

Spin-triplet superconducting pairing due to local Hund's rule and Dirac exchange

Jozef Spałek*

Marian Smoluchowski Institute of Physics, Jagiellonian University, ulica Reymonta 4, 30-059 Kraków, Poland

(Received 11 April 2000; revised manuscript received 22 August 2000; published 20 February 2001)

We discuss general implications of the local spin-triplet pairing among fermions induced by local ferromagnetic exchange, an example of which is the Hund's rule coupling. The quasiparticle energy and their wave function are determined for the three principal phases with the gap, which is momentum independent. We utilize the Bogolyubov–Nambu–de Gennes approach, which in the case of triplet pairing in the two-band case leads to the four-components wave function. Both gapless modes and those with an isotropic gap appear in the quasiparticle spectrum. A striking analogy with the Dirac equation is briefly explored. This type of pairing is relevant to relativistic fermions as well, since it reflects the fundamental discrete symmetry-particle interchange. A comparison with the local interband spin-singlet pairing is also made.

DOI: 10.1103/PhysRevB.63.104513

PACS number(s): 74.20.Mn, 03.65.Pm

I. INTRODUCTION

The discovery¹ of superconductivity in the orbitally degenerate system Sr_2RuO_4 , which is closely related to both ferromagnetic² SrRuO_3 and antiferromagnetic and Mott insulating³ Ca_2RuO_4 , poses a question about the role of short-range Coulomb and exchange interactions in stabilizing the spin-triplet superfluid state.³ In the case of Mott-Hubbard insulators the kinetic exchange interaction⁴ plays an essential role in stabilizing antiferromagnetism. This interaction is also instrumental in the form of *real-space pairing*⁵ in driving the system close to the Mott-Hubbard boundary towards spin-singlet superconducting state. In the case of orbitally degenerate systems, the ferromagnetic⁶ and antiferromagnetic kinetic exchange interactions compete with each other⁷ for the number of electrons per atom $n > 1$. Ferromagnetism (with a possible orbital ordering) usually wins⁸ for $n \rightarrow 1$, whereas the antiferromagnetism takes over when $n \rightarrow d$, where d is the orbital degeneracy. This type of competition should also be present in Sr_2RuO_4 , in which $4d^4$ configuration of Ru^{4+} contains two holes in t_{2g} shell composed of nominally triply degenerate $d_\epsilon = (d_{xy}, d_{yz}, d_{zx})$ orbitals. The two-dimensional antiferromagnetic spin fluctuations have been indeed observed in Sr_2RuO_4 system.⁹ From the symmetry point of view d_{xy} does not mix with d_{yz} and d_{zx} , so the fluctuations can be ascribed¹⁰ as solely due to the electrons in d_{xy} band. The Hund's rule coupling between d_{xy} and the remaining two bands (d_{yz}, d_{zx}) must then suppress the formation of the antiferromagnetic state. In effect, we are left with two electronic liquids: the doubly degenerate and hybridized $d_{yz} - d_{zx}$ band containing approximately one hole and the d_{xy} band containing the other. It must be underlined that all t_{2g} holes are delocalized, since one observes a well defined Baber-Landau-Pomeranchuk ($\sim T^2$) contribution to the resistivity in both $x-y$ (RuO_2) plane and in c direction.¹¹

From what has been said above it is important to formulate first the model of local pairing represented a doubly degenerate (or almost degenerate) band coupled by the Hund's rule and characterize the possible spin-triplet solutions induced by the Hund's rule (ferromagnetic) exchange. This type of model has been formulated by us recently.¹² We have shown there that sizeable (of the order of bare band-

width) Coulomb correlations renormalize the system properties, i.e., lead to an *almost localized Fermi liquid* with a nonretarded real-space and spin-triplet pairing. The value of the transition temperature has been estimated there in the situation when the magnitude of the Coulomb interaction and the bare bandwidth are comparable and at the proper band filling. The renormalized Fermi-liquid nature of our fermionic system will be a starting point in this paper, in which we consider basic features of the superconducting state such as the quasiparticle wave function (in the Fock space) and their energies. We list the possible solutions for our effective model with interorbital pairing. The question of coexistence of the A1 state with ferromagnetism, as well as the competition with the orbitally ordered-spin ferromagnetic state has been discussed separately.¹³ We believe that the present two-band model stands on its own ground, *independently* of the detailed nature of Sr_2RuO_4 superconductivity (which should include the third band and the anisotropic interband hybridization) and must be considered separately, to amplify the physical plausibility of this mechanism of spin-triplet pairing in a concrete situation (see also the discussion at the end). This is particularly so because the Hund's rule and associated with it ferromagnetic fluctuations¹⁴ represent probably the most natural determinants of spin-triplet pairing under these circumstances. Also, the present real-space pairing¹³ represents is formally analogous to the spin-singlet pairing⁵ and additionally, reflects a fundamental symmetry—the particle interchange. So, it contains fundamental physics in the sense, that the nature of the ground state, i.e., that of the spin-triplet superconductor, can appear instead of or together with an itinerant ferromagnetism.

II. NAMBU-DE GENNES METHOD FOR THE TRIPLET PAIRING IN THE TWO-BAND CASE

We consider a degenerate two-band Fermi-liquid system coupled by a local triplet pairing. The corresponding effective Hamiltonian is of the simple form¹²

$$\mathcal{H} = \sum_{\mathbf{k}\sigma l=1,2} E_{\mathbf{k}l} a_{\mathbf{k}l\sigma}^\dagger a_{\mathbf{k}l\sigma} - 2\tilde{J} \sum_{im} A_{im}^\dagger A_{im}, \quad (1)$$

where $E_{\mathbf{k}l}$ are the quasiparticle energies with enhanced masses by the band narrowing factor q^{-1} (calculated

self-consistently¹⁵) in the bands $l=1,2$, $\tilde{J} \sim Jt^2$ is the effective Hund's rule coupling (the local interorbital exchange), and t^2 is the probability of having interorbital local spin-triplet configurations, characterized by the creation operators $A_1^\dagger = a_{il\uparrow}^\dagger a_{il'\uparrow}^\dagger$, $A_{-1}^\dagger = a_{il\downarrow}^\dagger a_{il'\downarrow}^\dagger$, and $A_0^\dagger = (1/\sqrt{2})(a_{il\uparrow}^\dagger a_{il'\downarrow}^\dagger + a_{il\downarrow}^\dagger a_{il'\uparrow}^\dagger)$ for $l \neq l'$. The local exchange origin of the second term derives from the exact relation between the pairing operators in real space and the full exchange operator projecting the corresponding two-particle state onto the spin-triplet configuration,

$$\sum_{m=-1}^1 A_{im}^\dagger A_{im} = \mathbf{S}_{il} \cdot \mathbf{S}_{il'} + \frac{3}{4} n_{il} n_{il'}, \quad (2)$$

where \mathbf{S}_{il} and n_{il} are respectively the spin and the particle number operators for electron on site i and orbital l . Explicitly $n_{il} = \sum_{\sigma} n_{il\sigma}$, $n_{il\sigma} = a_{il\sigma}^\dagger a_{il\sigma}$, whereas the spin operators $\mathbf{S}_{il} \equiv (S_{il}^+, S_{il}^-, S_{il}^z) \equiv [a_{il\uparrow}^\dagger a_{il\downarrow}, a_{il\downarrow}^\dagger a_{il\uparrow}, (1/2)(n_{il\uparrow} - n_{il\downarrow})]$. The right-hand side of Eq. (3) represents thus the full exchange operator.

