

Comparison of superconductivity in Sr_2RuO_4 and copper oxides

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To compare the superconductivity in strongly correlated electron systems with the antiferromagnetic fluctuations in the copper oxides and with the ferromagnetic fluctuations in Sr_2RuO_4 a t - J - I model is proposed. The antiferromagnetic coupling J results in the superconducting state of $d_{x^2-y^2}$ symmetry and the ferromagnetic coupling I results in the spin-triplet p -type state. The difference in the gap anisotropies provides the large difference in T_c values, for the typical values of the coupling constants: $T_c \sim 1$ K for the ruthenate and $T_c \sim 100$ K for the cuprates.

I. INTRODUCTION

More than a decade of intensive research of the cuprate superconductors and related systems has raised fundamental challenges to our understanding of the mechanism of high-temperature superconductivity (SC). One of the most important questions is what is so specific in copper oxides, is it the unique chemistry of the planar Cu-O bond that determines the high value of T_c ? The discovery of SC in Sr_2RuO_4 with $T_c \sim 1$ K (Ref. 1) is of a particular interest because it has a similar crystal structure to the parent compound La_2CuO_4 , of one of the best studied families of the cuprate superconductors, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, but has four valence electrons (for Ru^{4+}) instead of one hole per formula unit. It is generally believed that comparison of normal and SC properties of the cuprates and the ruthenate will give more deeper understanding of the nature of high- T_c SC. While the normal state of doped cuprates looks like almost antiferromagnetic Fermi liquid,² the normal state of Sr_2RuO_4 is characterized by the strong ferromagnetic fluctuations.³ Properties of SC state are also different: the singlet pairing with major contribution of the $d_{x^2-y^2}$ symmetry was suggested for the cuprates,⁴ while the triplet pairing with p -type symmetry similar to the ^3He A_1 phase is proposed for Sr_2RuO_4 .⁵ The triplet SC in Sr_2RuO_4 is induced by the ferromagnetic spin fluctuations.⁶

To compare the SC in Sr_2RuO_4 and cuprates we have proposed here a t - J - I model containing both an indirect antiferromagnetic coupling J and a direct ferromagnetic coupling I between neighboring cations. This model is based on the electronic structure calculations. An important difference from the cuprates is that relevant orbitals to the states near the Fermi energy are Ru $d\epsilon(d_{xy}, d_{yz}, d_{xz})$ and O $p\pi$, instead of Cu $d_{x^2-y^2}$ and O $p\sigma$ states. Due to σ bonding in the cuprates a strong p - d hybridization takes place resulting in the strong antiferromagnetic coupling J , a direct $d_{x^2-y^2}$ Cu-Cu overlapping is negligible. In Sr_2RuO_4 with π bonding the Ru-O-Ru 180-degree antiferromagnetic superexchange coupling is weak⁷ while a direct d_{xy} Ru-Ru overlapping is not small. That is why we add the Heisenberg type direct Ru-Ru exchange interaction to the Hamiltonian of the t - J

model. The strong electron correlations are common features of the charge carriers both in cuprates and Sr_2RuO_4 in our model. These correlations for the cuprates are well known.⁸ The importance of electron correlations for Sr_2RuO_4 follows from the high value of the effective mass of electrons in the γ -band obtained by the quantum oscillations measurements.⁹

We have found different mean-field solutions for SC state in t - J - I model: with the singlet d -type pairing governed by the antiferromagnetic coupling J and with the triplet p -type pairing induced by the ferromagnetic coupling I . The equations for T_c in both states are similar. Nevertheless the same absolute value of the coupling constants results in quite different T_c values, $T_c^{(p)} \sim 1$ K and $T_c^{(d)} \sim 100$ K for typical values of parameters. The gap anisotropy is responsible for the large difference in the T_c values. For the p -type pairing the \mathbf{k} dependence of the gap provides cancellation of the singular van Hove contribution of the two-dimensional density of states, while the \mathbf{k} dependence of the d -type gap results in the significant contribution of the van Hove singularity.

II. HAMILTONIAN

The Hamiltonian of the proposed t - J - I model is written in the form

$$H = H_{\text{kin}} + H_{\text{int}}, \quad (1)$$

$$H_{\text{kin}} = \sum_{\mathbf{f}\sigma} (\varepsilon - \mu) X_{\mathbf{f}}^{\sigma\sigma} - t \sum_{\mathbf{f}\delta\sigma} X_{\mathbf{f}}^{\sigma 0} X_{\mathbf{f}+\delta}^{0\sigma}, \quad (2)$$

$$H_{\text{int}} = J \sum_{\mathbf{f}\delta} K_{\mathbf{f},\mathbf{f}+\delta}^{(-)} - I \sum_{\mathbf{f}\delta} K_{\mathbf{f},\mathbf{f}+\delta}^{(+)}, \quad (3)$$

$$K_{\mathbf{f}\mathbf{g}}^{(\pm)} = \tilde{S}_{\mathbf{f}} \cdot \tilde{S}_{\mathbf{g}} \pm \frac{1}{4} n_{\mathbf{f}} n_{\mathbf{g}}, \quad n_{\mathbf{f}} = \sum_{\sigma} X_{\mathbf{f}}^{\sigma\sigma}. \quad (4)$$

