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Coexistence of Spin-Triplet Superconductivity with Antiferromagnetism in Orbitally Degenerate System: Hartree–Fock Approximation

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We consider the coexistence of the Hund's-rule-exchange induced spin-triplet paired state with the antiferromagnetic ordering by starting from the extended Hubbard model for a doubly degenerate band. We use the density of states appropriate for the square lattice and treat the problem in the Hartree–Fock approximation. The temperature dependences of the superconducting gaps, the magnetic moment, and the chemical potential are presented. The free energy in the considered phase is evaluated, as well as the corresponding free energies in four additional phases: paramagnetic, ferromagnetic, superconducting of type A and superconducting of type $A1$ coexisting with ferromagnetism; they occur in the proper range of parameters: band filling n and the interaction parameters U/W and J/W. The low temperature values of the superconducting gaps and staggered magnetic moment are also analyzed as a function of band filling.

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1. Introduction

It is believed that the spin-triplet superconducting phase appears in Sr_2RuO_4 [1], UGe_2 [2] and URhGe [3]. In the last two compounds the considered type of superconducting phase occurs as coexisting with ferromagnetism. It has been shown [4–7] that the two phenomena may possibly have the same origin — the intra-atomic Hund's rule exchange, which can also lead to the coexistence of superconductivity with other type of magnetic ordering — antiferromagnetism. The coexisting superconducting and antiferromagnetic phase is discussed in this work for the extended two band Hubbard model with the use of the simplest Hartree–Fock approximation. For the sake of completeness, we also include some of the earlier results [7] concerning the superconducting phase of type A and the ferromagnetic phase coexisting with the superconducting phase of type $A1$.

2. Model

We consider the extended orbitally degenerate Hubbard Hamiltonian, which has the form

$$\hat{H} = \sum_{ij(i\neq j)l\sigma} t_{ij}\hat{a}^{\dagger}_{il\sigma}\hat{a}_{jl\sigma} + U\sum_{il}\hat{n}_{il\uparrow}\hat{n}_{il\downarrow} - J\sum_{ill'(l\neq l')}\left(\hat{\boldsymbol{S}}_{il}\cdot\hat{\boldsymbol{S}}_{il'} + \frac{3}{4}\hat{n}_{il}\hat{n}_{il'}\right), \quad (1)$$

where $l = 1, 2$ label the orbitals and the first term describes electron hopping between atomic sites i and j. The second term describes the intra-atomic Coulomb interaction between electrons on the same orbital. The third term introduces the (Hund's rule) ferromagnetic exchange between electrons localized on the same site, but on different orbitals. In this model we neglect the interaction-induced intra-atomic singlet-pair hopping $\sim J$ and the correlation induced hopping [8], as well as the inter-orbital Coulomb repulsion, as they should not introduce any important new feature in the considered here Hartree–Fock approximation. In this model for the sake of clarity, we neglect also the interorbital hybridization.

It can be shown that [4] one can represent the full exchange term with the help of the real-space pair operators, in the following manner

$$J\sum_{ill'(l\neq l')}\left(\hat{\boldsymbol{S}}_{il}\cdot\hat{\boldsymbol{S}}_{il'} + \frac{3}{4}\hat{n}_{il}\hat{n}_{il'}\right) \equiv 2J\sum_{i,m}\hat{A}^{\dagger}_{im}\hat{A}_{im}, \quad (2)$$

which are defined in the following way [9]

$$\hat{A}^{\dagger}_{i,m} \equiv \begin{cases} \hat{a}^{\dagger}_{i1\uparrow}\hat{a}^{\dagger}_{i2\uparrow} & m = 1 \\ \hat{a}^{\dagger}_{i1\downarrow}\hat{a}^{\dagger}_{i2\downarrow} & m = -1 \\ \frac{1}{\sqrt{2}}(\hat{a}^{\dagger}_{i1\uparrow}\hat{a}^{\dagger}_{i2\downarrow} + \hat{a}^{\dagger}_{i1\downarrow}\hat{a}^{\dagger}_{i2\uparrow}) & m = 0 \end{cases}. \quad (3)$$