After making the BCS-type approximation in the local form¹⁴

$$A_{im}^\dagger A_{im} \simeq A_{im}^\dagger \langle A_{im} \rangle + \langle A_{im}^\dagger \rangle A_{im} - \langle A_{im}^\dagger \rangle \langle A_{im} \rangle \quad (3)$$

we can cast Hamiltonian (1) into the four-component form, which in the reciprocal (\mathbf{k}) space takes the form¹²

$$\mathcal{H}_{BCS} = \sum_{\mathbf{k}} \mathbf{f}_{\mathbf{k}}^\dagger \mathbf{H}_{\mathbf{k}} \mathbf{f}_{\mathbf{k}} + \sum_{\mathbf{k}} E_{\mathbf{k}2}, \quad (4)$$

where the corresponding Nambu operators take the form: $\mathbf{f}_{\mathbf{k}}^\dagger = (f_{\mathbf{k}1\uparrow}^\dagger, f_{\mathbf{k}1\downarrow}^\dagger, f_{-\mathbf{k}2\uparrow}^\dagger, f_{-\mathbf{k}2\downarrow}^\dagger)$, $\mathbf{f}_{\mathbf{k}} = (\mathbf{f}_{\mathbf{k}}^\dagger)^\dagger$, and the Hamiltonian matrix for selected \mathbf{k} state reads

$$\mathbf{H}_{\mathbf{k}} = \begin{pmatrix} E_{\mathbf{k}1} - \mu, & 0, & \Delta_1, & \Delta_0 \\ 0, & E_{\mathbf{k}1} - \mu, & \Delta_0, & \Delta_{-1} \\ \Delta_1^*, & \Delta_0^*, & -E_{\mathbf{k}2} + \mu, & 0 \\ \Delta_0^*, & \Delta_{-1}^*, & 0, & -E_{\mathbf{k}2} + \mu \end{pmatrix} \\ \equiv \begin{pmatrix} E_{\mathbf{k}1} \hat{\sigma}_0, & \hat{\Delta} \\ \hat{\Delta}^*, & -E_{\mathbf{k}2} \hat{\sigma}_0 \end{pmatrix}, \quad (5)$$

where $\hat{\sigma}_0 \equiv \mathbf{1}$ is the unit 2×2 matrix, and μ is the chemical potential. The superconducting gap is parametrized as $\Delta_m \equiv -2\tilde{J} \sum_{\mathbf{k}} \langle f_{\mathbf{k}1\sigma}^\dagger f_{-\mathbf{k}2\sigma'}^\dagger \rangle$, with $m = (\sigma + \sigma')/2$, and $\sigma, \sigma' = \pm 1$. The 2×2 matrix $\hat{\Delta}$ is parametrized in the usual form,¹⁶

$$\hat{\Delta} = i(\mathbf{d} \cdot \tilde{\sigma}) \sigma_y = \begin{pmatrix} -d_x + id_y, & d_z \\ d_z, & d_x + id_y \end{pmatrix}, \quad (6)$$

where $\tilde{\sigma}$ is composed of the three Pauli matrices, whereas the vector \mathbf{d} in spin space has the components $d_x = (\Delta_{-1} - \Delta_1)/2$, $d_y = (\Delta_{-1} + \Delta_1)/2$, and $d_z = \Delta_0$. The form (5) is a generalization of the Nambu representation to the triplet case with three, in general different, gaps Δ_m .

It is straightforward to introduce the 4×4 Dirac matrices

$$\tilde{\beta} \equiv \begin{pmatrix} \mathbf{1}, & 0 \\ 0, & -\mathbf{1} \end{pmatrix} \quad \text{and} \quad \tilde{\alpha}_i = \begin{pmatrix} 0, & \sigma_i \\ \sigma_i, & 0 \end{pmatrix},$$

and then rewrite Eq. (5) for the degenerate case $E_{\mathbf{k}1} = E_{\mathbf{k}2}$ and for $\Delta_m = \Delta_m^*$ in the form

$$\mathbf{H}_{\mathbf{k}} = \tilde{\beta}(E_{\mathbf{k}} - \mu) + i(\mathbf{d} \cdot \tilde{\alpha}) \Sigma_2, \quad (7)$$

where

$$\Sigma_2 = \begin{pmatrix} 0, & \sigma_y \\ \sigma_y, & 0 \end{pmatrix}$$

is the y component of the relativistic spin operator. We discuss in detail the simple situation of degenerate electrons ($E_{\mathbf{k}1} = E_{\mathbf{k}2}$) with a real gap Δ_m in the next section.

One can also look at the approach from a different perspective. Let us introduce the four-component wave function for a single quasiparticle in the superconducting phase propagating in the real space as follows:

$$\Psi(\mathbf{x}, t) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \begin{pmatrix} \psi_{1\mathbf{k}} f_{\mathbf{k}1\uparrow} \\ \psi_{2\mathbf{k}} f_{\mathbf{k}1\downarrow} \\ \psi_{3\mathbf{k}} f_{-\mathbf{k}2\uparrow}^\dagger \\ \psi_{4\mathbf{k}} f_{-\mathbf{k}2\downarrow}^\dagger \end{pmatrix} \exp \left[i \left(\mathbf{k} \cdot \mathbf{x} - \frac{E_{\mathbf{k}}}{\hbar} t \right) \right], \quad (8)$$

where $\psi_{\mu\mathbf{k}}$ are the quasiparticle amplitudes which are determined for each eigenstate (see below). In this representation the Bogoliubov-de Gennes equation for a single quasiparticle in the superconducting states reads

$$i\hbar \partial_t \Psi = \tilde{\beta} \left[E_{\mathbf{k}} \left(\mathbf{k} \Rightarrow \frac{\nabla}{i} \right) - \mu \right] \Psi + i(\mathbf{d} \cdot \tilde{\alpha}) \Sigma_2 \Psi, \quad (9)$$

where $E_{\mathbf{k}}(\mathbf{k} \Rightarrow \nabla/i)$ represents now the differential operator $(1/i)\nabla$ replacing the wave vector \mathbf{k} in the dispersion relation $E_{\mathbf{k}}$ for quasiparticles. In the effective-mass approximation and in the stationary case this wave equation for quasiparticles in the superconducting phase has the following form:

$$\lambda \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = - \left(\frac{\hbar^2}{2m^*} \nabla^2 + \mu \right) \begin{pmatrix} \psi_1 \\ \psi_2 \\ -\psi_3 \\ -\psi_4 \end{pmatrix} + \begin{pmatrix} \Delta_1 \psi_3 + \Delta_0 \psi_4 \\ \Delta_0 \psi_3 + \Delta_{-1} \psi_4 \\ \Delta_1 \psi_1 + \Delta_0 \psi_2 \\ \Delta_0 \psi_1 + \Delta_{-1} \psi_2 \end{pmatrix}, \quad (10)$$

where $\psi_{\mu} \equiv \psi_{\mu}(\mathbf{x})$ and λ is an eigenvalue of quasiparticle state in the superconducting state with the above four-component wave function (Δ_m are regarded as real). The validity of this equation goes beyond the simple solution (8), as one can include the magnetic and electric fields and other

inhomogeneities if they appear on the mesoscopic or macroscopic scale. In the next section we will use explicitly the momentum representation of Eq. (10), as we will discuss exclusively homogeneous superconducting states. We will return to Eq. (10) when discussing the general features of this Hamiltonian in Sec. IV. One should also note that finding the eigenvalues for Hamiltonian in the forms (4) or (7) can be achieved by diagonalizing of the matrix 4×4 in general case, as discussed in analytic terms in Appendix A.