This Hamiltonian is given on d -dimensional lattice of N sites (\mathbf{f} is sites of the lattice), with z nearest neighbors (NN) and periodic boundary conditions (δ is vector connecting NN). It describes system of N_e electrons in subspace of local

states $|0\rangle$ and $|\sigma\rangle$, which are holes (empty sites of the lattice) and one-electron states with $\sigma = \uparrow$ and $\sigma = \downarrow$, so that $0 \leq n_e \leq N$. At this basis, states and transitions between these are described with Hubbard operators $X_f^{pq} = |p\rangle\langle q|$ with well known commutation relations, rule of multiplication on one site, and condition of fullness

$$X_f^{pq} \cdot X_f^{lm} = \delta_{ql} X_f^{pm}, \quad X_f^{00} + X_f^{\uparrow\uparrow} + X_f^{\downarrow\downarrow} = 1. \quad (5)$$

H_{kin} describes hopping of electrons onto nearest empty sites of the lattice (hopping integral $t > 0$), ε is energy of one-electron level (below, this energy is assumed to be 0), μ is chemical potential.

The antiferromagnetic ($J > 0$) and the ferromagnetic ($I > 0$) exchange interactions appear in the Hamiltonian H_{int} . \tilde{S}_f and n_f are the spin operator of $S = 1/2$ and operator of particles' number on site f . [The parameters J and I correspond to numerical value of the system's exchange energy per one bound (between NN). For example, the energy of the saturated ferromagnetic state $|F\rangle$ with $n = 1$ is equal to $E_F = \langle F | H_{\text{ex}}^{(+)} | F \rangle = -I \cdot \frac{1}{2} zN$, and the energy of the antiferromagnetic state, calculated with the Néel wave function $|AF\rangle$, is equal to $E_{AF} = \langle AF | H_{\text{ex}}^{(-)} | AF \rangle = -J \cdot \frac{1}{2} zN$, where $zN/2$ is the full number of bounds between all NN. Thus, the parameters I and J already contain square of the spin $S = 1/2$.] In general case, the exchange interaction between NN is sum of the antiferromagnetic kinetic exchange $J_{\text{kin}} = 2t^2/U$ and of direct exchange which may be as antiferromagnetic as ferromagnetic. If both exchanges are antiferromagnetic, then we assume $I = 0$ and use common parameter J . But if direct exchange is ferromagnetic, then J - I competition appears and this case is reflected in exchange part of the Hamiltonian H_{int} . For cuprates $J \gg I$ (or $I = 0$), and for Sr₂RuO₄ $I \gg J$.

To get SC the copper oxides should be doped while Sr₂RuO₄ is self-doped. According to the band structure calculations¹⁰ the electron α -band in Sr₂RuO₄ is half-filled, the hole β -band has $n_0 = 0.28$ holes and the electron γ -band with d_{xy} contribution is more than half-filled, $n_\gamma = 1 + n_0$. In our model, the strong electron correlations split the γ -band into filled lower Hubbard band (LHB) with $n_e = 1$ and partially filled upper Hubbard band (UHB) with the electron concentration $n_e = n_0$. We use the hole representation where the electron UHB transforms in the hole LHB with hole concentration $n_h = 1 - n_0$. All other bands (α and β) are treated here as an electron reservoir. Observation of a square flux-line lattice in Sr₂RuO₄ allows to suggest that SC resides mainly on the γ band.¹¹ For the cuprates the quasiparticle is a hole in the electron LHB with the electron concentration $n_e = 1 - n_0$, for La_{2-x}Sr_xCuO₄ $n_0 = x$.

For convenience, we normalize Hamiltonian (1) with the free electron half bandwidth $W = zt$. After Fourier transformations of Hubbard operators

$$X_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{f}} e^{i\mathbf{k}\mathbf{f}} X_{\mathbf{f}}^{0\sigma}, \quad X_{\mathbf{q}}^{\sigma\sigma'} = \frac{1}{\sqrt{N}} \sum_{\mathbf{f}} e^{i\mathbf{q}\mathbf{f}} X_{\mathbf{f}}^{\sigma\sigma'}, \quad (6)$$

where the vectors \mathbf{k} , \mathbf{q} belong to the first Brillouin zone, we obtain the dimensionless Hamiltonian of our model in the form

$$h = H/zt = h_{\text{kin}} + h_{\text{int}}, \quad (7)$$

$$H_{\text{kin}} = \sum_{\mathbf{k}\sigma} (\omega_{\mathbf{k}} - \tilde{\mu}) X_{\mathbf{k}\sigma}^+ X_{\mathbf{k}\sigma}, \quad \omega_{\mathbf{k}} = -\frac{1}{z} \sum_{\delta} e^{i\mathbf{k}\delta} = -\gamma_{\mathbf{k}}, \quad (8)$$