In our considerations the antiferromagnetic state reflects the simplest form of the spin-density-wave state. In this state, we can divide our system into two interpenetrating sublattices. We name those sublattices A and B. In the antiferromagnetic phase, the average magnetic (staggered) moment of electons on each of $N/2$ sublattice A sites is equal $\langle S^z_i\rangle = \langle S^z_A\rangle$, whereas the electrons on the remaining $N/2$ sublattice B sites have magnetic moment $\langle S^z_i\rangle = \langle S^z_B\rangle \equiv -\langle S^z_A\rangle$. In accordance with the division

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into the sublattices we define different annihilation operators for each sublattice, namely

$$\hat{a}_{il\sigma} = \begin{cases} \hat{a}_{il\sigma A} \\ \hat{a}_{il\sigma B} \end{cases}. \tag{4}$$

We do the same for the creation operators, $\hat{a}^{\dagger}_{il\sigma}$. For modeling purposes, we assume that the bands are identical and the charge ordering is absent. In this situation, we can write that

$$\langle \hat{S}^z_{i1A}\rangle = \langle \hat{S}^z_{i2A}\rangle \equiv \bar{S}^z, \quad \langle \hat{S}^z_{i1B}\rangle = \langle \hat{S}^z_{i2B}\rangle \equiv -\bar{S}^z, \tag{5}$$

$$\langle \hat{n}_{i1A}\rangle = \langle \hat{n}_{i2A}\rangle = \langle \hat{n}_{i1B}\rangle = \langle \hat{n}_{i2B}\rangle \equiv n/2. \tag{6}$$

In what follows, we treat the pairing and the Hubbard part in the mean field approximation. Applying (4) to (1) and making the Hartree–Fock approximation we can write down the Hamiltonian transformed to reciprocal ($\boldsymbol{k}$) space in the following form:

$$\begin{aligned}\hat{H}_{HF} = &\sum_{\boldsymbol{k}l\sigma}\Big(\epsilon_{\boldsymbol{k}}\big(\hat{a}^{\dagger}_{\boldsymbol{k}l\sigma A}\hat{a}_{\boldsymbol{k}l\sigma B} + \hat{a}^{\dagger}_{\boldsymbol{k}l\sigma B}\hat{a}_{\boldsymbol{k}l\sigma A}\big) \\ &-\sigma I\bar{S}^z\big(\hat{n}_{\boldsymbol{k}l\sigma A} - \hat{n}_{\boldsymbol{k}l\sigma B}\big)\Big) \\ &+\sum_{\boldsymbol{k},m=\pm 1}\big(\Delta^*_{mA}\hat{A}_{\boldsymbol{k}mA} + \Delta_{mA}\hat{A}^{\dagger}_{\boldsymbol{k}mA}\big) \\ &+\sum_{\boldsymbol{k},m=\pm 1}\big(\Delta^*_{mB}\hat{A}_{\boldsymbol{k}mB} + \Delta_{mB}\hat{A}^{\dagger}_{\boldsymbol{k}mB}\big) \\ &-\frac{\hat{N}}{4J}\big(|\Delta_{1A}|^2 + |\Delta_{-1A}|^2 + |\Delta_{1B}|^2 + |\Delta_{-1B}|^2\big) \\ &-\frac{\hat{N}}{8}(U-3J)n^2 + 2NI(\bar{S}^z)^2,\end{aligned} \tag{7}$$

where $I \equiv U + J$ is the effective magnetic coupling constant, N is the number of atomic sites and $\epsilon_{\boldsymbol{k}1} = \epsilon_{\boldsymbol{k}2} \equiv \epsilon_{\boldsymbol{k}}$ is the dispersion relation in the doubly degenerate band. One should note that the sum in (7) (and in all the corresponding equations below) is taken over N/2 independent $\boldsymbol{k}$ states. In the Hamiltonian above we also have introduced the superconducting spin-triplet gap parameters on the sublattices

$$\Delta_{\pm 1A} = -\frac{4J}{N}\sum_{\boldsymbol{k}}\langle \hat{A}_{\boldsymbol{k},\pm 1A}\rangle,$$

$$\Delta_{\pm 1B} = -\frac{4J}{N}\sum_{\boldsymbol{k}}\langle \hat{A}_{\boldsymbol{k},\pm 1B}\rangle. \tag{8}$$