III. SUPERCONDUCTING STATES AND THEIR QUASIPARTICLES

We now discuss three principal solutions of Eq. (10) by taking $\psi_\mu(\mathbf{x}) = \psi_\mu \exp(i\mathbf{k} \cdot \mathbf{x}) / \sqrt{V}$, where V is the system volume. We also assume that $\Delta_\mu = \Delta_\mu^*$ (e.g., neglect the applied magnetic fields), since we consider only spatially homogeneous solutions. Namely, rewriting Eq. (10) in components we obtain the combinations

$$\begin{cases} \lambda(\psi_1 + \psi_2) = (E_{\mathbf{k}} - \mu)(\psi_1 + \psi_2) + (\Delta_1 + \Delta_0)\psi_3 + (\Delta_0 + \Delta_{-1})\psi_4 \\ \lambda(\psi_3 + \psi_4) = -(E_{\mathbf{k}} - \mu)(\psi_3 + \psi_4) + (\Delta_1 + \Delta_0)\psi_1 + (\Delta_0 + \Delta_{-1})\psi_2, \end{cases} \quad (11)$$

and

$$\begin{cases} \lambda(\psi_1 - \psi_2) = (E_{\mathbf{k}} - \mu)(\psi_1 - \psi_2) + (\Delta_1 - \Delta_0)\psi_3 + (\Delta_0 - \Delta_{-1})\psi_4 \\ \lambda(\psi_3 - \psi_4) = -(E_{\mathbf{k}} - \mu)(\psi_3 - \psi_4) + (\Delta_1 - \Delta_0)\psi_1 + (\Delta_0 - \Delta_{-1})\psi_2. \end{cases} \quad (12)$$

Such combinations of particle (ψ_1 and ψ_2) and hole (ψ_3 and ψ_4) components contain basic symmetry, as we will see on example of particular solutions, which we discuss next.

A. Isotropic solution: $\Delta_0 = \Delta_{-1} = \Delta_1 \equiv \Delta$

In that situation Eqs. (11) and (12) take a simple form,

$$\begin{cases} \lambda(\psi_1 + \psi_2) = (E_{\mathbf{k}} - \mu)(\psi_1 + \psi_2) + 2\Delta(\psi_3 + \psi_4) \\ \lambda(\psi_3 + \psi_4) = -(E_{\mathbf{k}} - \mu)(\psi_3 + \psi_4) + 2\Delta(\psi_1 + \psi_2), \end{cases} \quad (13)$$

and

$$\begin{cases} \lambda(\psi_1 - \psi_2) = (E_{\mathbf{k}} - \mu)(\psi_1 - \psi_2) \\ \lambda(\psi_3 - \psi_4) = -(E_{\mathbf{k}} - \mu)(\psi_3 - \psi_4). \end{cases} \quad (14)$$

The first two equations lead to the modes with a gap

$$\lambda = \lambda_{\mathbf{k}1,2} = \pm \sqrt{(E_{\mathbf{k}} - \mu)^2 + 4\Delta^2} \equiv \pm \lambda_{\mathbf{k}}. \quad (15)$$

For those two modes $\psi_1 = \psi_2$ and $\psi_3 = \psi_4$ and their eigenstates are characterized by the following quasiparticle operators:

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} \frac{1}{\sqrt{2}} (f_{\mathbf{k}1\uparrow} + f_{\mathbf{k}1\downarrow}) - v_{\mathbf{k}} \frac{1}{\sqrt{2}} (f_{-\mathbf{k}2\uparrow}^\dagger + f_{-\mathbf{k}2\downarrow}), \quad (16)$$

and

$$\beta_{-\mathbf{k}}^\dagger = v_{\mathbf{k}} \frac{1}{\sqrt{2}} (f_{\mathbf{k}1\uparrow} + f_{\mathbf{k}1\downarrow}) + u_{\mathbf{k}} \frac{1}{\sqrt{2}} (f_{-\mathbf{k}2\uparrow}^\dagger + f_{-\mathbf{k}2\downarrow}), \quad (17)$$

with the Bogoliubov coherence factors

$$u_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(1 + \frac{E_{\mathbf{k}} - \mu}{\lambda_{\mathbf{k}}} \right)^{1/2}, \quad v_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(1 - \frac{E_{\mathbf{k}} - \mu}{\lambda_{\mathbf{k}}} \right)^{1/2}. \quad (18)$$

The quasiparticle operators contain symmetric combinations $(f_{\mathbf{k}1\uparrow} + f_{\mathbf{k}1\downarrow})/\sqrt{2}$ and $(f_{-\mathbf{k}2\uparrow} + f_{-\mathbf{k}2\downarrow})/\sqrt{2}$. The wave function is symmetric with respect to particle-spin interchange ($\uparrow \leftrightarrow \downarrow$) and describes quasiparticle states of energy $\pm \lambda_{\mathbf{k}}$, respectively.

Equations (14) lead to the gapless modes of the form,

$$\lambda = \lambda_{\mathbf{k}3,4} = \pm (E_{\mathbf{k}} - \mu), \quad (19)$$

and correspond to the eigenstates characterized by the operators

$$\gamma_{\mathbf{k}} = \frac{1}{\sqrt{2}} (f_{\mathbf{k}1\uparrow} - f_{\mathbf{k}1\downarrow}), \quad \text{and} \quad \delta_{-\mathbf{k}}^\dagger = \frac{1}{\sqrt{2}} (f_{-\mathbf{k}2\uparrow}^\dagger - f_{-\mathbf{k}2\downarrow}^\dagger) \quad (20)$$

and constitute the antisymmetric-in-spin operators, representing the unpaired electrons. These gapless modes disappear when the gap components are not equal, as shown in Appendix A. One should note that the gapless modes appear even though the superconducting gap here is \mathbf{k} independent.

Combining the solutions (16)–(18) and (19) and (20) we can express the original (“old”) particle operators in terms of quasiparticle (“new”) operators in the following manner:

$$\begin{pmatrix} f_{\mathbf{k}1\uparrow} \\ f_{\mathbf{k}1\downarrow} \\ f_{-\mathbf{k}2\uparrow}^\dagger \\ f_{-\mathbf{k}2\downarrow}^\dagger \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} & 1 & 0 \\ u_{\mathbf{k}} & v_{\mathbf{k}} & -1 & 0 \\ -v_{\mathbf{k}} & u_{\mathbf{k}} & 0 & 1 \\ -v_{\mathbf{k}} & u_{\mathbf{k}} & 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}} \\ \beta_{-\mathbf{k}}^\dagger \\ \gamma_{\mathbf{k}} \\ \delta_{-\mathbf{k}}^\dagger \end{pmatrix}. \quad (21)$$

This transformation is necessary for determining the self-consistent equation for the gap and for the chemical potential μ . First, we rewrite the Hamiltonian (4) in the diagonal form

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \lambda_{\mathbf{k}} (\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} - \beta_{-\mathbf{k}} \beta_{-\mathbf{k}}^\dagger) + E_{\mathbf{k}} (\gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}} - \delta_{-\mathbf{k}} \delta_{-\mathbf{k}}^\dagger) + \sum_{\mathbf{k}} E_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} \lambda_{\mathbf{k}} (\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{-\mathbf{k}}^\dagger \beta_{-\mathbf{k}} - 1) + E_{\mathbf{k}} (\gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}} + \delta_{-\mathbf{k}}^\dagger \delta_{-\mathbf{k}}). \end{aligned} \quad (22)$$