$$h_{\text{int}} = \frac{1}{2} \sum_{\mathbf{q}} \gamma_{\mathbf{q}} \left\{ g \sum_{\sigma} (X_{\mathbf{q}}^{\sigma\bar{\sigma}} X_{-\mathbf{q}}^{\bar{\sigma}\sigma} - X_{\mathbf{q}}^{\sigma\sigma} X_{-\mathbf{q}}^{\bar{\sigma}\bar{\sigma}}) - r \sum_{\sigma} (X_{\mathbf{q}}^{\sigma\bar{\sigma}} X_{-\mathbf{q}}^{\bar{\sigma}\sigma} + X_{\mathbf{q}}^{\sigma\sigma} X_{-\mathbf{q}}^{\sigma\sigma}) \right\}, \quad (9)$$

where $\bar{\sigma} = -\sigma$ and the dimensionless parameters $g = J/t$, $r = I/t$, and $\tilde{\mu} = \mu/zt$ have started being using. We call reader's attention to participation of factor $(1/z)$ in formation of dispersion law $\omega_{\mathbf{k}}$ for hopping and for all interactions between NN.

III. EQUATION OF MOTION

There are many ways to get the mean-field solutions for SC state; we have used the irreducible Green function method¹²⁻¹⁵ projecting the higher-order Green functions onto subspace of normal $\langle\langle X_{\mathbf{k}}^{0\sigma} | X_{\mathbf{k}}^{\sigma 0} \rangle\rangle$ and abnormal $\langle\langle X_{-\mathbf{k}}^{-\sigma 0} | X_{\mathbf{k}}^{\sigma 0} \rangle\rangle$ Green functions coupled via the Gorkov system of equations.

Using the dimensionless Hamiltonian $h = H/zt$ and the algebra of the X operators, we derive the equation of motion for the quasi-Fermi operator ($\hbar = 1$):

$$i\dot{X}_{\mathbf{k}\sigma} = [X_{\mathbf{k}\sigma}, h] = (\omega_{\mathbf{k}} - \tilde{\mu}) X_{\mathbf{k}\sigma} + L_{\mathbf{k}\sigma}, \quad (10)$$

$$L_{\mathbf{k}\sigma} = L_{\mathbf{k}\sigma}^{(\text{kin})} + L_{\mathbf{k}\sigma}^{(\text{int})}, \quad (11)$$

$$L_{\mathbf{k}\sigma}^{(\text{kin})} = \frac{1}{\sqrt{N}} \sum_{\mathbf{p}} \omega_{\mathbf{p}} (X_{\mathbf{k}-\mathbf{p}}^{\bar{\sigma}\sigma} X_{\mathbf{p}\sigma} - X_{\mathbf{k}-\mathbf{p}}^{\bar{\sigma}\bar{\sigma}} X_{\mathbf{p}\sigma}), \quad (12)$$

$$L_{\mathbf{k}\sigma}^{(\text{int})} = \frac{1}{\sqrt{N}} \sum_{\mathbf{p}} \gamma_{\mathbf{k}-\mathbf{p}} \{ (g-r) X_{\mathbf{k}-\mathbf{p}}^{\bar{\sigma}\sigma} X_{\mathbf{p}\sigma} - g X_{\mathbf{k}-\mathbf{p}}^{\bar{\sigma}\bar{\sigma}} X_{\mathbf{p}\sigma} - r X_{\mathbf{k}-\mathbf{p}}^{\sigma\sigma} X_{\mathbf{p}\sigma} \}, \quad (13)$$

where the nonlinear operator $L_{\mathbf{k}\sigma}$ describes the electron correlations both with the opposite and with the same spin projections.

Let us introduce the irreducible operator (refer to Ref. 12)

$$\bar{L}_{\mathbf{k}\sigma} = L_{\mathbf{k}\sigma} - \frac{\langle\{L_{\mathbf{k}\sigma}, X_{\mathbf{k}\sigma}^+\}\rangle}{\langle\{X_{\mathbf{k}\sigma}, X_{\mathbf{k}\sigma}^+\}\rangle} X_{\mathbf{k}\sigma} - \frac{\langle\{L_{\mathbf{k}\sigma}, X_{-\mathbf{k}\sigma}^-\}\rangle}{\langle\{X_{-\mathbf{k}\sigma}^-, X_{-\mathbf{k}\sigma}^-\}\rangle} X_{-\mathbf{k}\sigma}^-, \quad (14)$$

possessing ‘‘orthogonality at the average’’ property: $\langle\{\bar{L}_{\mathbf{k}\sigma}, X_{\mathbf{k}\sigma}^+\}\rangle = \langle\{\bar{L}_{\mathbf{k}\sigma}, X_{-\mathbf{k}\sigma}^-\}\rangle = 0$. Then Eq. (10) is written in the form

$$i\dot{X}_{\mathbf{k}\sigma} = \left(\omega_{\mathbf{k}} - \tilde{\mu} + \frac{C_{\mathbf{k}\sigma}}{1 - n_{\bar{\sigma}}} \right) X_{\mathbf{k}\sigma} + \frac{\Delta_{\mathbf{k}\sigma}}{1 - n_{\sigma}} X_{-\mathbf{k}\sigma}^+ + \bar{L}_{\mathbf{k}\sigma}, \quad (15)$$

where $C_{\mathbf{k}\sigma} = \langle\{L_{\mathbf{k}\sigma}, X_{\mathbf{k}\sigma}^+\}\rangle$ and $\Delta_{\mathbf{k}\sigma} = \langle\{L_{\mathbf{k}\sigma}, X_{-\mathbf{k}\sigma}^-\}\rangle$.