Because we are considering the superconducting phase coexisting with antiferromagnetism in which all lattice sites have a nonzero magnetic moment, the Cooper pairs in the spin-triplet state for $m = 0$ and spin $S^z = 0$ (that correspond to the pair operator $\hat{A}_{\boldsymbol{k},0}$) are not likely to be created. The phase, in which the gap parameters corresponding to the mentioned spin-triplet state of the Cooper pairs are nonzero, is not going to be stable, so we have neglected the term that contains $\Delta_{0A} = -\frac{4J}{\sqrt{2}N}\sum_{\boldsymbol{k}}\langle \hat{A}_{\boldsymbol{k},0A}\rangle$ and $\Delta_{0B} = -\frac{4J}{\sqrt{2}N}\sum_{\boldsymbol{k}}\langle \hat{A}_{\mathbf{k},0B}\rangle$.

By introducing the composite fermion creation operator

$$\begin{aligned}\hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{k}} \equiv \big(&\hat{a}^{\dagger}_{\boldsymbol{k}1\uparrow A}, \hat{a}^{\dagger}_{\boldsymbol{k}1\downarrow A}, \hat{a}_{-\boldsymbol{k}2\uparrow A}, \hat{a}_{-\boldsymbol{k}2\downarrow A}, \hat{a}^{\dagger}_{\boldsymbol{k}1\uparrow B}, \hat{a}^{\dagger}_{\boldsymbol{k}1\downarrow B}, \\ &\hat{a}_{-\boldsymbol{k}2\uparrow B}, \hat{a}_{-\boldsymbol{k}2\downarrow B}\big),\end{aligned} \tag{9}$$

we can construct the 8×8 Hamiltonian matrix and write

$$\hat{H}_{HF} - \mu\hat{N} = \sum_{\boldsymbol{k}}\hat{f}^{\dagger}_{\boldsymbol{k}}H_{\boldsymbol{k}}\hat{f}_{\boldsymbol{k}} - 4\mu\hat{N}, \tag{10}$$

where $\hat{f}_{\boldsymbol{k}} \equiv (\hat{f}^{\dagger}_{\boldsymbol{k}})^{\dagger}$, and

$$H_{\boldsymbol{k}} = \begin{pmatrix} -I\bar{S}^z-\mu & 0 & \Delta_{1A} & 0 & \epsilon_{\boldsymbol{k}} & 0 & 0 & 0 \\ 0 & I\bar{S}^z-\mu & 0 & \Delta_{-1A} & 0 & \epsilon_{\boldsymbol{k}} & 0 & 0 \\ \Delta^*_{1A} & 0 & I\bar{S}^z+\mu & 0 & 0 & 0 & -\epsilon_{\boldsymbol{k}} & 0 \\ 0 & \Delta^*_{-1A} & 0 & -I\bar{S}^z+\mu & 0 & 0 & 0 & -\epsilon_{\boldsymbol{k}} \\ \epsilon_{\boldsymbol{k}} & 0 & 0 & 0 & I\bar{S}^z-\mu & 0 & \Delta_{1B} & 0 \\ 0 & \epsilon_{\boldsymbol{k}} & 0 & 0 & 0 & -I\bar{S}^z-\mu & 0 & \Delta_{-1B} \\ 0 & 0 & -\epsilon_{\boldsymbol{k}} & 0 & \Delta^*_{1B} & 0 & -I\bar{S}^z+\mu & 0 \\ 0 & 0 & 0 & -\epsilon_{\boldsymbol{k}} & 0 & \Delta^*_{-1B} & 0 & I\bar{S}^z+\mu \end{pmatrix}. \tag{11}$$

In our considerations we limit to the case with the real gap parameters $\Delta^*_{\pm 1A(B)} = \Delta_{\pm 1A(B)}$. After diagonalization of (11), we can write down the Hamiltonian in the following form

$$\begin{aligned}\hat{H}_{HF} - \mu\hat{N} = &\sum_{\boldsymbol{k}d}(-1)^{d+1}\lambda_{\boldsymbol{k}d}\hat{\alpha}^{\dagger}_{\boldsymbol{k}d}\hat{\alpha}_{\boldsymbol{k}d} - 4\mu\hat{N} \\ &+\sum_{\boldsymbol{k}}(\lambda_{\boldsymbol{k}2} + \lambda_{\boldsymbol{k}4} + \lambda_{\boldsymbol{k}6} + \lambda_{\boldsymbol{k}8}),\end{aligned} \tag{12}$$

