de Haas-van Alphen effect and effective masses in KFe_2As_2 from LDA+DMFT

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de Haas-van Alphen effect

- density of states at the Fermi level oscillates as a function of inverse magnetic field
- oscillations can be observed in ρ, τ, χ and c_V
- measure extremal cross sections S of the Fermi surface and effective masses m^* of the charge carriers
- frequencies are given by $F = \hbar/2\pi e \cdot S$
- band masses are given by $m^* = \frac{\hbar^2}{2\pi}\frac{dS}{dk}\frac{dk}{dE}$
- compare experiment and calculations quantitatively

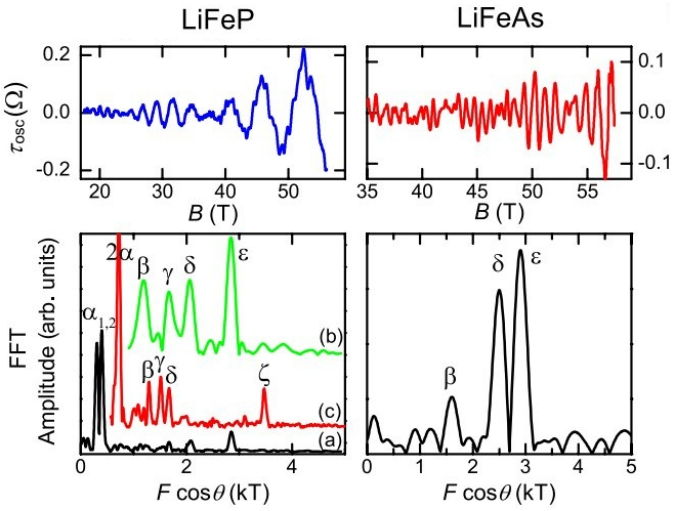


Figure: Putzke et al., PRL **108**, 047002 (2012)

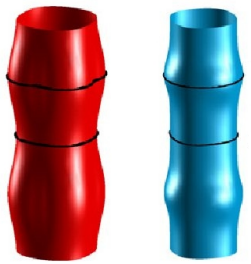


Figure: Carrington, Rep. Prog. Phys. **74**, 124507 (2011)

Calculating de Haas-van Alphen frequencies *ab-initio*

- calculate electronic bands with DFT (+DMFT)
- construct super cell with band energies on a dense grid using interpolation
- find Fermi surface with stepping algorithm on slices
- match orbits to sheets
- single out extremal orbits
- calculate frequencies and effective masses
- algorithm described in Rourke & Julian, Comput. Phys. Commun. **183**, 324–332 (2012)

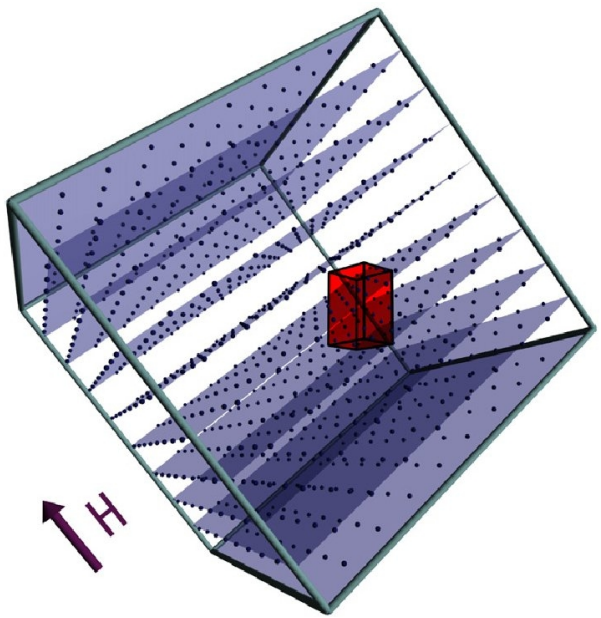
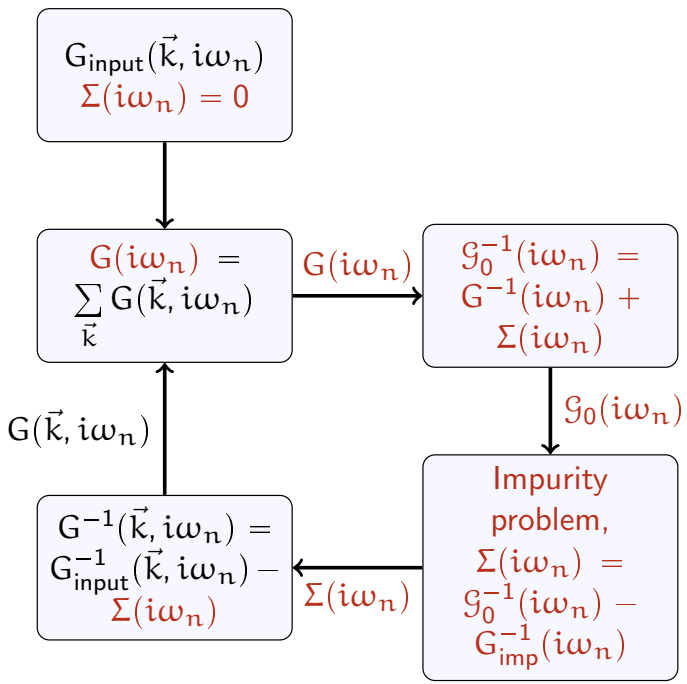