The equation for the gap, e.g., $\Delta_1 = \langle f_{\mathbf{k}_1 \uparrow}^\dagger f_{-\mathbf{k}_2 \uparrow}^\dagger \rangle$ is obtained by substituting the relevant transformed operators in Eq. (21) to Δ_1 . In effect, we obtain the usual BCS form ($E_{\mathbf{k}} \equiv E_{\mathbf{k}} - \mu$)

$$\langle f_{\mathbf{k}_1 \uparrow}^\dagger f_{-\mathbf{k}_2 \uparrow}^\dagger \rangle = -\frac{1}{2} \frac{\Delta}{\sqrt{E_{\mathbf{k}}^2 + 4\Delta^2}} \tanh\left(\frac{\beta \sqrt{E_{\mathbf{k}}^2 + 4\Delta^2}}{2}\right), \quad (23)$$

where $\beta \equiv (k_B T)^{-1}$. So, the gap equation has two solutions: 1°, $\Delta \equiv 0$,

$$2^\circ, \quad 1 = \frac{J}{N} \sum_{\mathbf{k}} \frac{1}{\sqrt{E_{\mathbf{k}}^2 + 4\Delta^2}} \tanh\left(\frac{\beta \sqrt{E_{\mathbf{k}}^2 + 4\Delta^2}}{2}\right). \quad (24)$$

The last equation tells us that the physical gap is 2Δ . The self-consistent equation for the chemical potential must include gapless modes, i.e., takes the form

$$n = \frac{1}{N} \sum_{\mathbf{k}\sigma} \langle f_{\mathbf{k}_1 \sigma}^\dagger f_{\mathbf{k}_1 \sigma} + f_{\mathbf{k}_2 \sigma}^\dagger f_{\mathbf{k}_2 \sigma} \rangle = \frac{2}{N} \sum_{\mathbf{k}} \langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}} \rangle. \quad (25)$$

Normally, as we shall see, $\Delta \ll |\mu|$, and hence approximately half of all particles will have the spectrum gapped. The details must be analyzed numerically for a concrete structure of the density of states. In the limit $\tilde{W} \ll \tilde{J}$ we have the estimate of the gap value at $T=0$ in the form $\Delta = (\tilde{W}/2) \exp(-\tilde{W}/(2\tilde{J}))$; this yields the value $\Delta/\tilde{W} \sim 10^{-3} - 10^{-4}$, or in the regime 1–10 K for $\tilde{W} \approx 1$ eV and $\tilde{J} \sim 0.1\tilde{W}$.

We need also the expression for the ground-state energy, as various solutions are possible. In the present case, this energy can be written as

$$\begin{aligned} \frac{E_G}{N} &= \frac{2}{N} \sum_{\mathbf{k}} (\sqrt{E_{\mathbf{k}}^2 + \tilde{\Delta}^2} \langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} \rangle + E_{\mathbf{k}} \langle \gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}} \rangle \\ &\quad - \sqrt{E_{\mathbf{k}}^2 + \tilde{\Delta}^2}) + \frac{\tilde{\Delta}^2}{2J}, \end{aligned} \quad (26)$$

where $\tilde{\Delta} = 2\Delta$.

B. Equal-spin pairing: $\Delta_0 \equiv 0$

To obtain the explicit solution we now combine separately the first and third components of Eq. (10) on one side, and the second and the fourth on the other. Adding and subtracting the corresponding terms we obtain

$$\begin{cases} (\Delta_1 - \lambda)(\psi_1 + \psi_3) + (E_{\mathbf{k}} - \mu)(\psi_1 - \psi_3) = 0 \\ (E_{\mathbf{k}} - \mu)(\psi_1 + \psi_3) - (\Delta_1 + \lambda)(\psi_1 - \psi_3) = 0, \end{cases} \quad (27)$$

and

$$\begin{cases} (\Delta_{-1} - \lambda)(\psi_2 + \psi_4) + (E_{\mathbf{k}} - \mu)(\psi_2 - \psi_4) = 0 \\ (E_{\mathbf{k}} - \mu)(\psi_2 + \psi_4) - (\Delta_{-1} + \lambda)(\psi_2 - \psi_4) = 0. \end{cases} \quad (28)$$

Thus the two pairs of components (27) and (28) separate from each other and it is sufficient to solve, e.g., the first system (27) to be able to reproduce the other. Explicitly, the two solutions can be combined into the form, in which the eigenvalues take the form

$$\lambda \equiv \lambda_{\mathbf{k}_1 \dots \mathbf{k}_4} = \pm \sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_\sigma^2} \equiv \pm \lambda_{\mathbf{k}}^{(\sigma)}, \quad (29)$$

where for each spin orientation $\sigma = \pm 1$ of the quasiparticles we have two solutions with the gap $\pm \sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_\sigma^2}$. The quasiparticle operators ($\alpha_{\mathbf{k}\sigma}, \beta_{-\mathbf{k}\sigma}^\dagger$) diagonalizing Hamiltonian (4) in this case are

$$\alpha_{\mathbf{k}\sigma} = u_{\mathbf{k}}^{(\sigma)} \frac{1}{\sqrt{2}} (f_{\mathbf{k}_1 \sigma} + f_{-\mathbf{k}_2 \sigma}^\dagger) - v_{\mathbf{k}}^{(\sigma)} \frac{1}{\sqrt{2}} (f_{\mathbf{k}_1 \sigma} - f_{-\mathbf{k}_2 \sigma}^\dagger), \quad (30)$$

and

$$\beta_{-\mathbf{k}\sigma}^\dagger = -v_{\mathbf{k}}^{(\sigma)} \frac{1}{\sqrt{2}} (f_{\mathbf{k}_1 \sigma} + f_{-\mathbf{k}_2 \sigma}^\dagger) + u_{\mathbf{k}}^{(\sigma)} \frac{1}{\sqrt{2}} (f_{\mathbf{k}_1 \sigma} - f_{-\mathbf{k}_2 \sigma}^\dagger), \quad (31)$$

with the coherence factors

$$u_{\mathbf{k}}^{(\sigma)} = \frac{1}{\sqrt{2}} \left(1 + \frac{\Delta_\sigma}{\lambda_{\mathbf{k}}^{(\sigma)}} \right)^{1/2}, \quad v_{\mathbf{k}}^{(\sigma)} = \frac{1}{\sqrt{2}} \left(1 - \frac{\Delta_\sigma}{\lambda_{\mathbf{k}}^{(\sigma)}} \right)^{1/2}. \quad (32)$$

In general, we have two gaps $\Delta_\sigma = (\Delta_1, \Delta_{-1})$. In the situation $\Delta_\sigma = \Delta_{-\sigma} = \Delta$ we have a doubly (spin) degenerate solutions. It can be easily verified that the operators (30) and (31) obey the fermion anticommutation relations. The diagonalized Hamiltonian has the form

$$\mathcal{H} = \sum_{\mathbf{k}} \lambda_{\mathbf{k}}^{(\sigma)} (\alpha_{\mathbf{k}\sigma}^\dagger \alpha_{\mathbf{k}\sigma} + \beta_{\mathbf{k}\sigma}^\dagger \beta_{\mathbf{k}\sigma} - 1) + E_0. \quad (33)$$

To determine the gap equation we have to find the transformation which is reverse of Eqs. (30) and (31). It is of the form

$$\begin{pmatrix} f_{\mathbf{k}1\uparrow} \\ f_{\mathbf{k}1\downarrow} \\ f_{-\mathbf{k}2\uparrow}^\dagger \\ f_{-\mathbf{k}2\downarrow}^\dagger \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} u_{\mathbf{k}}^{(+)} + v_{\mathbf{k}}^{(+)}, & u_{\mathbf{k}}^{(+)} - v_{\mathbf{k}}^{(+)}, & 0, & 0 \\ 0, & 0, & u_{\mathbf{k}}^{(-)} + v_{\mathbf{k}}^{(-)}, & u_{\mathbf{k}}^{(-)} - v_{\mathbf{k}}^{(-)} \\ u_{\mathbf{k}}^{(+)} - v_{\mathbf{k}}^{(+)}, & -u_{\mathbf{k}}^{(+)} - v_{\mathbf{k}}^{(+)}, & 0, & 0 \\ 0, & 0, & u_{\mathbf{k}}^{(-)} - v_{\mathbf{k}}^{(-)}, & -u_{\mathbf{k}}^{(-)} - v_{\mathbf{k}}^{(-)} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}\uparrow} \\ \beta_{-\mathbf{k}\uparrow}^\dagger \\ \alpha_{\mathbf{k}\downarrow} \\ \beta_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix}. \quad (34)$$

