Ferromagnetic fluctuation and superconductivity in Na$_{0.35}$CoO$_2$·1.3H$_2$O: FLEX study of multi-orbital Hubbard model

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Abstract

Spin and charge fluctuations and superconductivity in Na$_{0.35}$CoO$_2$·1.3H$_2$O are studied based on a multi-orbital Hubbard model. By applying the fluctuation exchange (FLEX) approximation, we show that the Hund’s-rule coupling between the Co $t_{2g}$ orbitals causes ferromagnetic spin fluctuation. Triplet pairing is favored by this ferromagnetic fluctuation on the hole-pocket band. We propose that, in Na$_{0.35}$CoO$_2$·1.3H$_2$O, Co $t_{2g}$ orbitals and inter-orbital Hund’s-rule coupling play important roles on the triplet pairing, and this compound can be a first example of the triplet superconductor mediated by inter-orbital-interaction-induced ferromagnetic fluctuation.

Key words: Na$_{0.35}$CoO$_2$·1.3H$_2$O, orbital degree of freedom, Hund’s-rule coupling, triplet superconductivity

The mechanism and nature of superconductivity in Na$_{0.35}$CoO$_2$·1.3H$_2$O is currently attracting great interest [1]. However, in spite of a lot of attempt and effort, even the paring symmetry has not been resolved yet. In this paper, we study the electronic structure and superconductivity in this compound by employing a multi-orbital Hamiltonian given by $H = H_{\text{cry}} + H_{\text{kin}} + H_{\text{int}}$. Here, the first term $H_{\text{cry}}$ expresses the crystal field from the O ions acting on the Co $t_{2g}$ orbitals, and the second term $H_{\text{kin}}$ represents the kinetic energy. The tight-binding parameters are deduced by fitting the LDA band structure, and we find that up to the third nearest-neighbor hoppings between Co $t_{2g}$ orbitals are necessary at least. In Fig. 1, we show the band dispersions and the Fermi surfaces for non-interacting Hamiltonian ($H_{\text{cry}} + H_{\text{kin}}$). Both reproduce very well the LDA results [2], especially near the Fermi level. The Fermi surfaces consist of a large cylindrical one around the Γ-point and six hole pockets near the K-points. The cylindrical Fermi surface has a dominant $a_{1g}$-orbital character, while the hole pockets have an $e'_{g}$-orbital character.

The term $H_{\text{on-site}}$ represents the on-site $d$-$d$ Coulomb interactions, which consists of following four contributions: $H_{\text{int}} = H_U + H_{U'} + H_{J_H} + H_{J'}$ where $H_U$ and $H_{U'}$ are the intra- and inter-orbital Coulomb interactions, respectively, and $H_{J_H}$ and $H_{J'}$ are the Hund’s-rule coupling and the pair-hopping interactions, respectively. These interactions are expressed using Kanamori parameters, $U$, $U'$, $J_H$ and $J'$. The
value of $U$ has been estimated experimentally as 3-5.5 eV, and $J_H$ for Co $^{3+}$ ion is 0.84 eV. Thus, the ratio $J_H/U$, which gives the strength of Hund’s-rule coupling, is 0.15-0.28 in this compound.

We apply the FLEX approximation to this multi-orbital Hubbard model. Figure 2 shows the spin susceptibility for various values of $J_H/U$ at $T = 0.02$. As shown in this figure, a peak structure around the $\Gamma$-point is strongly enhanced as $J_H/U$ increases, while the small peak at the M-point hardly changes. Since $J_H/U$ is 0.15-0.28 in the actual compound, the enhanced peak at the $\Gamma$-point at $J_H/U = 0.18$ indicates that the ferromagnetic fluctuation actually exists in this compound. Further, the structure at the $\Gamma$-point is considerably small without Hund’s-rule coupling ($J_H/U = 0$), indicating a substantial importance of the Hund’s-rule coupling for emergence of the ferromagnetic fluctuation. On the other hand, the charge-orbital susceptibility does not exhibit any remarkable structures, implying an absence of the charge- and orbital-density-wave instabilities.

By solving the Eliashberg equations, we find that the dominant superconducting instability at $J_H/U = 0.18$ is $f_{y(y^2-3z^2)}$-wave pairing mediated by this ferromagnetic fluctuation arises mainly on the $e'_{g}$ band with the pocket Fermi surfaces. The pocket Fermi surfaces as well as a large DOS due to the vHS near the Fermi level are crucially important for the $f_{y(y^2-3z^2)}$-wave pairing instability on the $e'_{g}$ band. We have pointed out that this material can be a first example of the inter-orbital-interaction-induced triplet superconductivity.

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Note added. — After the submission of this paper, our further study found a tiplet $p$-wave state which is nearly degenerate with the $f$-wave one proposed in this paper. This $p$-wave state is also mediated by the FM fluctuation due to the Hund’s-rule coupling, and the hole pockets and the vHS singularity also play substantial roles. For details, see cond-mat/0407094.

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