Generalized Hartree-Fock approximation (GHFA) or mean field approximation corresponds to the linear part of

Eq. (15), i.e., neglecting the irreducible operator $\bar{L}_{\mathbf{k}\sigma}$. Just in this approach we shall consider the possibility of superconductivity appearance. In Eq. (15), $C_{\mathbf{k}\sigma}/(1-n_{\bar{\sigma}})$ determines the renormalization of spectrum and $\Delta_{\mathbf{k}\sigma}$ describes possible superconducting gap. The spectral renormalization can be calculated in general case, however it is enough to use the simplest approximation of the Hubbard I type, and then in the nonmagnetic ground state ($n_{\uparrow}=n_{\downarrow}=n/2$) dependency on spin projection disappears and the modified spectrum can be represented in the form

$$\xi_{\mathbf{k}}=c(n)(\omega_{\mathbf{k}}-m), \quad m=\left[(g+r)\frac{n}{4}+\tilde{\mu}\right]/c(n),$$

$$c(n)=1-\frac{n}{2}, \quad (16)$$

where m is the effective chemical potential.

The expression for the gap $\Delta_{\mathbf{k}\sigma}$ is reduced to the form

$$\Delta_{-\mathbf{k}\downarrow}=-\Delta_{\mathbf{k}\uparrow}=\Delta_{\mathbf{k}},$$

$$\Delta_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{p}}[2\omega_{\mathbf{p}}+g(\gamma_{\mathbf{k}+\mathbf{p}}+\gamma_{\mathbf{k}-\mathbf{p}})-r\gamma_{\mathbf{k}+\mathbf{p}}]B_{\mathbf{p}}, \quad (17)$$

where $B_{\mathbf{p}}=\langle X_{-\mathbf{p}\downarrow}X_{\mathbf{p}\uparrow} \rangle$ are the abnormal averages. The first term in Eq. (17) is caused by kinematic correlations of electrons and derives from the kinetic term in the Hamiltonian (so-called kinematic mechanism of pairing¹⁶); the rest is effects of the exchange interaction. [We must note that in Refs. 18 and 19 a similar expression for the gap is derived for the t - J model with diagram method, however, there, beneath sign of sum, $g\gamma_{\mathbf{k}-\mathbf{p}}$ appears (in our notation) instead of symmetric in momentum combinations $g(\gamma_{\mathbf{k}+\mathbf{p}}+\gamma_{\mathbf{k}-\mathbf{p}})$ in formula (17).]

On the base of the equations (15) (irreducible operator $\bar{L}_{\mathbf{k}\sigma}$ is discarded) and formulas (16) and (17), at the mean field approximation we derive the system of equations

$$i\dot{X}_{\mathbf{k}\uparrow}=\xi_{\mathbf{k}}X_{\mathbf{k}\uparrow}-\frac{\Delta_{\mathbf{k}}}{c(n)}X_{-\mathbf{k}\downarrow}^+,$$

$$i\dot{X}_{-\mathbf{k}\downarrow}^+=-\xi_{\mathbf{k}}X_{-\mathbf{k}\downarrow}^+-\frac{\Delta_{\mathbf{k}}^*}{c(n)}X_{\mathbf{k}\uparrow}. \quad (18)$$

Using Eq. (18), we get the Gorkov type system of equations for retarding anticommutator Green functions and its solution:

$$\langle\langle X_{\mathbf{k}\uparrow}|X_{\mathbf{k}\uparrow}^+ \rangle\rangle_E=c(n)\frac{E+\xi_{\mathbf{k}}}{E^2-E_{\mathbf{k}}^2},$$

$$\langle\langle X_{-\mathbf{k}\downarrow}^+|X_{\mathbf{k}\uparrow}^+ \rangle\rangle_E=-\frac{\Delta_{\mathbf{k}}^*}{E^2-E_{\mathbf{k}}^2}, \quad (19)$$

where

$$E_{\mathbf{k}}^2=\xi_{\mathbf{k}}^2+\frac{|\Delta_{\mathbf{k}}|^2}{c(n)^2}. \quad (20)$$

General physical requirement of $E_{\mathbf{k}}=E_{-\mathbf{k}}$ leads to

$$|\Delta_{\mathbf{k}}|^2=|\Delta_{-\mathbf{k}}|^2. \quad (21)$$

IV. SELF-CONSISTENT EQUATIONS FOR DIFFERENT PAIRING SYMMETRIES

According to the spectral theorem,¹² we find the normal and the abnormal averages:

$$n_{\mathbf{k}}=\langle X_{\mathbf{k}\uparrow}^+X_{\mathbf{k}\uparrow} \rangle$$

$$=\langle X_{\mathbf{k}\downarrow}^+X_{\mathbf{k}\downarrow} \rangle$$

$$=c(n)\cdot\frac{1}{2}\left[1-\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\tanh\frac{E_{\mathbf{k}}}{2\tau}\right]\equiv c(n)\cdot f_{\mathbf{k}}, \quad (22)$$

$$B_{\mathbf{k}}^*=\langle X_{\mathbf{k}\uparrow}^+X_{-\mathbf{k}\downarrow}^+ \rangle=\frac{\Delta_{\mathbf{k}}^*}{2E_{\mathbf{k}}}\tanh\frac{E_{\mathbf{k}}}{2\tau}, \quad (23)$$

where $E_{\mathbf{k}}>0, \tau=k_B T/zt$ is the dimensionless temperature.