The difference with the isotropic pairing (21) is that here the coherence factors appear in combinations. Those appear also in the self-consistent equation for the gap

$$\langle f_{-\mathbf{k}2\sigma}^\dagger f_{\mathbf{k}1\sigma}^\dagger \rangle = -(u_{\mathbf{k}}^{(\sigma)2} - v_{\mathbf{k}}^{(\sigma)2}) [1 - \langle \alpha_{\mathbf{k}\sigma}^\dagger \alpha_{\mathbf{k}\sigma} \rangle - \langle \beta_{\mathbf{k}\sigma}^\dagger \beta_{\mathbf{k}\sigma} \rangle]. \quad (35)$$

In result, the self-consistent equation will have the following three solutions: 1° $\Delta_\sigma \equiv 0$, 2° $\Delta_{(-\sigma)} = 0$, but $\Delta_\sigma \neq 0$ is the solution of equation

$$1 = \frac{J}{N} \sum_{\mathbf{k}} \frac{1}{\sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_\sigma^2}} \tanh\left(\frac{\beta}{2} \sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_\sigma^2}\right) \quad (36)$$

3° $\Delta_\sigma \neq 0$, $\Delta_{-\sigma} \neq 0$, and each of them is determined from Eq. (36).

One should note that the coupling constant above (J) is the same as for the isotropic phase [cf. Eq. (24)]. For the sake of completeness, we reproduce the ground-state-energy expression which is

$$\begin{aligned} \frac{E_G}{N} &= \frac{2}{N} \sum_{\mathbf{k}\sigma} \sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_\sigma^2} \langle \alpha_{\mathbf{k}\sigma}^\dagger \alpha_{\mathbf{k}\sigma} \rangle + \frac{\Delta_\uparrow^2 + \Delta_\downarrow^2}{2J} \\ &\quad - \frac{1}{N} \sum_{\mathbf{k}\sigma} \sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_\sigma^2} + \frac{1}{N} \sum_{\mathbf{k}} E_{\mathbf{k}}. \end{aligned} \quad (37)$$

This phase represents a starting point when discussing the coexistence of ferromagnetism and the spin-triplet superconductivity.

C. Spin-polarized phase: $\Delta_0 = \Delta_\uparrow = \Delta_\downarrow = 0$

In this limit the system is totally spin polarized, i.e., is a *spin-saturated superconductor*. In that limit we recover again the spectrum both with and without gap, i.e., $\lambda_{\mathbf{k}1,2} = \pm \sqrt{(E_{\mathbf{k}} - \mu)^2 + \Delta_\uparrow^2}$, $\lambda_{\mathbf{k}3,4} = \pm (E_{\mathbf{k}} - \mu)$. Thus paired and unpaired states coexist also in this phase, as can be easily seen from Eqs. (30) and (31), which yield the form written there for $\sigma = \uparrow$ and $\alpha_{\mathbf{k}\downarrow} = f_{\mathbf{k}1\downarrow}$ and $\beta_{-\mathbf{k}\downarrow}^\dagger = -f_{\mathbf{k}2\downarrow}^\dagger$.

Summarizing Secs. III A–C, the lowest energy will have the homogeneous state with $\Delta_\uparrow = \Delta_\downarrow = \Delta_0$ so that the effective gap is equal to 2Δ . The most interesting feature of the results is that the gapless modes coexist in A and C and represent half of the spectrum. Also, the condensed phases described by A–C above correspond roughly to the solutions for superfluid ^3He , which are labeled¹⁷ B, A, and A1. However, under the present circumstances here we have momentum *independent* gaps, since the pairing is of the local (intrasite, but interorbital) nature. For the sake of comparison

we present in Appendix B the case of spin-singlet pairing induced by the same type of local interband pairing induced by antiferromagnetic exchange.

IV. REMARK ON THE TRIPLET PAIRING FOR RELATIVISTIC FERMIONS

The two-band situation with a local ferromagnetic exchange can be easily generalized to the explicitly relativistic form modeling thus the triplet configuration of spin, isospin, or color (the singlet case was considered by Nambu and Jona-Lasinio¹⁶ and in Ref. 19). The paired quasiparticles²⁰ obey the following modified Dirac wave equation:

$$i\hbar \partial_t \Psi = (c \tilde{\alpha} \cdot \hat{\mathbf{p}} + \tilde{\beta} m c^2) \Psi + i(\mathbf{d} \cdot \tilde{\alpha}) \Sigma_2 \Psi, \quad (38)$$

where the last term supplements the Dirac equation with the contact pairing. By taking the analogy with the original approach by Nambu²¹ one can write down the stationary version of this equation as the following system in the two-component (Weyl) representation:

$$\begin{aligned} \lambda \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} &= (c \tilde{\sigma} \cdot \hat{\mathbf{p}} - \mu) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} + m c^2 \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix} \\ &\quad + \begin{pmatrix} \Delta_1 \psi_3 + \Delta_0 \psi_4 \\ \Delta_0 \psi_3 + \Delta_{-1} \psi_4 \end{pmatrix}, \end{aligned} \quad (39)$$

$$\begin{aligned} \lambda \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix} &= -(c \tilde{\sigma} \cdot \hat{\mathbf{p}} - \mu) \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix} + m c^2 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \\ &\quad + \begin{pmatrix} \Delta_1 \psi_1 + \Delta_0 \psi_2 \\ \Delta_0 \psi_1 + \Delta_{-1} \psi_2 \end{pmatrix}. \end{aligned} \quad (40)$$

This system of equations can be directly compared with Eq. (10) for nonrelativistic electrons. In the present situation the mass term mixes the upper and the lower two components of the bispinor, as does the pairing part. Apart from a modification in the kinetic-energy part, the system of Eqs. (39)–(40) can be solved in the manner as discussed in Sec. III. The detailed discussion must include also the gauge fields, which lead to one-exchange pairing (analogous to the phonon-mediated pairing), a topic intensively discussed in recent literature.²² In general, the singlet pairing^{16,19–22} is mutually exclusive with the triplet pairing proposed here and therefore the latter requires first a detailed discussion of exchange interactions represented by relativistic spin $\{\Sigma_{ij}\}$.

V. DISCUSSION

In this paper we have formulated the quasiparticle language for local triplet pairing between fermions (interband pairing in the nonrelativistic case) induced by the local (Hund's rule or Dirac) exchange. In particular, we have determined explicitly the quasiparticle states and the de Gennes wave equation for them, which can be useful when considering spatially inhomogeneous situations.²³ The principal feature of the results is the existence of the gapless modes, existence of which can also be proved on a phenomenological level.²⁴ The circumstance that the pairing is induced by the ferromagnetic exchange means that this interaction can lead not only to an itinerant ferromagnetic state, but also to either spin-triplet superconductor or to a coexistence of both these states (for a brief discussion of this issue, see Ref. 13). The present paper represents only the first step in this direction. Furthermore, our mechanism of pairing expressing the fundamental symmetry (the particle interchange) may have an important astrophysical application: the pairing in the neutron-proton matter in pulsar, but this intriguing possibility requires a separate study.