where $d = 1, 2, 3, \ldots, 8$ and $\lambda_{\boldsymbol{k}d}$ are the eigenvalues of the matrix Hamiltonian (11) and $\hat{\alpha}_{\boldsymbol{k}d}$, $\hat{\alpha}^{\dagger}_{\boldsymbol{k}d}$ are the quasiparticle annihilation and creation operators, which can be expressed by the initial creation and annihilation operators via generalized Bogoliubov transformation, i.e.,

$$\hat{\boldsymbol{g}}_{\boldsymbol{k}} = U_{\boldsymbol{k}}\hat{\boldsymbol{f}}_{\boldsymbol{k}}, \tag{13}$$

with $\hat{\boldsymbol{g}}^{\dagger}_{\boldsymbol{k}} \equiv \big(\hat{\alpha}^{\dagger}_{\boldsymbol{k}1}, \hat{\alpha}_{-\boldsymbol{k}2}, \hat{\alpha}^{\dagger}_{\boldsymbol{k}3}, \hat{\alpha}_{-\boldsymbol{k}4}, \hat{\alpha}^{\dagger}_{\boldsymbol{k}5}, \hat{\alpha}_{-\boldsymbol{k}6}, \hat{\alpha}^{\dagger}_{\boldsymbol{k}7}, \hat{\alpha}_{-\boldsymbol{k}8}\big)$ and $\hat{\boldsymbol{g}}_{\boldsymbol{k}} = (\hat{\boldsymbol{g}}^{\dagger}_{\boldsymbol{k}})^{\dagger}$. Eigenvectors of the Hamiltonian matrix (11) are the columns of the diagonalization matrix $U_{\boldsymbol{k}}$. Using the definitions of gap parameters $\Delta_{\pm 1A}$, $\Delta_{\pm 1B}$, the average number of particles per atomic site $n = \sum_l\langle \hat{n}_{il\uparrow A} + \hat{n}_{il\downarrow A}\rangle$, and the average magnetic moment

per band per site $S^z = \langle \hat{n}_{il\uparrow A} - \hat{n}_{il\downarrow A} \rangle /2$, we can construct the set of self consistent equations for all mean-field parameters ($\Delta_{\pm 1A}$, $\Delta_{\pm 1B}$, $\bar{S}^z$) and the chemical potential. The averages that appear in the set of self consistent equations $\langle \hat{\alpha}^{\dagger}_{\boldsymbol{k}d} \hat{\alpha}_{\boldsymbol{k}d} \rangle$ can be replaced by the corresponding Fermi-Dirac distribution function

$$f((-1)^{d+1}\lambda_{\boldsymbol{k}d}) = 1/[\exp(\beta(-1)^{d+1}\lambda_{\boldsymbol{k}d}) + 1].$$

The eigenvalues and eigenvectors of matrix (11) are evaluated numerically during the procedure of solving the set of self consistent equations. The detailed procedure of calculating the free energies and corresponding order parameters is similar as in our previous work [7]. The numerical results are obtained by assuming the square lattice with the hopping t between the nearest neighbors.

3. Results and discussion

In all presented below figures the energies have been normalized to the bare band-width $W = 8|t|$, as well as T corresponds to the reduced temperature $T \equiv k_B T/W$.

