Theory of superconducting mechanism and gap structure of Sr_2RuO_4

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Abstract

We discuss a possible mechanism of the spin-triplet superconductivity and a gap structure of Sr_2RuO_4. We calculate transition temperature as a function of the on-site Coulomb energy, and determine the momentum dependences of the superconducting gap, by solving the linearized Éliashberg equation for a realistic three-band Hubbard model. Here the effective pairing interaction is expanded perturbatively with respect to the on-site Coulomb interaction up to the third order. In the present article we display the results of the calculations of transition temperature and specific heat in the superconducting state. We obtain a relatively high transition temperature as a result of the effective interaction favoring p-wave pairing. The theoretical gap structure reproduces the experimental temperature dependence of specific heat very well.

Key words: Sr_2RuO_4; superconducting mechanism; gap structure; specific heat

One of the most intriguing aspects in the physics of Sr_2RuO_4 is the spin-triplet superconductivity [1]. The possibility of the parallel-spin pairing state was proposed theoretically soon after the discovery of the superconductivity in Sr_2RuO_4 [2]. Many experiments support the realization of the triplet superconductivity in Sr_2RuO_4. In particular, NMR Knight shift measurement revealed that the in-plane spin susceptibility does not change at the superconducting transition, and strongly excludes the possibility of the spin-singlet pairing [3].

Microscopic origin of the spin-triplet superconductivity in Sr_2RuO_4 has been discussed intensively. In the early stage, it was expected plausibly that some strong ferromagnetic spin fluctuations mediate the triplet superconductivity. However, the neutron scattering experiment observed not any enhanced ferromagnetic fluctuations but sizeable incommensurate fluctuations [4]. Therefore the picture that some strong ferromagnetic fluctuations mediate the triplet superconductivity will not be valid for Sr_2RuO_4.

The superconducting gap structure also has been still opened to intensive discussions. Sigrist et al. theoretically singled out the most promising form of $\boldsymbol{d}$-vector, $\boldsymbol{d}(\boldsymbol{k}) \sim (k_x \pm ik_y)\hat{z}$ [5]. This form of the $\boldsymbol{d}$-vector is widely accepted today. However, this form of the $\boldsymbol{d}$-vector usually gives nodeless energy gap, and seems inconsistent with the power-law temperature dependences observed experimentally in many quantities, e.g. specific heat [6].

In this short article, we would like to insist the following points: (I) We can regard the spin-triplet superconductivity in Sr_2RuO_4 as one of the natural results of the electron correlations. (II) The strong momentum dependences of the gap structure derived microscopically provide a line-node-like power-law behavior of the specific heat, even if we postulate the symmetry, $\boldsymbol{d}(\boldsymbol{k}) \sim (k_x \pm ik_y)\hat{z}$. As a result, the calculation results of specific heat agree with the experimental results quite well for moderately strong inter-orbit couplings.

Sr_2RuO_4 is a strongly correlated system where Ru4dε electrons play the important roles for the electronic properties. We consider a realistic three band

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Hubbard model for Ru4dε-like electrons. The Hamiltonian H consists of two parts: the kinetic part,

$$H_0 = \sum_{\boldsymbol{k},\ell,\sigma} \xi_\ell(\boldsymbol{k}) c^\dagger_{\boldsymbol{k}\ell\sigma} c_{\boldsymbol{k}\ell\sigma} + \sum_{\boldsymbol{k},\sigma} \lambda(\boldsymbol{k})(c^\dagger_{\boldsymbol{k}\,yz\,\sigma} c_{\boldsymbol{k}\,xz\,\sigma} + c^\dagger_{\boldsymbol{k}\,xz\,\sigma} c_{\boldsymbol{k}\,yz\,\sigma}), \quad (1)$$