Two problems should be tackled next. First, the analysis of the Meissner effect, since in the present situation the orbital diamagnetism will compete with the ferromagnetic spin polarization (particularly, if the triplet superconducting and ferromagnetic phases can coexist). An intriguing question here is: can we reach the limiting superconducting phase (corresponding to A1 phase in the case of superfluid ³He), the critical temperature T_c of which can be enhanced by the applied magnetic field?

Second, one should derive microscopically the Ginzburg-Landau equation for the condensed pairs. Note that the de Gennes Eqs. (9) or (10) is useful in describing the quasiparticle tunneling, whereas the Ginzburg-Landau equation is useful when considering the Josephson (pair) tunneling. Here an intriguing question to what extent the gapless quasiparticles influence the tunneling between the spin-singlet and the spin-triplet superconductors or between the triplet superconductor and normal metal. We should be able to see the progress in answering those questions in a near future.

Finally, returning to the question of the nature of the paired state in Sr_2RuO_4 one can make the following two remarks. First, the existence of gapless modes in B- and A1-like phases leads to the persistence of the linear term in the specific heat in the superconducting phase at its 50% value, if the pairing is the pure spin-triplet state of electrons pairs derived from d_{zx} bands. The recent measurements²⁵ in very pure samples contradict such earlier claims¹¹ that a half of the linear specific heat survives in the superconducting phases. Does that mean that the full phase diagram involves more than one phase depending on the doping degree, as in the heavy fermion system $\text{U}_{1-x}\text{Th}_x\text{Be}_{13}$?²⁶ In connection with this one can say that because of the reasons mentioned in Sec. I it is conceivable that a singlet pairing in d_{xy} band induced by antiferromagnetic fluctuations⁹ can compete in the triplet state in the other two bands.²⁷ The nature of the resultant state should be determined then. Obviously, our approach is not directly applicable to any concrete system, as

we neglect the realistic structure of, e.g., Sr system.²⁸ We should be able to see a progress in those matters in near future (the results will be presented separately, Ref. 27).

Second, an important question concerns the nature of the pairing potential. In more standard approach^{28,14} one introduces the effective triplet pairing via the paramagnon exchange. In that situation the coupling constant is determined by the susceptibility $\chi(\mathbf{q}=\mathbf{k}-\mathbf{k}')$ and hence, is wave-vector (\mathbf{q}) dependent. In the approach developed here the exchange interaction itself provides real-space pairing, as in the case of high-temperature superconductors.⁵ In the case of Hund's rule coupling the pairing potential is then \mathbf{k} independent. We believe that the latter approach is relevant when the particles are strongly correlated. Sr_2RuO_4 is a systems close to (but below) the Mott-Hubbard localization threshold, i.e., the halfway between the weak-correlation and the strong-correlation asymptotic regimes. Therefore the real-space pairing is certainly worth of analyzing, as it allows for an analytic approach.

One methodological remark at the end. In the analytical analysis of the spin-triplet pairing one usually uses^{17,29} the \mathbf{d} vector in expressing the pairing part. Here we decided to use the original BCS gap parameters, a completely equivalent procedure, but probably a bit more direct, at least in the spatially homogenous situation. In connection with this a difference of the present description with that for superfluid *helium*-3 should be stressed. Namely, in the *helium*-3 case, the $L=1$ orbital moment \mathbf{l} and the spin vector \mathbf{d} determine the (many-component) nature of the gap. The $\mathbf{d}\cdot\mathbf{l}$ and $\mathbf{d}\times\mathbf{l}$ combinations determine the order-parameter dynamics. Here, no \mathbf{l} vector appears and therefore the order parameter can have up to three independent components.

One should note that the present pairing is operative for arbitrary anisotropic bands, since the symmetry $E_{\mathbf{k}}=E_{-\mathbf{k}}$ takes place if only the time reversal symmetry is obeyed, e.g., in the absence of either applied magnetic field or if the superconducting state does not coexist with ferromagnetism. In those situations the Fulde-Ferrell-Larkin-Ovchinnikov state should be considered.³⁰

ACKNOWLEDGMENTS

I am grateful to my student Andrzej Klejberg for the cooperation which led to this effective model. I am also grateful to Włodek Wójcik for many discussions and a technical help. Additionally, I was partially motivated by the question posed by Mark Jarrell from the University of Cincinnati, who asked if a simpler model representation of the work presented in Ref. 12 was possible. The work was supported by KBN, Grant No. 2P03B 092 18.

APPENDIX A: GENERAL SOLUTION: $\Delta_1 \neq \Delta_2 \neq \Delta_3 \neq \Delta_1$, $E_{\mathbf{k}1} \neq E_{\mathbf{k}2}$

The most general case of finding the eigenvalues for quasiparticles in the superconducting phase is to diagonalize matrix 4×4 , i.e., to solve the equation (we assume that $E_{\mathbf{k}1,2} - \mu = E_{\mathbf{k}}$ and that $\Delta_1 = \Delta_1^*$)

$$\det \begin{pmatrix} E_{\mathbf{k}_1} - \lambda, & 0, & \Delta_1, & \Delta_0 \\ 0, & E_{\mathbf{k}_1} - \lambda, & \Delta_0, & \Delta_{-1} \\ \Delta_1, & \Delta_0, & -E_{\mathbf{k}_2} - \lambda, & 0 \\ \Delta_0, & \Delta_{-1}, & 0, & -E_{\mathbf{k}_2} - \lambda \end{pmatrix} = 0. \quad (\text{A1})$$

By a straightforward evaluation one obtains the eigenvalues

$$\lambda_{\mathbf{k}_1 \dots 4} = \frac{1}{2} (E_{\mathbf{k}_1} - E_{\mathbf{k}_2}) \pm \frac{1}{2} [(E_{\mathbf{k}_1} + E_{\mathbf{k}_2})^2 + 2\tilde{\Delta}^2 \pm 2\sqrt{\tilde{\Delta}^4 - 4\tilde{\delta}^4}]^{1/2}, \quad (\text{A2})$$

where

$$\tilde{\Delta} = (\Delta_1^2 + \Delta_{-1}^2 + 2\Delta_0^2)^{1/2} \quad (\text{A3})$$

is the total gap, and

$$\tilde{\delta} = \sqrt{|\Delta_0^2 - \Delta_1 \Delta_{-1}|} \quad (\text{A4})$$

is its anisotropy in fermion-pair spin space. In this general case all four modes are each with a different gap and the results reduce nicely to the eigenvalues discussed as Secs. III A–C. In general, the superconducting coupling at the level of energies amounts to hybridizing the different fermion fields ($l=1,2$) and their spin ($\sigma=\uparrow,\downarrow$) states. The general form of the eigenstates can also be found in a straightforward manner, but will not be discussed here.

APPENDIX B: LOCAL SPIN-SINGLET PAIRING IN TWO-BAND CASE

For the sake of comparison with the spin-triplet case we outline here the solution for the corresponding spin-singlet situation. In this case the Hamiltonian with the spin-singlet exchange coupling has the form in the real space

$$\mathcal{H} = \sum_{\mathbf{k}\sigma l=1,2} E_{\mathbf{k}l} n_{\mathbf{k}l\sigma} + J \sum_{ill'} \left(\mathbf{S}_{il} \mathbf{S}_{il'} + \frac{1}{4} n_{il} n_{il'} \right). \quad (\text{B1})$$

Note that now the exchange operator in the present situation differs from Eq. (2) introduced in the triplet case. Introducing the corresponding local pairing operators in the singlet state

$$B_i^\dagger = \frac{1}{\sqrt{2}} (a_{i1\uparrow}^\dagger a_{i2\downarrow}^\dagger - a_{i1\downarrow}^\dagger a_{i2\uparrow}^\dagger) \quad (\text{B2})$$

we can write down the second term in Eq. (B1) as $-2J \sum_i B_i^\dagger B_i$.