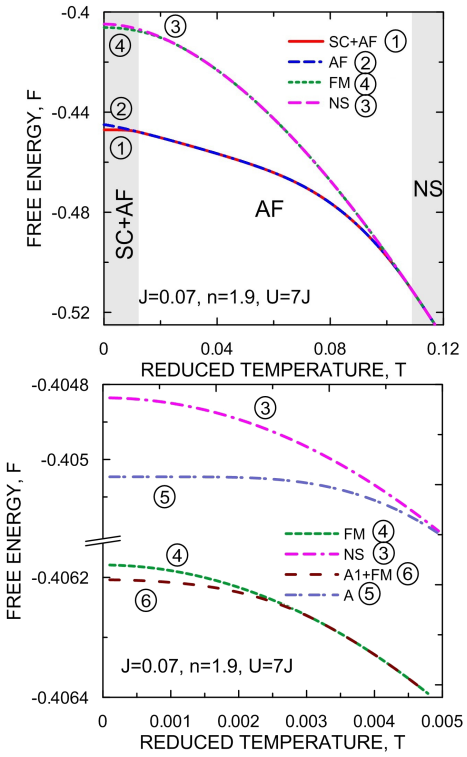

Fig. 1. (a) — temperature dependences of free energy in phases: coexisting superconducting–antiferromagnetic (SC+AF), antiferromagnetic (AF), normal state (NS), ferromagnetic (FM); (b) — free energies for A, NS, $A1$+FM and FM phases in the low-T regime. The free energy for A and $A1$+FM phases are not shown in Fig. 1a for the sake of clarity. For the selected parameters, AF+SC and AF phases are the only stable phases in proper temperature intervals.

In Fig. 1 we present the temperature dependence of free energies for the six different phases: NS — normal state, A — superconducting phase A ($\Delta_{\pm 1A} = \Delta_{\pm 1B} \neq 0$), $A1$+FM — coexistent superconducting phase $A1$ ($\Delta_{1A} = \Delta_{1B} \neq 0$ and $\Delta_{-1A} = \Delta_{-1B} = 0$) and the non-saturated ferromagnetic phase, $A1$+SFM — coexistent superconducting $A1$ and saturated ferromagnetic phase, SC+AF — coexistent superconducting and antiferromagnetic phase. Because the free-energy values of the A and NS phases are very close, we exhibit their temperature dependences zoomed in Fig. 1b). The same is shown for the phases $A1$+FM and FM (bottom part). As one can see from the Fig. 1, the phase SC+AF has the lowest free energy below the reduced temperature $T_S \approx 0.0123$ for the specified values of the microscopic parameters.

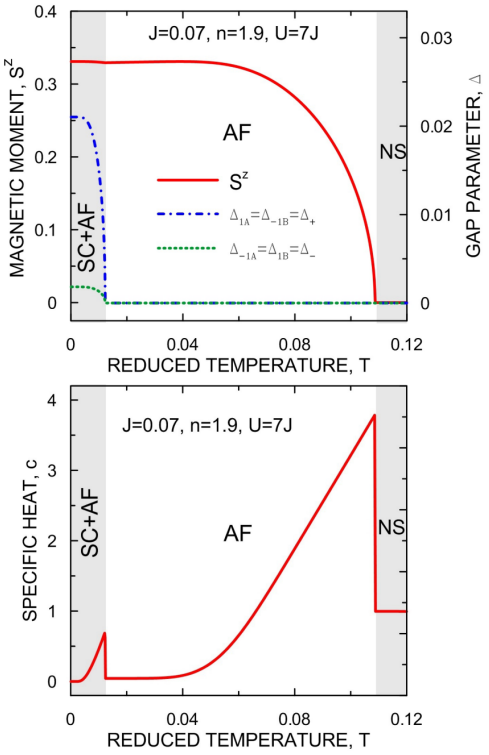

Fig. 2. (a) — temperature dependence of the superconducting gaps and the staggered magnetic moment; (b) — temperature dependence of the specific heat for the to the stable phases.

Temperature dependence of superconducting gaps and staggered magnetic moment in the SC+AF phase are shown in Fig. 2. Below T_S the staggered magnetic moment and the superconducting gaps, have all nonzero values. In the SC+AF phase the gap parameters that correspond to Cooper pairs with the spin aligned in the same direction as the magnetic moment on the sublattice have equal values ($\Delta_{1A} = \Delta_{-1B} \equiv \Delta_+$). Gap parameters that correspond to Cooper pairs with spin aligned in the opposite direction to the magnetic moment on the sublattice also have equal values ($\Delta_{-1A} = \Delta_{1B} \equiv \Delta_-$), but much smaller than the gap parameters Δ_{1A}, Δ_{-1B}.

