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Enhanced spin fluctuations and $s\pm$ pairing by diagonal electron hopping in Fe-based superconductors

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In the itinerant spin picture of the iron-based superconductors, the nesting between electron and hole Fermi surfaces is usually considered to be the origin of the spin fluctuation and thus the pairing glue. However, there have appeared some experimental observations suggesting absence of Fermi surface nesting. For instance, in the 1111 materials $Ln\text{FeAsO}_{1-x}\text{H}_x$ (Ln=La,Sm, etc.) [1], electron doping rate x reaches up to 50%, which in a rigid band picture would wipe out the hole Fermi surfaces. Still, superconductivity not only survives, but is even enhanced in the largely doped regime, in contradiction to the expectation from the bad nesting. Another example is $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$, where the ARPES experiments show the absence of hole Fermi surfaces[2-5]. In the present talk, we first focus on $Ln\text{FeAsO}_{1-x}\text{H}_x$, where the band structure is actually not rigid against doping, and the hole Fermi surface originating from the d_{xy} orbital remains nearly unchanged. The origin of this can be traced back to real space, where the nearest neighbor hopping t_1 within the d_{xy} orbital is found to be strongly suppressed with doping [6]. Although the nesting itself is degraded, the spin fluctuation in the largely electron doped regime is enhanced due to $t_2 > t_1$, where t_2 is the 2nd neighbor diagonal hopping. This re-enhances s± pairing superconductivity, and explains the double dome x-T_c phase diagram of $\text{LaFeAsO}_{1-x}\text{H}_x$[1]. From this viewpoint, it is also interesting to look into the relation between t_1 and t_2 in other materials. For instance, our first principles estimation for KFe_2Se_2 gives $t_1 = -0.008$ eV and $t_2 = 0.056$ eV, and from this strong reduction of t_1, both electron and hole Fermi surfaces are expected to be present around the Γ point, in contradiction to previous experimental observations. Results of a recent ARPES experiment will be discussed from this viewpoint. References [1] S. Iimura et al., Nat. Commun. **3**, 943 (2012). [2] T. Qian et al., Phys. Rev. Lett. **106**, 187001 (2011). [3] Y. Zhang et al., Nature Mat. **10**, 273 (2011). [4] D. Mou et al., Phys. Rev. Lett. **106**, 107001 (2011). [5] M. Yi et al., Phys. Rev. Lett. **110**, 067003 (2013). [6] K. Suzuki et al., Phys. Rev. Lett. **113**, 027002 (2014).