldsymbol{k},\boldsymbol{k}'} = (I_{\rm s}^2/4)\chi_{\rm s}(|k - k'|)$, where $\tilde{U}$ simulates the short-range irreducible repulsion and

Table 1. Transition temperatures T_c^s (T_c^t) for singlet (triplet) pairing and their ratio T_c^s/T_c^t.

	$\alpha = 0.2$	$\alpha = 0.3$
T_c^s/t	4.09×10^{-4}	5.95×10^{-3}
T_c^t/t	6.60×10^{-5}	2.45×10^{-3}
T_c^s/T_c^t	~ 6.2	~ 2.4

I_c (I_s) is the constant of coupling of quasiparticles to the charge (spin) fluctuation modes. The pairing interaction is then written as

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \begin{Bmatrix} \tilde{U} \\ 0 \end{Bmatrix} + \frac{1}{2} \begin{Bmatrix} 3a_s - a_c \\ -a_s - a_c \end{Bmatrix} \chi_{1D}(k_x - k_x') \tag{4}$$

for SP (upper) and TP (lower), with $a_{c,s} = I_{c,s}^2 K_{c,s} v_F / v_{c,s}$.

We determine the transition temperature T_c and the gap function Δ_k from the linearized gap equation

$$\Delta_k = -\sum_{\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'} \frac{\Delta_{k'}}{2\xi_{\boldsymbol{k}'}} \tanh \frac{\xi_{\boldsymbol{k}'}}{2k_B T_c}. \tag{5}$$

In order to search in the low-temperature region, $T_c \ll t$, we need to divide the k-space into finer meshes around the Fermi points[3]. We performed calculations for a wide variety of parameter sets and obtained qualitatively the same results. In the following, we show the results for $\tilde{U} = 3.0t$, $I_c^2 K_c v_F / v_c = 0.75\tilde{U}^2$, $I_s^2 K_s v_F / v_s = \tilde{U}^2$, and $k_F = \pi/4$ (quarter-filling).

The transition temperature T_c is finite for both SP and TP. It is far below $10^{-6}t$ for $\alpha = 0$, but increases appreciably to $10^{-(2-3)}t$ as α is increased to 0.3 (see table 1). It is remarked that, while T_c for TP (T_c^t) is generally lower than T_c for SP (T_c^s), they are comparable in magnitude, i.e., the ratio $R_{T_c} \equiv T_c^s/T_c^t$ is of the order of unity. This ratio, R_{T_c}, becomes even smaller for larger α, as seen in table 1; in other words, intrachain interaction makes the difference between T_c^s and T_c^t smaller. With such small R_{T_c} of the order of unity, T_c^t can exceed T_c^s under a moderately large magnetic field along the direction for which the orbital effects are negligible, since SP is suppressed due to the paramagnetic effect while TP is not. This field-induced changeover from SP to TP will show itself as an anomalous T-dependence of H_{c2}. This may provide an explanation for such anomalous H_{c2} as observed in $(TMTSF)_2PF_6$ [5]. For this changeover to occur under moderate magnetic fields ($\gtrsim 2$ T), it is necessary that the interaction mediated by charge fluctuations is comparable to that mediated by spin fluctuations. It is remarked that the former character cannot be taken into account by the FLEX approximation.

The gap function Δ_k is sharply peaked on both sides of the Fermi point and quickly approaches zero away from it. The behaviour near the Fermi point $k_F = \pi/4$ is shown in figure 1. The most impressive feature is that it changes sign across the Fermi points, $\Delta_{k_F} = 0$. This type of gap, a radial-node gap, whose variation occurs in the radial direction, is quite different from the conventional anisotropic gap whose sign changes in the angular direction. The peak position depends on temperature, and the distance from the Fermi point is proportional to the transition temperature. This is the only reason that the peak for TP with lower T_c is closer to the Fermi point compared to that for SP.

The peculiar k-dependence of Δ_k may be understood as follows. With a conventional gap function, which does not change sign across the Fermi point, the pairing potential $V_{\boldsymbol{k},\boldsymbol{k}'}\Delta_k\Delta_{k'}$ is positive for a dominant momentum transfer of $\pm 2k_F$ (e.g., $k = -k_F$ and $k' = k_F$). This means that $V_{\boldsymbol{k},\boldsymbol{k}'}$ acts as a repulsive interaction for both SP and TP (see figure 2(a)). On the

[3] The size of the mesh is $\sim 10^{-10}$ near the Fermi points, and 3000 points are taken in the region $0 < k < \pi$.