In Fig. 2b one can observe that there are two discontinuities in the specific-heat temperature dependence. The

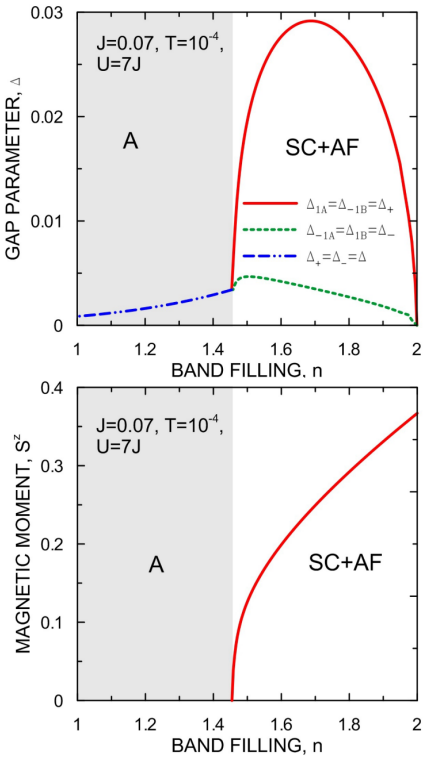

Fig. 3. (a) — gap parameters Δ_+ and Δ_- and (b) — staggered magnetic moment both as a function of band filling n. The coexistent phase appears near the half filling.

first, at lower T, corresponds to the phase transition from the SC+AF phase to the pure AF phase, while the second corresponds to the transition from the AF phase to the normal phase (NS). Near the Néel temperature, $T_N \approx 0.11$, the staggered magnetic moment decreases continuously to zero. The low temperature values of gap parameters for the AF+SC phase for different values of band filling are presented in Fig. 3. One can see that gap components Δ_+ and Δ_- tend to zero when the system is approaching the half filling ($n \to 2$). On the contrary, the staggered magnetic moment $\bar{S}^z$ reaches then maximum. Below the critical value of band filling, $n_c \approx 1.45$, the gap parameters Δ_+ and Δ_- become equal and the staggered magnetic moment vanishes. In this regime the superconducting phase of type A is the stable phase. One should mention that the easiness, with which the superconducting triplet state is accommodated within the antiferromagnetic phase stems from the fact that the SC gaps have an intra-atomic origin and the spins are parallel. Therefore, the pairs respect the Hund's rule and do not disturb the staggered-moment structure at the same time.

4. Conclusions

We have obtained the stable coexistent superconducting and antiferromagnetic phase within the extended two band Hubbard model using the Hartree–Fock approximation. For selected values of the microscopic parameters, that correspond to zero-temperature stability of SC+AF phase, with the rise of temperature, one can observe two phase transitions. The first is from the SC+AF phase to the antiferromagnetic phase and the second form the antiferromagnetic phase to paramagnetic state. The transition temperature ratio is $T_N/T_S \approx 9$. In the superconducting phase coexisting with antiferromagnetism we have introduced two different gap parameters on different sublattices. The calculated gap parameters fulfill the relations

$$\Delta_{1A} = \Delta_{-1B} \equiv \Delta_+, \ \Delta_{-1A} = \Delta_{1B} \equiv \Delta_-, \ \Delta_+ > \Delta_-.$$

Full discussion including details of the phase diagram that contains all considered here phases will be provided elsewhere.

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References

[1] Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J.G. Bednorz, F. Lichtenberg, *Nature* **372**, 532 (1994).

[2] S.S. Saxena, P. Agarwal, K. Ahilan, F.M. Grosche, R.K.W. Haselwimmer, M.J. Steiner, E. Pugh, I.R. Walker, S.R. Julian, P. Monthoux, G.G. Lonzarich, A. Huxley, I. Sheikin, D. Braithwaite, J. Flouquet, *Nature* **406**, 587 (2000).

[3] N. Tateiwa, T.C. Kobayashi, K. Hanazono, K. Amaya, Y. Haga, R. Settai, Y. Onuki, *J. Phys. Condens. Matter* **13**, 117 (2001).

[4] K. Klejnberg, J. Spałek, *J. Phys. Condens. Matter* **11**, 6553 (1999).

[5] J. Spałek, *Phys. Rev. B* **63**, 104513 (2001).

[6] K. Klejnberg, J. Spałek, *Phys. Rev. B* **61**, 15542 (2000).

[7] M. Zegrodnik, J. Spałek, *Acta. Phys. Pol. A*, in press.

[8] T. Nomura, K. Yamada, *J. Phys. Soc. Jpn.* **71**, 1993 (2002).

[9] P. Wróbel, Ph.D. Thesis, Jagiellonian University, Kraków, (2004), unpublished.