Fermi Surface Topology of LaFePO and LiFeP

Johannes Ferber, Harald O. Jeschke, and Roser Valentí
Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main, Germany

–Supplemental Material–

Effect of different double counting corrections, interaction parameters, and structures on the Fermi surfaces

We investigated the robustness of our results with respect to a different double counting correction, variations in the interaction parameters, and other structures reported in the literature. Figure 1 shows the Fermi surfaces of LaFePO and LiFeP under these changes along the cuts where the predicted topological change occurs ($k_z = 0$ for LaFePO, $k_z = 0.5$ for LiFeP). While being affected quantitatively, the topology change is consistent among all calculations with only minimal changes in the pocket sizes.

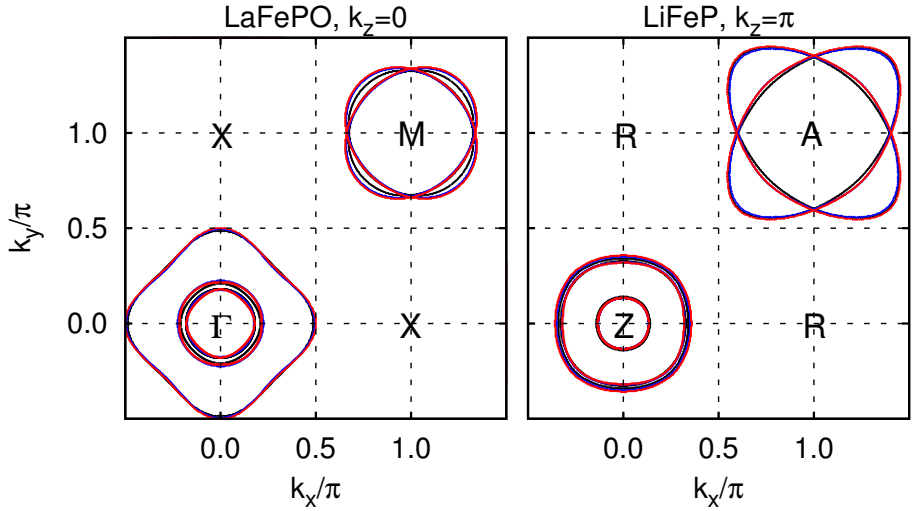

Figure 1: Fermi surfaces at $k_z = 0$ ($k_z = \pi$) for LaFePO (LiFeP) for different interaction parameters/double countings/structures compared to the paper. Black: as in Paper, but FLL (fully localized limit) double counting; Blue: as in Paper, but $U = 3.5$ eV, $J = 0.7$ ($U = 4$ eV, $J = 0.7$) eV for LaFePO (LiFeP); Red: as in Paper, but structure taken from Ref. [McQueen08] (Ref. [Putzke12]) for LaFePO (LiFeP).

Inclusion of the rotational invariant Hund's rule coupling on the example of LiFeAs

Our work only considers density-density terms of the Hund's rule coupling J in the interaction vertex. Whereas we can give no definitive statement concerning the effects of the neglected J terms on the Fermi surface properties for the systems under consideration, we have performed a comparison of LDA+DMFT calculations with and without inclusion of the full Hund's rule coupling for the Fermi surfaces of the more correlated LiFeAs as shown in Fig. 2.