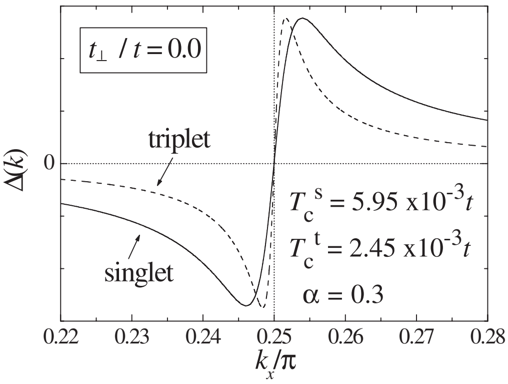

Figure 1. The gap function at the transition temperature in the 1D model. The solid (dashed) curve represents the gap for singlet (triplet) pairing. The vertical dotted line indicates the Fermi point $k_F = \pi/4$.

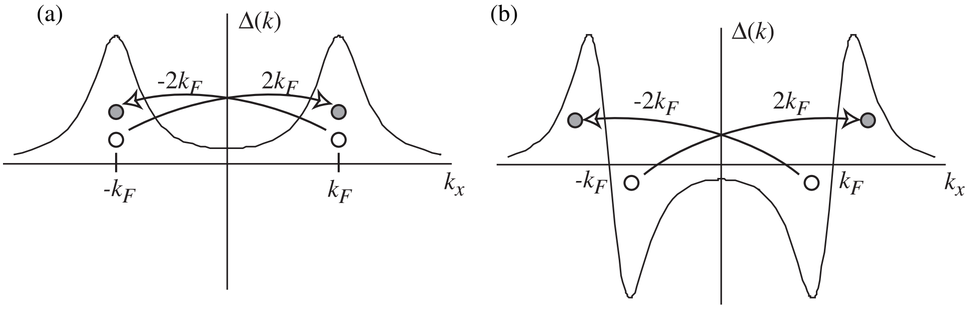

Figure 2. An illustration of the $2k_F$ pair scattering processes via 1D fluctuations χ_{1D} and the relation with the gap function $\Delta(k)$ (even parity is assumed). (a) For the conventional gap, the sign of $\Delta(k)$ does not change through the $2k_F$ scattering and χ_{1D} acts as a 'repulsive' interaction. (b) For the radial-node gap, $\Delta(k)$ changes sign through the $2k_F$ scattering and $\chi_{1D}(q \sim 2k_F)$ mediates an 'attractive' interaction. The same argument applies to the odd-parity TP also.

other hand, with the radial-node gap, $V_{\boldsymbol{k},\boldsymbol{k}'}\Delta_k\Delta_{k'}$ can be negative and $V_{\boldsymbol{k},\boldsymbol{k}'}$ acts as an attractive interaction (see figure 2(b)). Due to this sign change, the present gap does not feel the 'on-site' repulsion $\tilde{U}$. In fact, we observed that T_c does not depend on the value of $\tilde{U}$ as long as $\tilde{U} > 0$. This type of pairing has not been considered in the conventional renormalization group theory (g-ology) of 1D Fermi gas [8]. Work in this direction is in progress [13].

3. Quasi-one-dimensional case

So far we have considered purely 1D systems. The problem there is that the SDW instability is actually stronger than the pairing instability examined, and the SDW phase, rather than the present superconducting state, will be stabilized once the three-dimensionality of the system is assumed. We now switch on the interchain hopping $t_\perp$ and show that the SDW is quickly suppressed, whereas the essential character of the present superconductivity remains valid. We limit ourselves to finite but very small values for $t_\perp$ and assume that the $q_\perp$-dependence is negligible in the pairing interaction—that is, that the pairing interaction is mediated only by intrachain fluctuations. The gap function thus depends only on k (not on $k_\perp$).

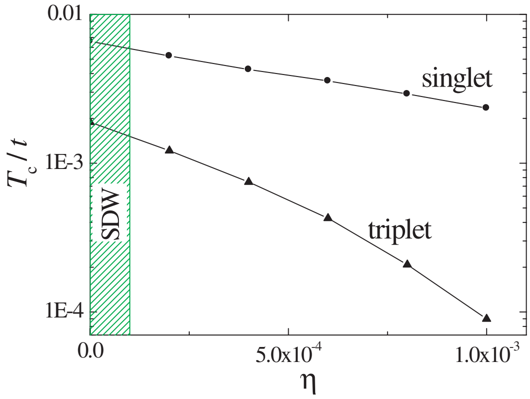

Figure 3. The dependence of T_c^s and T_c^t on η. The SDW ordering is destroyed at η_{SDW} satisfying $\chi_{chain}(2k_F, \eta_{SDW}) = g_\perp^{-1}$. Here, we set $g_\perp/t = 2.34 \times 10^{-1}$.
(This figure is in colour only in the electronic version)