and the on-site Coulomb interaction,

$$H' = \frac{1}{2}U \sum_i \sum_{\sigma\neq\sigma'} \sum_\ell c^\dagger_{i\ell\sigma} c^\dagger_{i\ell\sigma'} c_{i\ell\sigma'} c_{i\ell\sigma} + \frac{1}{2}U' \sum_i \sum_{\sigma,\sigma'} \sum_{\ell\neq\ell'} c^\dagger_{i\ell\sigma} c^\dagger_{i\ell'\sigma'} c_{i\ell'\sigma'} c_{i\ell\sigma} + \frac{1}{2}J \sum_i \sum_{\sigma,\sigma'} \sum_{\ell\neq\ell'} c^\dagger_{i\ell\sigma} c^\dagger_{i\ell'\sigma'} c_{i\ell\sigma'} c_{i\ell'\sigma} + \frac{1}{2}J' \sum_i \sum_{\sigma\neq\sigma'} \sum_{\ell\neq\ell'} c^\dagger_{i\ell\sigma} c^\dagger_{i\ell\sigma'} c_{i\ell'\sigma'} c_{i\ell'\sigma}, \quad (2)$$

where $\ell^{(\prime)}$ and $\sigma^{(\prime)}$ denote the Wannier states (xy, yz, xz) and spin state, respectively. We take the following band dispersions, $\xi_{xy}(\boldsymbol{k}) = 2t_1(\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y - \mu_{xy}, \xi_{yz}(\boldsymbol{k}) = 2t_3 \cos k_y + 2t_4 \cos k_x - \mu_{yz}, \xi_{xz}(\boldsymbol{k}) = 2t_3 \cos k_x + 2t_4 \cos k_y - \mu_{xz}, \lambda(\boldsymbol{k}) = 4\lambda_0 \sin k_x \sin k_y$, where the transfer integrals are determined to reproduce the electronic structure suggested by the de Haas-van Alven measurement [7].

We expand the effective pairing interaction perturbatively with respect to H' up to the third order, and obtain the Éliashberg equation in the following multiband form:

$$\Sigma^{\mathrm{A}}_{a,\sigma_1\sigma_2}(q) = -\frac{T}{N} \sum_{k,a',\sigma_4\sigma_3} \left|G_{a'}(k)\right|^2 \Sigma^{\mathrm{A}}_{a',\sigma_4\sigma_3}(k) \Gamma_{a,\sigma_1\sigma_2;a',\sigma_3\sigma_4}(q,k), \quad (3)$$

where $a^{(\prime)}$ denotes the diagonalized three bands, which are usually named α, β and γ [7].

Here we show the results of the calculation. In Fig. 1, we show the calculated transition temperature as a function of U. In the present calculations we have taken $U' = J = J'$ simply. In Fig. 2, we show the result of specific heat, which is comapared with experimental results. According to our discussions, the superconducting gap has a node-like structure along the c-axis on one of the three bands, β.

We summarize the concluding remarks suggested by the present discussion. the spin-triplet p-wave superconductivity in Sr_2RuO_4 would be understood as a natural result from the electron correlations. The superconducting gap has a large anisotropy, and the gap magnitude has a strong band dependence. The experimental result of specific heat is naturally explained by taking into account the anisotropy and the many-band effects. The details of the calculations of transition temperature and specific heat are given in the Refs. [9] and [10], respectively.

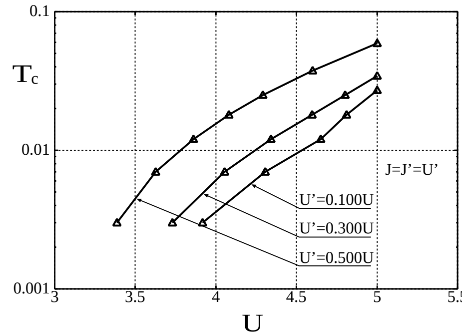

Fig. 1. Transition temperature as a function of U for spin-triplet p-wave state. $J = J' = U'$.

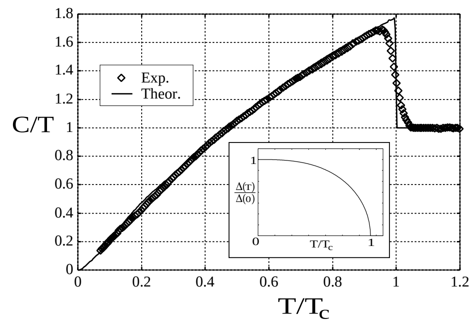

Fig. 2. Calculation result of specific heat divided by temperature (solid curve), which is compared with experimental data (◇) from Refs. [6] and [8]. The inter-orbit couplings are moderately strong, $J = J' = U' = 0.360U$. The inset shows the temperature dependence of gap magnitude $\Delta(T)$ obtained by solving BCS gap equation.

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