After taking the space Fourier transform, and including only $(\mathbf{k}, -\mathbf{k})$ pairs we obtain

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}l} n_{\mathbf{k}l\sigma} - \frac{J}{N} \sum_{\mathbf{k}\mathbf{k}'} (f_{\mathbf{k}_1\uparrow}^\dagger f_{-\mathbf{k}_2\downarrow}^\dagger - f_{\mathbf{k}_1\downarrow}^\dagger f_{-\mathbf{k}_2\uparrow}^\dagger) \times (f_{-\mathbf{k}_2\downarrow} f_{\mathbf{k}_1\uparrow} - f_{-\mathbf{k}_2\uparrow} f_{\mathbf{k}_1\downarrow}). \quad (\text{B3})$$

Making subsequently, as in Sec. II the BCS approximation, we obtain (the chemical potential is included in $E_{\mathbf{k}l} \equiv E_{\mathbf{k}l} - \mu$)

$$\mathcal{H}_{BCS} = \sum_{\mathbf{k}l\sigma} [E_{\mathbf{k}l} n_{\mathbf{k}l\sigma} + \Delta_{\mathbf{k}}^* (f_{\mathbf{k}_1\uparrow}^\dagger f_{-\mathbf{k}_2\downarrow}^\dagger - f_{\mathbf{k}_1\downarrow}^\dagger f_{-\mathbf{k}_2\uparrow}^\dagger) + \text{H.c.}] - \frac{\Delta^2}{2J} N, \quad (\text{B4})$$

where

$$\Delta \equiv -\frac{2J}{N} \sum_{\mathbf{k}} \langle f_{\mathbf{k}_1\uparrow}^\dagger f_{-\mathbf{k}_2\downarrow}^\dagger \rangle. \quad (\text{B5})$$

Introducing, as before, the four-dimensional vectors $\mathbf{f}^\dagger \equiv (f_{\mathbf{k}_1\uparrow}^\dagger, f_{\mathbf{k}_1\downarrow}^\dagger, f_{-\mathbf{k}_2\uparrow}^\dagger, f_{-\mathbf{k}_2\downarrow}^\dagger)$ and their conjugate as one column vectors, we can write down the Hamiltonian in the form of the following 4×4 matrix:

$$\mathcal{H}_{BCS} = E_0 + \begin{pmatrix} f_{\mathbf{k}_1\uparrow}^\dagger & f_{\mathbf{k}_1\downarrow}^\dagger & f_{-\mathbf{k}_2\uparrow}^\dagger & f_{-\mathbf{k}_2\downarrow}^\dagger \end{pmatrix} \times \begin{pmatrix} E_{\mathbf{k}_1} & 0 & 0 & \Delta \\ 0 & E_{\mathbf{k}_1} & -\Delta & 0 \\ 0 & -\Delta^* & -E_{\mathbf{k}_2} & 0 \\ \Delta^* & 0 & 0 & -E_{\mathbf{k}_2} \end{pmatrix} \begin{pmatrix} f_{\mathbf{k}_1\uparrow} \\ f_{\mathbf{k}_1\downarrow} \\ f_{-\mathbf{k}_2\uparrow} \\ f_{-\mathbf{k}_2\downarrow} \end{pmatrix} \quad (\text{B6})$$

with $E_0 = 2 \sum_{\mathbf{k}} E_{\mathbf{k}2} + \Delta^2 / (2J)$. Diagonalization of this 4×4 matrix leads to the eigenvalues

$$\lambda_{1,2} = \frac{1}{2} (E_{\mathbf{k}_1} - E_{\mathbf{k}_2}) \pm \sqrt{\left(\frac{E_{\mathbf{k}_1} + E_{\mathbf{k}_2}}{2} \right)^2 + |\Delta|^2}. \quad (\text{B7})$$

Both eigenmodes are doubly degenerate and with an isotropic gap Δ . We take the form of usual dispersion relation for degenerate bands $E_{\mathbf{k}_1} = E_{\mathbf{k}_2}$.

The corresponding combinations¹⁸ of the wave-function components are (for $\Delta = \Delta^*$)

$$\begin{cases} (E_{\mathbf{k}_1} - \lambda)(\psi_1 + \psi_2) - \Delta(\psi_3 - \psi_4) = 0 \\ \Delta(\psi_1 + \psi_2) + (E_{\mathbf{k}_2} + \lambda)(\psi_3 - \psi_4) = 0, \end{cases} \quad (\text{B8})$$

and

$$\begin{cases} (E_{\mathbf{k}_1} - \lambda)(\psi_1 - \psi_2) + \Delta(\psi_3 + \psi_4) = 0 \\ \Delta(\psi_1 - \psi_2) - (E_{\mathbf{k}_2} + \lambda)(\psi_3 + \psi_4) = 0. \end{cases} \quad (\text{B9})$$

For the sake of simplicity we consider here only the case $E_{\mathbf{k}_1} = E_{\mathbf{k}_2} = E_{\mathbf{k}}$, as it provides the main character of the eigenstates. Moreover, it is sufficient to consider only the system (B10) due to the double degeneracy of the eigenvalues. By standard method (including the wave-function normalization) we obtain the quasiparticle operators

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} \frac{1}{\sqrt{2}} (f_{\mathbf{k}_1\uparrow} + f_{\mathbf{k}_1\downarrow}) + v_{\mathbf{k}} \frac{1}{\sqrt{2}} (f_{-\mathbf{k}_2\uparrow}^\dagger - f_{-\mathbf{k}_2\downarrow}^\dagger), \quad (\text{B10})$$

$$\beta_{-\mathbf{k}}^\dagger = -v_{\mathbf{k}} \frac{1}{\sqrt{2}} (f_{\mathbf{k}1\uparrow} + f_{\mathbf{k}1\downarrow}) + u_{\mathbf{k}} \frac{1}{\sqrt{2}} (f_{-\mathbf{k}2\uparrow}^\dagger - f_{-\mathbf{k}2\downarrow}), \quad (\text{B11})$$

where

$$u_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(1 + \frac{E_{\mathbf{k}}}{\sqrt{E_{\mathbf{k}}^2 + \Delta^2}} \right)^{1/2},$$

$$v_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(1 - \frac{E_{\mathbf{k}}}{\sqrt{E_{\mathbf{k}}^2 + \Delta^2}} \right)^{1/2}. \quad (\text{B12})$$

Again, we have a combination of the two types of states. The corresponding wave equation which replaces the

Bogoliubov–de Gennes equation for one-band singlet superconductor reads in the effective-mass approximation

$$i\hbar \partial_t \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \left(-\frac{\hbar^2}{2m^*} \nabla^2 - \mu \right) \begin{pmatrix} \psi_1 \\ \psi_2 \\ -\psi_3 \\ -\psi_4 \end{pmatrix} + \Delta \begin{pmatrix} \psi_4 \\ -\psi_3 \\ -\psi_2 \\ \psi_1 \end{pmatrix}. \quad (\text{B13})$$

We see that the pairing couples explicitly the particle and hole components (ψ_1 with ψ_4 , ψ_2 with $-\psi_3$, etc.). This equation forms a basis for the discussion of inhomogeneous paired states.

*Electronic address: ufspalek@if.uj.edu.pl

¹Y. Maeno, H. Hashimoto, K. Yoshida, S. NishiZaki, S. Fujita, and J.G. Bednorz, *Nature (London)* **372**, 532 (1994); T. Akima, S. NishiZaki, and Y. Maeno, *J. Phys. Soc. Jpn.* **68**, 694 (1999).

²P.B. Allen *et al.*, *Phys. Rev. B* **53**, 4393 (1996).

