Transition from antiferromagnetic to ferromagnetic fluctuation under charge doping in $Pb_9Cu(PO_4)_6O$ so-called LK-99

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In 2023, room-temperature superconductivity was reported in a copper doped lead apatite, $Pb_9Cu(PO_4)_6O$, so-called LK-99 [1, 2]. The hope of room-temperature superconductor has largely been dashed by global research efforts. A problem was a magnetic half-levitation. It is suggested that the origin of the half-levitation be ferromagnetism by and experiment [3]. However, mechanism of the ferromagnetism is not clear.

In this study [4], we investigate electronic and magnetic structures of $Pb_9Cu(PO_4)_6O$ based on density functional theory (DFT) and spin fluctuation theory. We calculate electronic structure of $Pb_9Cu(PO_4)_6O$ based on DFT, and construct four-band Hubbard model including Cu $3d$ and O $2p$ orbitals. The Cu $3d$ orbitals construct a three-dimensional triangular lattice. The upper band is half-filled.

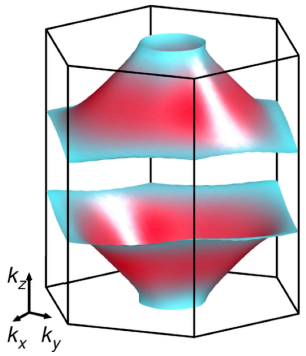

Figure 1: Fermi surface of $Pb_9Cu(PO_4)_6O$. It shows a large k_z dependence.

We apply fluctuation exchange (FLEX) approximation to the Hubbard model and calculate spin susceptibility. We find antiferromagnetic fluctuations in the stoichiometric compound. Magnetic fluctuations transfers to ferromagnetic fluctuations with slight charge doping ($\Delta n \sim 0.1$). The half-levitation can be explained by our results; slight inhomogeneity of samples makes slight charge doping, and the samples show ferromagnetism. This ferromagnetic situation is similar to a two-dimensional one-band triangular lattice Hamiltonian with charge doping ($\Delta n = 0.5$).

Interestingly, the doping level to reach ferromagnetism in LK-99 is much smaller than that in a two-dimensional one-band triangular lattice. This difference would originate from the three-dimensionality or/and the orbital degree of freedom.

[1] S. Lee, J.-H. Kim, and Y.-W. Kwon, arXiv:2307.12008.

[2] S. Lee, J. Kim, H.-T. Kim, S. Im, S. An, and K. H. Auh, arXiv:2307.12037.

[3] K. Guo, Y. Li, and S. Jia, Sci. China Phys. Astron. **66**, 107411 (2023).

[4] M. Shimizu, J. Otsuki, and H. O. Jeschke, Phys. Rev. B **108**, L201105 (2023).