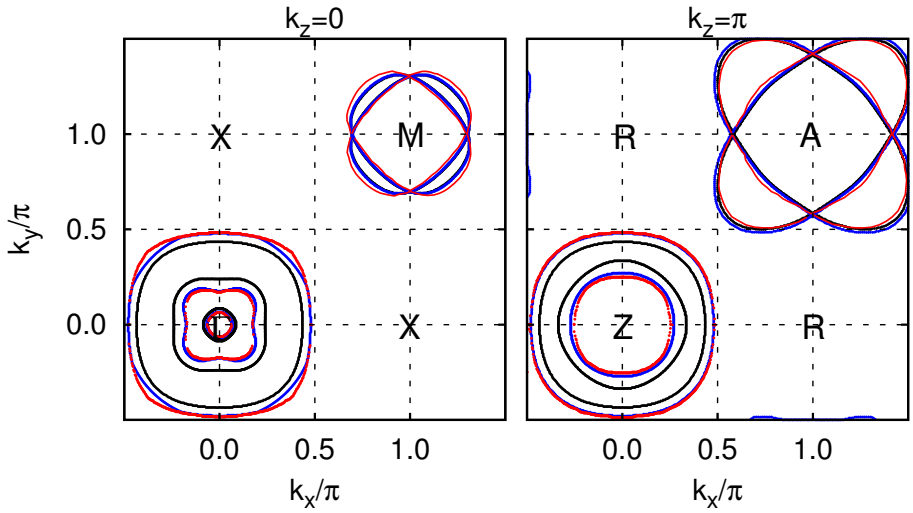

Figure 2: Comparison of Fermi surfaces for LiFeAs. Black: LDA; blue: LDA+DMFT, density-density terms in J only, $U = 4$ eV, $J = 0.9$ eV from Ref. [Ferber12]; red: LDA+DMFT, full J coupling, $U = 5$ eV, $J = 0.8$ eV, data taken from Ref. [Lee12].

No substantial difference between consideration of the full Hund's rule coupling and only density-density terms is visible from Fig. 2, both predict a shrinking of the middle hole pocket and an increase of the outer hole pocket at Γ/Z (note, however, the slightly different interaction parameters; we also don't have information about which double counting correction was used in the work by Lee *et al.*). Furthermore, as LiFeAs in general shows stronger dependence on J than LaFePO and LiFeP (see evolution of calculated effective masses with J for both LiFeAs and LiFeP in Fig. 3), we expect the difference to be even smaller for these systems.

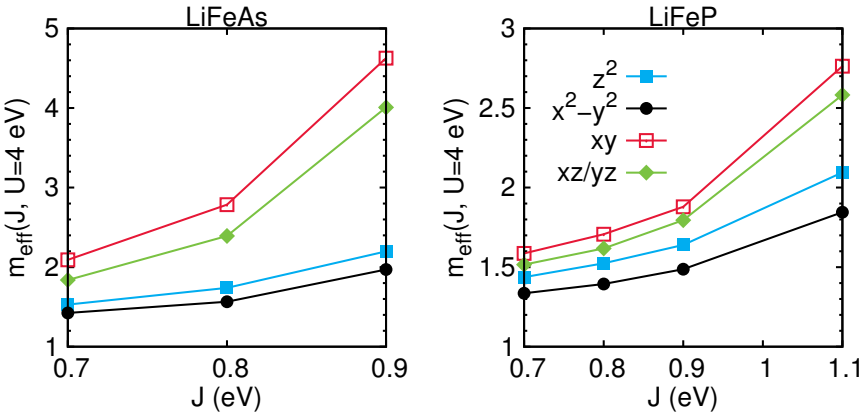

Figure 3: Dependence of orbital-resolved effective masses in LiFeAs and LiFeP. The effective masses are generally higher in LiFeAs compared to LiFeP and depend more strongly on J (note the larger range of J shown for LiFeP).

References

[Ferber12] J. Ferber, K. Foyevtsova, R. Valentí and H. O. Jeschke. Phys. Rev. B **85**, 094505 (2012).

[Lee12] G. Lee, H. S. Ji, Y. Kim, C. Kim, K. Haule, G. Kotliar, B. Lee, S. Khim, K. H. Kim, K. S. Kim, K.-S. Kim and J. H. Shim. Phys. Rev. Lett. **109**, 177001 (2012).

[McQueen08] T. M. McQueen, M. Regulacio, A. J. Williams, Q. Huang, J. W. Lynn, Y. S. Hor, D. V. West, M. A. Green and R. J. Cava. Phys. Rev. B **78**, 024521 (2008).

[Putzke12] C. Putzke, A. I. Coldea, I. Guillamón, D. Vignolles, A. McCollam, D. LeBoeuf, M. D. Watson, I. I. Mazin, S. Kasahara, T. Terashima, T. Shibauchi, Y. Matsuda and A. Carrington. Phys. Rev. Lett. **108**, 047002 (2012).