3D Spin Fluctuation Calculations of Pairing Strength in Iron-based Superconductors

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Introduction

The discovery of superconductivity at ~50-70K in the Fe-based superconducting materials has caused considerable excitement in the condensed matter community [1]. It is believed that most of these differences arise due to differences in electronic structure and local interactions, which lead to "sign-changing s-wave" order [2], as shown in Fig. 1(Left). Most calculations of pairing have used a Hubbard-Hund Hamiltonian with 5 d-orbitals in two dimensions. Since in some systems significant 3D corrugations of Fermi surfaces occur, and because the true symmetry of these crystals requires two distinct Fe atoms per unit cell, a 10-orbital model is the minimal one respecting crystal symmetry in 122 Fe-based systems.

Results and Discussion

We performed 10-orbital, 3D spin fluctuations calculations of pairing in various materials using the Berk-Schrieffer approximation for the pairing vertex, generalized to multiorbital systems. The first system considered was LiFeAs, which is unusual for a lack of nesting, and disagreement of angle-resolved photoemission spectroscopy (ARPES) measurements of hole Fermi surfaces with density functional theory (DFT) calculations. We therefore collaborated with the Dresden ARPES group to fit a band structure to their data, and used it as an input to the calculation of the pairing function, Fig. 1 (Middle).

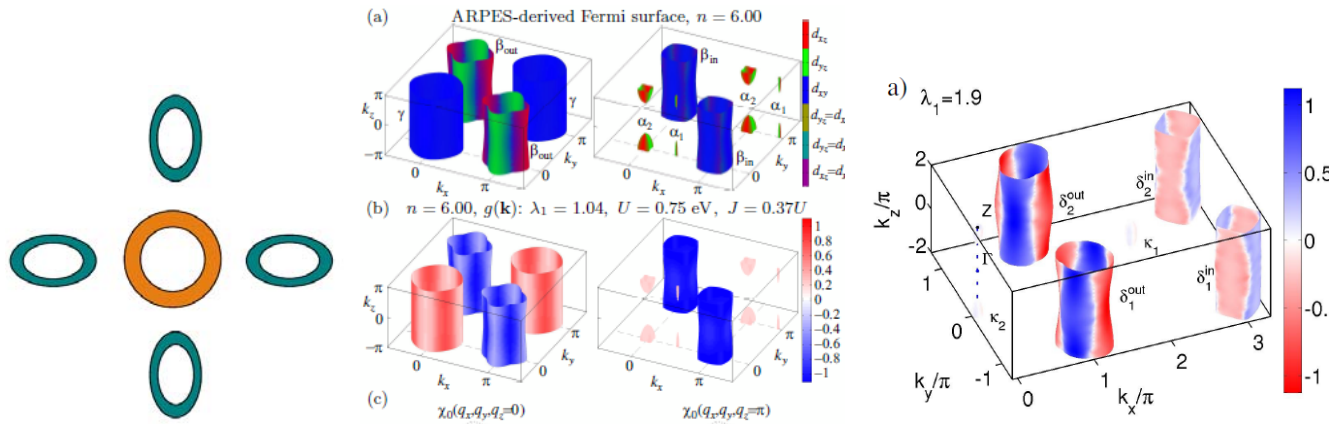

Figure 1 (Left) Cartoon of $s_{+/-}$ -wave state. Color indicates sign of superconducting gap D. (Middle) (a) inner and outer sheets of the Fermi surface; color indicates d-orbital character as in legend; (b) s-wave LiFeAs gap function from theory for parameters in Hubbard – Hund Hamiltonian as shown. (Right) d-wave pairing function in KFe_2Se_2.

The system KFe_2Se_2 is of great current interest since according to ARPES experiments it has no hole pockets, so that the scenario based on Fig. 1(Left) is apparently inadequate. Indeed in our calculations (Fig. 1 (Right)), we find that the system has d-wave pairing. The 122 symmetry requires quasinodes on the Fermi surface, as seen in the figure, due to hybridization of the electron bands.

Conclusions

The superconducting state in most Fe-based superconductors is probably of multiband anisotropic s type due to spin fluctuations, including in LiFeAs where Fermi surfaces are not well nested, but has a stronger tendency to be d-wave if hole pockets are absent.

Acknowledgements

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References

[1] For review see P.J. Hirschfeld, M.M. Korshunov, and I.I. Mazin, Reports on Progress in Physics 74, 124508 (2011) [2] S. Graser P.J. Hirschfeld, T. Maier, and D.J. Scalapino, New J. Phys. 11, 025016 (2009). [3] A. Kreisel, T. Maier, Y. Wang, D.J. Scalapino and P.J. Hirschfeld, Phys. Rev. B 88, 094522 (2013).