In the superconducting phase we have a system of three equations of self-consistency: (i) The interdependence of concentration n and effective chemical potential m on the base of Eq. (23) for the normal averages; (ii) the equation for the energy gap $\Delta_{\mathbf{k}}$ which is defined by Eq. (17) and meets condition (22); and (iii) a sum rule for abnormal averages $B_{\mathbf{p}}$ as a result of X -operators' algebra in the subspace of states $|0\rangle, |\sigma\rangle$.

The multiplication rule (5) results in

$$\frac{1}{N}\sum_{\mathbf{k}}B_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{k}}\langle X_{-\mathbf{p}\downarrow}X_{\mathbf{p}\uparrow} \rangle=\frac{1}{N}\sum_{\mathbf{f}}\langle X_{\mathbf{f}}^{0\downarrow}X_{\mathbf{f}}^{0\uparrow} \rangle=0. \quad (24)$$

This constraint is the direct result of the strong electron correlation and is the most essential difference between our approach and the traditional mean-field theory.

We must remark that while handling superconductivity in a system with full basis of Hubbard model states $|0\rangle, |\sigma\rangle, |2\rangle$ the condition (24) must be modified. Since Fermi operator $c_{\mathbf{f}\sigma}=X_{\mathbf{f}}^{0\sigma}+\eta(\sigma)X_{\mathbf{f}}^{\bar{\sigma}2}$, the abnormal average $B_{\mathbf{p}}=\langle c_{-\mathbf{p}\downarrow}c_{\mathbf{p}\uparrow} \rangle$ must meet the sum rule

$$\frac{1}{N}\sum_{\mathbf{p}}B_{\mathbf{p}}=\frac{1}{N}\sum_{\mathbf{f}}\langle c_{\mathbf{f}\downarrow}c_{\mathbf{f}\uparrow} \rangle=\frac{1}{N}\sum_{\mathbf{f}}\langle X_{\mathbf{f}}^{02} \rangle\equiv A$$

and again we have a system of three self-consistency equations.

We will demonstrate just which solutions exist and meet all the three equations.

Let us represent the abnormal averages $B_{\mathbf{p}}\equiv\langle X_{-\mathbf{p}\downarrow}X_{\mathbf{p}\uparrow} \rangle$ in the form

$$B_{\mathbf{k}}=B_{\mathbf{k}}^{(s)}+B_{\mathbf{k}}^{(a)}, B_{\mathbf{k}}^{(s)}=\frac{1}{2}(B_{\mathbf{k}}+B_{-\mathbf{k}})=B_{-\mathbf{k}}^{(s)},$$

$$B_{\mathbf{k}}^{(a)}=\frac{1}{2}(B_{\mathbf{k}}-B_{-\mathbf{k}})=-B_{-\mathbf{k}}^{(a)}, \quad (25)$$

i.e., as a sum of symmetric (s) and antisymmetric (a) parts. At once we remark that sum rule (24) is fulfilled automati-

cally for the antisymmetric part $B_{\mathbf{k}}^{(a)}$. It is easy to show that $B_{\mathbf{k}}^{(s)}$ describes the singlet pairings and $B_{\mathbf{k}}^{(a)}$ describes the triplet pairings with $S^z=0$.

We consider the bipartite lattices ($z=2d, d=2,3$) for which

$$\gamma_{\mathbf{k}} = \frac{1}{d} \sum_j \cos k_j \quad (26)$$

(lattice parameter $a=1$). Because of

$$\gamma_{\mathbf{k}\pm\mathbf{p}} = \frac{1}{d} \sum_j (\cos k_j \cos p_j \pm \sin k_j \sin p_j),$$

the gap (17) can be represented in the form

$$\Delta_{\mathbf{k}} = \Delta_{\mathbf{k}}^{(s)} + \Delta_{\mathbf{k}}^{(a)},$$

$$\Delta_{\mathbf{k}}^{(s)} = 2\Delta_0 + (2g-r) \frac{1}{d} \sum_j C_j \cos k_j,$$

$$\Delta_0 = \frac{1}{N} \sum_{\mathbf{p}} \omega_{\mathbf{p}} B_{\mathbf{p}}^{(s)}, \quad (27)$$

$$\Delta_{\mathbf{k}}^{(a)} = r \frac{1}{d} \sum_j S_j \sin k_j, \quad (28)$$

where

$$C_j = \frac{1}{N} \sum_{\mathbf{p}} \cos p_j B_{\mathbf{p}}^{(s)}, \quad S_j = \frac{1}{N} \sum_{\mathbf{p}} \sin p_j B_{\mathbf{p}}^{(a)}. \quad (29)$$

Here the gap $\Delta_{\mathbf{k}}^{(s)}$ (27) corresponds to the singlet pairings and $\Delta_{\mathbf{k}}^{(a)}$ (28) to the triplet pairings.