The effect of $t_\perp$ will be to destroy the perfect nesting of the Fermi surface and thereby suppress the $2k_F$ singularity of χ_{1D} [12]. We model this suppression as

$$\left|\tan\frac{(q \pm 2k_F)}{4}\right|^{-\alpha} \rightarrow \left|\tan^2\frac{(q \pm 2k_F)}{4} + \eta^2\right|^{-\alpha/2} \tag{6}$$

by introducing a smearing factor η. Even a small value of η considerably suppresses the singularity; $\chi_{1D}(2k_F, \eta) \simeq 17.9/t$ for $\eta = 10^{-6}$ and $4.28/t$ for $\eta = 10^{-4}$, which leads to a strong suppression of the SDW ordering. In figure 3, the phase boundary of SDW is determined by $\chi_{s,Q1D}^{-1} \equiv \chi_{s,1D}^{-1}(2k_F, \eta) - g_\perp = 0$, with the small interchain interaction $g_\perp \ll t$. On the other hand, for the present superconductivity, the change of T_c (figure 3) is moderate and the superconducting ground state persists in a relatively wide region after the SDW phase is destroyed. This feature is consistent with the pressure dependence of the ground state of $(TMTSF)_2PF_6$ [4]. Below, we take $t_\perp = 0.03t$ (other parameters being the same as before) and see how the 1D pairing state is modified by $t_\perp$.

The gap function, shown in figure 4(a), has similar k-dependence to that of the 1D case for both SP and TP. The positions of the peaks, however, are fixed at the k-values of the extremum points of the 'Fermi line', in contrast to the 1D case where they were T-dependent. This feature seems robust against variations of T, η, or $t_\perp$ as long as $t_\perp \ll t$. Since the Fermi surface is slightly warped (due to $t_\perp$) and the nodes of the gap are independent of $k_\perp$, the gap inevitably has four nodes on the Fermi surface; in this case nodes are located at $(\pm\pi/4, \pm\pi/2)$ (see figure 4(b)). A similar gap function was obtained by the FLEX approximation in [7], although the value of T_c were not mentioned there. In [7] attention was paid only to the sign change of the gap function in the angular direction, not to that in the radial direction as proposed here. Topologically the same gaps were also used in a study of quasiparticle density of states (DOS) near the surface [15].

4. Effect of unitary impurities

In this section, we study the effect of impurities on DOS in the superconducting state. We first determine the magnitude, $\Delta_0(T)$, of the gap below T_c. For this we use the gap equation as an approximation assuming that the gap has the same k-dependence as the one obtained at

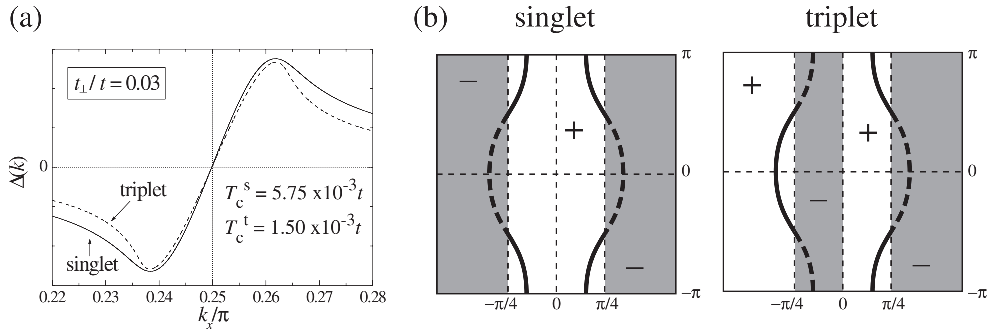

Figure 4. (a) The gap function at the transition temperature for the Q1D case. The solid (dashed) curve represents the gap for singlet (triplet) pairing. (b) The sign of the gap function on the Fermi surface for Q1D systems. The solid (dashed) curve indicates $\Delta_k > 0$ (<0).

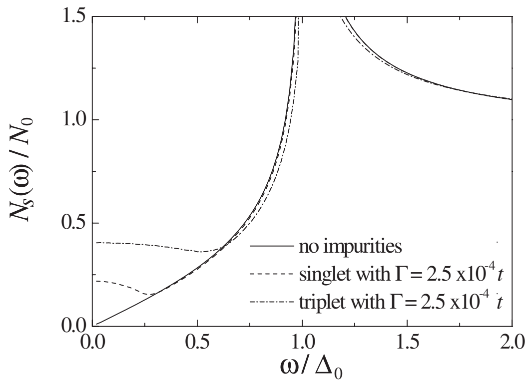

Figure 5. Quasiparticle DOS $N_s(\omega)/N_0$ versus reduced energy ω/Δ_0 in Q1D systems.

T_c. At $T = 0$, we obtained $\Delta_0(0) = 1.18 \times 10^{-2} t$ for SP and $2.82 \times 10^{-3} t$ for TP. The ratio $2\Delta_0(0)/k_B T_c$ is estimated as 4.1 for SP and 3.8 for TP.