³G. Cao, S. McCall, M. Shepard, J.E. Crow, and R.P. Guertin, *Phys. Rev. B* **56**, R2916 (1997); S. Nakatsuji, S. Ikeda, and Y. Maeno, *J. Phys. Soc. Jpn.* **66**, 1868 (1997).

⁴P.W. Anderson, *Phys. Rev.* **115**, 2 (1959); in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, San Diego, 1963), Vol. 14, pp. 99–214.

⁵P.W. Anderson, *Science* **235**, 1196 (1987); A.E. Ruckenstein, P.J. Hirschfeld, and J. Appel, *Phys. Rev. B* **36**, 857 (1987); J. Spałek, *ibid.* **37**, 533 (1988); F.C. Zhang and T.M. Rice, *ibid.* **37**, 3759 (1988).

⁶K.I. Kugel and D.I. Khomskii, *Zh. Éksp. Teor. Fiz.* **64**, 1429 (1973) [*JETP* **37**, 725 (1973)].

⁷S. Inagaki, *J. Phys. Soc. Jpn.* **39**, 596 (1975); M. Cyrot and C. Lyon-Caen, *J. Phys. (Paris)* **36**, 253 (1975); J. Spałek and K.A. Chao, *J. Phys. C* **13**, 5241 (1980); S. Ishikara, I. Inoue, and S. Maekawa, *Phys. Rev. B* **55**, 8280 (1997).

⁸S. Inagaki and R. Kubo, *Int. J. Magn.* **4**, 139 (1973); K. Held and D. Vollhardt, *Eur. Phys. J. B* **5**, 473 (1998).

⁹Y. Sidis, M. Braden, P. Bourges, B. Hennion, S. NishiZaki, Y. Maeno, and Y. Mori, *Phys. Rev. Lett.* **83**, 3320 (1999).

¹⁰M. Sato and M. Kohmoto, cond-mat/0003046 (unpublished).

¹¹Y. Maeno, S. NishiZaki, K. Yosida, S. Ikeda, and T. Fujita, *J. Low Temp. Phys.* **105**, 1577 (1996).

¹²A. Klejnberg and J. Spałek, *J. Phys.: Condens. Matter* **11**, 6553 (1999). We start here with the *effective renormalized Hamiltonian* obtained in that paper.

¹³A. Klejnberg and J. Spałek, *Phys. Rev. B* **61**, 15 542 (2000).

¹⁴The possibility of spin-triplet pairing induced by the ferromagnetic spin fluctuations has been considered in a number of papers; see, e.g., D. Fay and J. Appel, *Phys. Rev. B* **16**, 2325 (1977); A. Layzer and D. Fay, *Int. J. Magn.* **1**, 135 (1971); *Solid State Commun.* **15**, 599 (1974). Following Ref. 12 we start from real-space pairing, which is obtained for renormalized (almost-localized) Fermi liquid. In connection with this the related work is D. Agterberg, T.M. Rice, and M. Sigrist, *Phys. Rev. Lett.* **78**, 3374 (1997), and G. Baskaran, *Physica B* **223-224**, 498 (1996).

However, in our previous works Refs. 12 and 13 we put quantitative emphasis on the Hund's rule coupling and locating the other Coulomb terms in the effective-mass renormalization, the chemical potential shift, and the Hund's rule exchange renormalization ($J \rightarrow Jt^2$). Here they represent thus the *quasiparticle characteristic*, also if the starting bands are hybridized. The importance of the Hund's rule in the possible triplet pairing has been noticed also in D. van der Marel and G. Sawatzky, *Solid State Commun.* **55**, 937 (1985), where it was applied to the Anderson lattice with degenerate f level to account for the properties of heavy fermion superconductors. The influence of the Hund's rule on electron states of Sr_2RuO_4 was also discussed in M. Cuoco, C. Noce, and A. Romano, *Phys. Rev. B* **57**, 11 989 (1998).

¹⁵The quasiparticle bandwidth $\bar{W} = Wq$ is much larger than the coupling constant Jt^2 , since even close to the Mott-Hubbard localization $q \approx 1/2$ and $t^2 \approx 0.1$ (cf. Ref. 12).

¹⁶Y. Nambu, *Phys. Rev.* **117**, 648 (1960); P.W. Anderson, *ibid.* **112**, 1900 (1958); Y. Nambu and G. Jona-Lasinio, *ibid.* **122**, 345 (1961); **124**, 246 (1961).

¹⁷R. Balian and N.R. Werthamer, *Phys. Rev.* **131**, 1553 (1963). For review, see M. Sigrist and K. Ueda, *Rev. Mod. Phys.* **63**, 239 (1991). Note that here the order-parameter components are \mathbf{k} independent as we have local (interorbital) pairing.

¹⁸Obviously, because the system of Eqs. (13) is linear and homogeneous, one has supplemented it with the normalization condition, which for the amplitude sum takes the form $(\psi_1 + \psi_2)^2 + (\psi_3 + \psi_4)^2 = 2$ for $\psi_1 = \psi_2$ and $\psi_3 = \psi_4$.

¹⁹For relatively recent review, see S.P. Klevansky, *Rev. Mod. Phys.* **64**, 649 (1992).

²⁰Paranthenically, the *asymptotically free* particles represent state very similar to that of Landau-Fermi liquid, particularly if the gauge fields are ignored (we make that assumption to simplify the argument here, as we want to point only the connection to the formalism in the two-band case in nonrelativistic situation).

²¹Y. Nambu, *Midwest Conference on Theoretical Physics* (Purdue University, 1960).

²²D. Balian and A. Love, *Phys. Rep.* **107**, 325 (1984); M. Alford, K. Rajagopal, and F. Wilczek, *Phys. Lett. B* **422**, 247 (1998); R. Rapp, T. Schäfer, E.V. Shuryak, and M. Velkovsky, *Phys. Rev.*

- Lett. **81**, 53 (1998); T. Schäfer and F. Wilczek, *ibid.* **82**, 3956 (1999).
- ²³P.G. de Gennes, *Superconductivity of Metals and Alloys* (Addison-Wesley, Reading, MA, 1989), Chap. 5.
- ²⁴M. Sigrist and M.E. Zhitomirsky, J. Phys. Soc. Jpn. **65**, 3452 (1996); K. Machida, M. Ozaki, and T. Ohmi, *ibid.* **65**, 3720 (1996).
- ²⁵S. NishiZaki, Y. Maeno, and Z. Mao, J. Low Temp. Phys. **117**, 1581 (1999).
- ²⁶H.R. Ott, H. Rudigier, Z. Fisk, and I.L. Smith, Phys. Rev. B **31**, 1651 (1985); U. Rauchschwalde, U. Ahlheim, H. Mayer, C.D. Bredl, and F. Steglich, J. Magn. Magn. Mater. **63-64**, 447(1987).
- ²⁷J. Spałek and W. Wójcik (unpublished).
- ²⁸I.I. Mazin and D.J. Singh, Phys. Rev. Lett. **79**, 733 (1997); Phys. Rev. B **56**, 2556 (1997); M. Sigrist *et al.*, cond-mat/9902214 (unpublished).
- ²⁹A.J. Leggett, Rev. Mod. Phys. **47**, 331 (1975); D. Vollhardt and P. Wölfle, *The Superfluid Phases of Helium 3* (Taylor & Francis, London, 1990), Chaps. 3 and 5.
- ³⁰P. Fulde and R.A. Ferrell, Phys. Rev. **135**, A550 (1964); A.I. Larkin and Yu.N. Ovchinnokov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964) [Sov. Phys. JETP **20**, 762 (1965)]; in quasi-two-dimensional systems: H. Shimahara, J. Phys. Soc. Jpn. **66**, 541 (1997).