In limits of each class, with fulfilling Eq. (21), in principle, several solutions can exist, and each of these is a definite combination of cosines (for S pairings) and sines (for T pairings). In general case, we number the solutions with symbol l and denote the gap of l -type as $\Delta_{\mathbf{k}l}$ and the spectrum as $E_{\mathbf{k}l}$.

Symmetric solutions for S-pairing of s-type, $l=0$. If $C_x = C_y = C_z$ for $d=3$ or $C_x = C_y$ for $d=2$, then we have

$$\Delta_{\mathbf{k}0} = (2 + \lambda_0 \omega_{\mathbf{k}}) \Delta_0, \quad \lambda_0 = 2g - r, \quad (30)$$

where λ_0 is a dimensionless coupling constant for singlet (S) pairing. In this case, the sum of the abnormal averages (while $T=0$)

$$\frac{1}{N} \sum_{\mathbf{p}} B_{\mathbf{p}0} = \Delta_0 \frac{1}{N} \sum_{\mathbf{p}} \frac{2 + \lambda_0 \omega_{\mathbf{p}}}{\sqrt{\xi^2 + |\Delta_{\mathbf{p}0}|^2/c^2(n)}} \neq 0. \quad (31)$$

The constraint condition (24) is not fulfilled for the abnormal averages $B_{\mathbf{k}0}$ with gap $\Delta_{\mathbf{k}0}$ and due to this reason *the solutions of s-type are not present*.^{14,15,18,19} We note that the s -type gap solutions were cited earlier (for example, Refs. 16 and 17); however, the constraint condition was not taken into account.

Further, we restrict ourselves with the analysis of the case $d=2$.

The antisymmetric solutions of p -type ($l=1$) and the symmetric solutions of d -type ($l=2$) can be represented in the single form

$$\Delta_{\mathbf{k}l} = \lambda_l \psi_l(\mathbf{k}) \Delta_l, \quad \Delta_l = \frac{1}{N} \sum_{\mathbf{p}} \psi_l(\mathbf{p}) B_{\mathbf{p}l}. \quad (32)$$

We have the next types of solutions in the explicit form

(1) *Antisymmetric solutions of p-type (triplet pairing), $l=1$:*

$$\psi_p(\mathbf{k}) = \frac{1}{2} (\sin k_x + i \cdot \sin k_y), \quad \lambda_p = r. \quad (33)$$

(2) *Symmetric solutions of d-type (singlet pairing), $l=2$:*

$$\psi_d(\mathbf{k}) = \frac{1}{2} (\cos k_x - \cos k_y), \quad \lambda_d = 2g - r. \quad (34)$$

The sum rule (24) can be written as

$$\frac{1}{N} \sum_{\mathbf{p}} \frac{\psi_l(\mathbf{p})}{E_{\mathbf{p}l}} = 0 \quad (35)$$

and is fulfilled automatically for the p -type and is proven easily for the d -type (34) using the symmetry properties.

The gap equations for the p, d states are

$$\frac{1}{\lambda_l} = \frac{1}{N} \sum_{\mathbf{p}} \frac{|\psi_l(\mathbf{p})|^2}{2E_{\mathbf{p}l}} \tanh\left(\frac{E_{\mathbf{p}l}}{2\tau}\right), \quad (36)$$

where

$$E_{\mathbf{p}l} = \sqrt{c^2(n)(\omega_{\mathbf{p}} - m)^2 + \frac{|\Delta_{\mathbf{p}l}|^2}{c^2(n)}}.$$

The equation for T_c in p and d states is given by

$$\frac{2c(n)}{\lambda_l} = \frac{1}{N} \sum_{\mathbf{p}} \frac{|\psi_l(\mathbf{p})|^2}{|\omega_{\mathbf{p}} - m|} \tanh\left(\frac{c(n)|\omega_{\mathbf{p}} - m|}{2\tau_c^{(l)}}\right). \quad (37)$$

The same equation for the $d_{x^2-y^2}$ pairing has been derived by the diagram technique for the t - J model.¹⁵

V. RESULTS OF CALCULATIONS

At the numerical solution of the equation (37) more than 10^6 points of the Brillouin zone have been taken. Results of $T_c(n)$ computations are shown in the Figs. 1 and 2 for several values of the coupling constants λ_l . These results have revealed the remarkable difference in T_c values: $T_c^{(p)} \ll T_c^{(d)}$ when $\lambda_p = \lambda_d$. The moderate values of $\lambda \approx 0.4 - 0.5$ and $zt \approx 0.5$ eV result in $T_c^{(p)} \sim 1$ K, $T_c^{(d)} \sim 100$ K. The mean-field stability criterion for the p pairing is $\lambda_p > 0$ and for the d pairing is $\lambda_d > 0$. As concerns the stability of the mean-field solution to the charge density and spin fluctuations, recently, this stability has been proved using the same approach in Ref. 13 where the self-energy corrections have been considered.