We then model the k-dependence of the gap function used above by the form

$$\Delta_k = \frac{\Delta_0(T)}{Z} \frac{\tanh(k - k_F)}{(k - k_F)^2 + a^2} \tag{7}$$

for $k > 0$. Here, Z is a normalization factor such that Δ_0 gives the maximum value of Δ_k. For $a = 4.25 \times 10^{-2} (Z = 11.8)$, equation (7) reproduces the numerically obtained one (at T_c) quite well.

With Δ_k thus determined, we have studied the effect of impurities in the unitary limit following the standard method [15, 16]. In figure 5, we plot $N_s(\omega)/N_0$ for the pure system (solid curve) and that with impurities $\Gamma = 2.5 \times 10^{-4} t$ for different $\Delta_0(0)$ at $T = 0$. Here, Γ is the electron damping due to the impurity scattering and is proportional to the impurity concentration. Without impurities, the DOS is linear in ω at low energy ($\omega \ll \Delta_0(T)$) and is divergent at $\omega = \Delta_0(T)$. A small level of impurity produces a finite DOS, $N_s(0)$, at $\omega = 0$ as in conventional anisotropic superconductors. We see that $N_s(0)$ is approximately proportional to $\sqrt{\eta \ln(2/\eta)}$ ($\eta \equiv \Gamma/\Delta_0(T)$) [17], and the relation $N_s(0; T = 0) \sim \sqrt{(\ln T_c)/T_c}$ holds if Γ is assumed to be constant (see figure 5).

We propose the following scenario to account for the anomalous behaviour of $1/T_1$ observed in $(TMTSF)_2PF_6$ [6]. Under zero magnetic field, SP sets in at $T = T_c^s$. This SP is relatively *strong* against impurities due to its higher T_c, so it has a small residual DOS leading to the T-dependence $1/T_1 \propto T^3$ over a rather wide T-region below T_c^s. On the other hand, under moderately large magnetic fields, SP is destroyed by the paramagnetic effect and TP with lower T_c^t will arise instead. This TP state is *weak* against the impurity scattering, and may allow a large residual DOS leading to the gapless behaviour as observed in $1/T_1$.

In conclusion, we have investigated a new type of superconducting state in Q1D metals, which are mediated by singular spin and charge fluctuations at $2k_F$, and have discussed the relevance of this state to the unusual behaviours of $(TMTSF)_2PF_6$. The novel gap found in this letter may have relevance to a wide class of Q1D superconductors.

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References

[1] Miyake K, Schmitt-Rink S and Varma C M 1986 *Phys. Rev.* B **34** 6554
[2] Scalapino D J, Loh E Jr and Hirsch J E 1986 *Phys. Rev.* B **34** 8190
[3] Emery V J 1986 *Synth. Met.* **13** 21
[4] Jérome D 1982 *Mol. Cryst. Liq. Cryst.* **79** 155
[5] Lee I J, Chaikin P M and Naughton M J 1997 *Phys. Rev. Lett.* **78** 3555
[6] Lee I J, Brown S E, Clark W G, Strouse M J, Naughton M J, Kang W and Chaikin P M 2002 *Phys. Rev. Lett.* **88** 017004
[7] Kuroki K, Arita R and Aoki H 2001 *Phys. Rev.* B **63** 094509
[8] See, for example,
Sólyom J 1979 *Adv. Phys.* **28** 201
[9] Coexistence of $2k_F$ CDW and $2k_F$ SDW has been suggested on the basis of the x-ray scattering experiments in Pouget J P and Ravy S 1996 *Synth. Met.* **85** 1523
[10] Nakajima S 1973 *Prog. Theor. Phys.* **50** 1101
[11] Anderson P W and Brinkman W F 1975 *The Helium Liquids* ed J G M Armitage and I E Farquhar (London: Academic) p 315
[12] It is true that $t_\perp$ drives the 1D fluctuations into 3D ordering, as studied in
Suzumura Y and Fukuyama H 1978 *J. Low. Temp. Phys.* **31** 273
We, however, do not incorporate this effect of $t_\perp$ in the calculation. Instead, we make an implicit assumption of three-dimensionality as a mechanism leading to the ordered states (SDW or superconductivity).
[13] Fuseya Y *et al* in preparation
[14] Tanuma Y, Kuroki K, Tanaka V and Kashiwaya S 2001 *Phys. Rev.* B **64** 214510
[15] Schmitt-Rink S, Miyake K and Varma C M 1986 *Phys. Rev. Lett.* **57** 2575
[16] Hirschfeld P J, Vollhardt D and Wölfle P 1986 *Solid State Commun.* **59** 111
Hirschfeld P J, Wölfle P and Einzel D 1988 *Phys. Rev.* B **37** 83
[17] Miyake K 1987 *J. Magn. Magn. Mater.* **63+64** 411