It is clear from definitions (33), (34) that the p -type SC is formed by the ferromagnetic interaction; that is the case of Sr₂RuO₄, and the d -type SC is induced by the antiferromag-

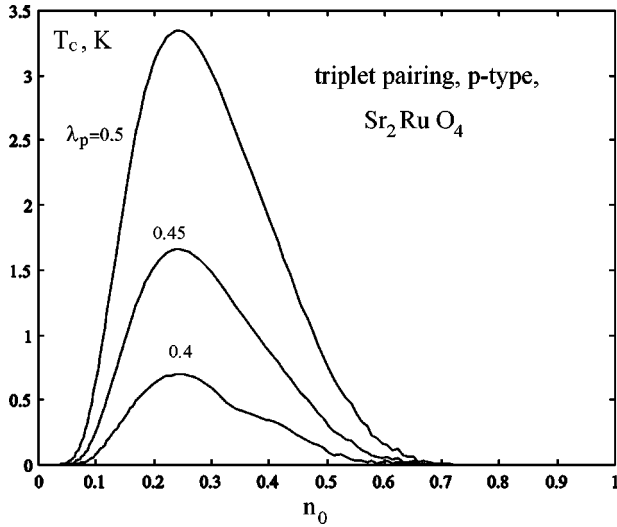


FIG. 1. Concentration dependence of T_c for the triplet pairing of the p -type, $\lambda_p = I/t$, I is a parameter of the antiferromagnetic exchange, and t is the hopping integral. Here $t = 0.1$ eV.

netic interaction in copper oxides. The d -type cannot arise in ruthenates because of the inappropriate sign of the parameter λ_d , the p -type is displaced by the d -type in cuprates for the reason that the λ_p is very low. To understand why $T_c^{(d)} \gg T_c^{(p)}$ we have analyzed the Eq. (37) analytically. Using integration over the constant energy surfaces $\omega_{\mathbf{k}} = \omega$ it can be rewritten as

$$\frac{2c(n)}{\alpha_l} = \int_{-1}^{+1} \frac{\psi_l^2(\omega)}{|\omega - m|} \tanh\left(\frac{c(n)|\omega - m|}{2\tau_c}\right) d\omega, \quad (38)$$

$$\psi_l^2(\omega) = \frac{1}{(2\pi)^2} \oint_{(\sigma_\omega)} \frac{|\psi_l(\mathbf{k})|^2}{|\nabla_{\mathbf{k}}\omega_{\mathbf{k}}|} d\sigma_\omega. \quad (39)$$

The sum rule for the $\psi_l^2(\omega)$ functions is the same for $l=p$ and $l=d$:

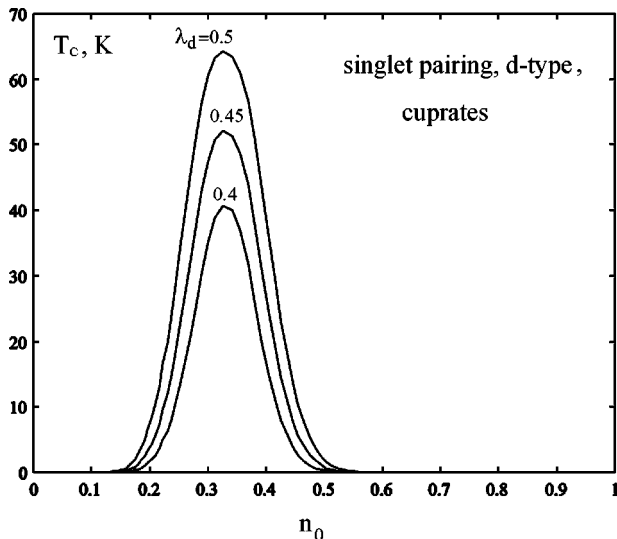


FIG. 2. Concentration dependence of T_c for the singlet pairing of the d -type, $\lambda_d = (2J - I)/t$, J is a parameter of the antiferromagnetic exchange, and I and t are the same as in Fig. 1.

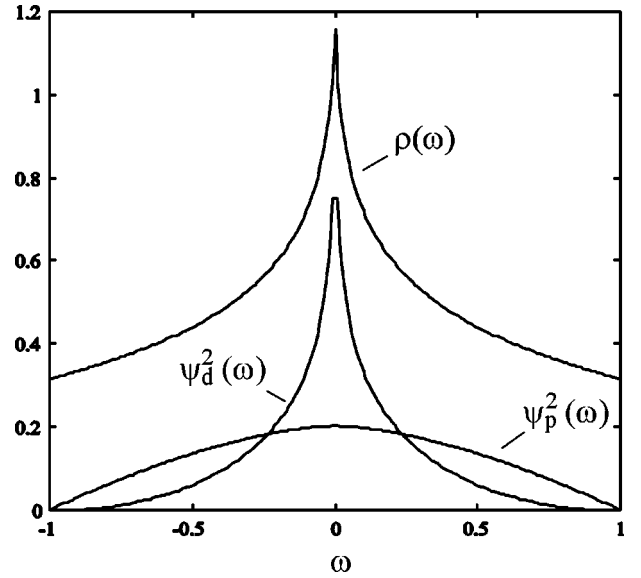


FIG. 3. Energy dependence of the effective gap anisotropy ψ_p^2 and ψ_d^2 and single-particle density of states $\rho(\omega)$ in square lattice.

$$\frac{1}{N} \sum_{\mathbf{k}} |\psi_l(\mathbf{k})|^2 = \int_{-1}^{+1} \psi_l^2(\omega) d\omega = 1/4. \quad (40)$$

For the p state

$$\frac{|\psi_p(\mathbf{k})|}{|\nabla_{\mathbf{k}}\omega_{\mathbf{k}}|} = |\nabla_{\mathbf{k}}\omega_{\mathbf{k}}| \quad (41)$$

and $\psi_p^2(\omega)$ is rather small with smooth energy dependence,

$$\begin{aligned} \psi_p^2(\omega) &= \frac{2}{\pi^2} [\mathbf{E}(\sqrt{1-\omega^2}) - \omega^2 \mathbf{K}(\sqrt{1-\omega^2})] \\ &\approx \frac{2}{\pi^2} (1 - |\omega|^{1.61}), \end{aligned} \quad (42)$$

where \mathbf{K} and \mathbf{E} are the Legendre's complete elliptic integrals of the first and the second kinds. For the d state

$$\frac{\psi_d^2(\mathbf{k})}{|\nabla_{\mathbf{k}}\omega_{\mathbf{k}}|} = \frac{1}{2} \frac{(\cos k_x - \cos k_y)^2}{\sqrt{\sin^2 k_x + \sin^2 k_y}} \quad (43)$$

has the same singularity as the van Hove singularity in the density of states $\rho(\omega)$. The result of calculation is

$$\psi_d^2(\omega) = (1 - \omega^2)\rho(\omega) - 2\psi_p^2(\omega),$$

where

$$\rho(\omega) = \frac{2}{\pi^2} \mathbf{K}(\sqrt{1-\omega^2}) \approx \frac{1}{\pi} - \left(\frac{1}{2} - \frac{1}{\pi}\right) \ln(|\omega|). \quad (44)$$

The comparison of $\psi_p^2(\omega)$ and $\psi_d^2(\omega)$ has shown that the van Hove singularity is cancelled in the p state and does not cancel in the d state (Fig. 3).

The similar conclusion on the large van Hove singularity contribution in the case of $d_{x^2-y^2}$ pairing in the strongly correlated holes in the CuO_2 plane have been obtained previously in the frame work in Ref. 20 of the t - J model.

The parameters t and I can be estimated from some experimental data. While concentration of “double states” is low in the upper Hubbard subband (those are equivalent to holes in the lower Hubbard subband), the dispersion law is well described in effective mass approximation: $\varepsilon_{\mathbf{k}} = -zt\gamma_{\mathbf{k}} \approx \varepsilon_0 + \mathbf{p}^2/2m^*$, i.e., $1/m^* = 2ta^2/\hbar^2$, where a is distance between atoms. Substituting values of the effective mass $m^* = (5-10)m_e$ ($m^*/m_e = 12$ according to Ref. 9) and distances $a = (2-4)$ (angstrom), we obtain t in interval $t = (0.02-0.2)$ eV with typical average $t \sim 0.1$ eV.

The spin-wave theory formula $k_B T_C \sim zI_{(xy)}/\ln[I_{(xy)}/I_{(z)}]$ may be used for Curie temperature T_C , here $I_{(xy)} \equiv I$ is the intraplanar exchange and $I_{(z)}$ is the interplanar exchange. The ratio of this interaction may be 10^4-10^5 and the Curie temperature T_C may reach the value $\sim (100-200)$ K. For example, in the recently synthesized hybrid Cu-Ru oxide systems with superconducting CuO_2 layers, the RuO_2 layers demonstrate ferromagnetic order with $T_C = 132$ K.²¹ Then $I \sim (2-5) \times 10^{-2}$ eV. Thus, the ruthenats’ values $r = I/t \sim (0.2-0.5)$ are equal roughly to the cuprates’ dimensionless parameter $\lambda_d = 2J/t$.

In conclusion we have presented the model of strongly correlated electrons in two dimensional lattice that allows us

to consider the cuprates ($J \gg I$) and Sr_2RuO_4 ($J \ll I$) on the same footing. The singlet SC in the s state is absent in the strong correlation limit, the triplet p pairing occurs due to the ferromagnetic fluctuations and the singlet d pairing is induced by the antiferromagnetic fluctuations. The reason why T_c in the cuprates is much higher than in Sr_2RuO_4 is the different gap anisotropies. For the p -state \mathbf{k} -dependence of the gap results in the cancellation of the van Hove singularity while for the d state the gap anisotropy permits large van Hove singularity contribution in the equation for T_c . For the question what is so specific in the copper oxides for high- T_c superconductivity the possible answer may be as follows: it is the planar Cu-O σ bonding resulting in the strong antiferromagnetic Cu-Cu interaction, that induced the singlet pairing with $d_{x^2-y^2}$ symmetry.

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