Figure: Rourke & Julian, Comput. Phys. Commun. **183**, 324–332 (2012)

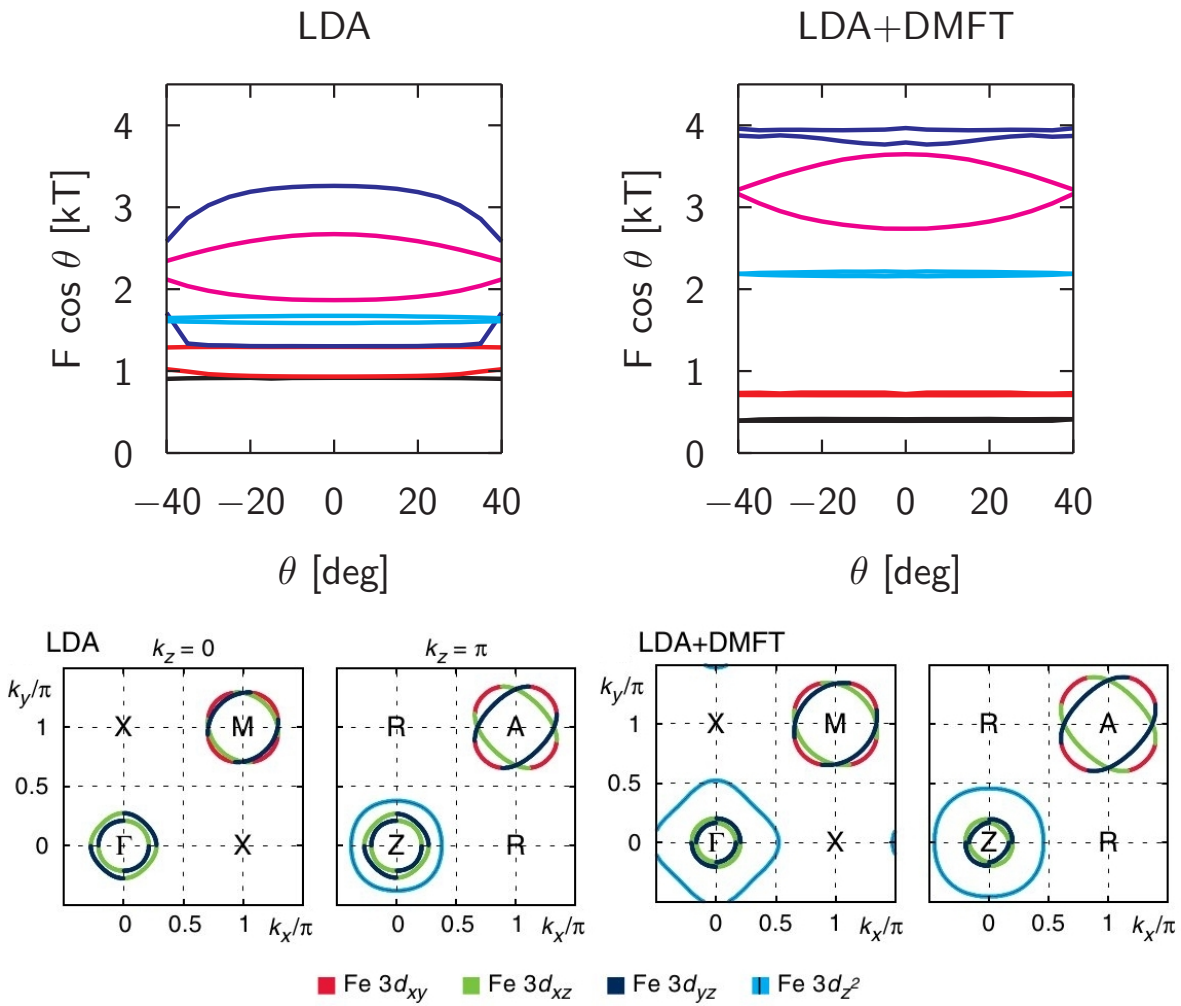
Density functional theory + Dynamical mean field theory

- calculate electronic bands with density functional theory
- project out Fe-d states for which multi-orbital Hubbard Hamiltonian is solved
- calculate the lattice Green's function from projection
- map lattice problem (3+1 dim.) to impurity problem (0+1 dim.)
- solve impurity problem with QMC
- impurity self-energy $\Sigma(i\omega_n)$ contains all local correlations of the lattice problem
- loop until self-energy is converged



Example: dHvA frequencies in LaFePO

- dHvA frequencies strongly altered when going from LDA to LDA+DMFT
- results very similar to Ferber et al., PRL **109**, 236403 (2012)
- successfully tested on various other materials



Summary of experiment and theory regarding superconductivity and electronic structure in KFe_2As_2

- nodal $s^{\pm}$-symmetry seen in Laser ARPES
  (Okazaki et al., Science **337**, 1314–1317 (2012))
- d-wave observed in thermal conductivity
  (Reid et al., PRL **109**, 087001 (2012))
- possible phase transition between two superconducting phases under pressure
  (Tafti et al., Nature Physics **9**, 359–352 (2013))
- close competition between s- and d-wave predicted (Maiti et al., PRL **107**, 147002 (2011))
- d-wave predicted (Thomale et al., PRL **107**, 117001 (2011))
- very bad agreement between dHvA frequencies derived from DFT and experiment (Terashima et al., PRB **87**, 224512 (2013))

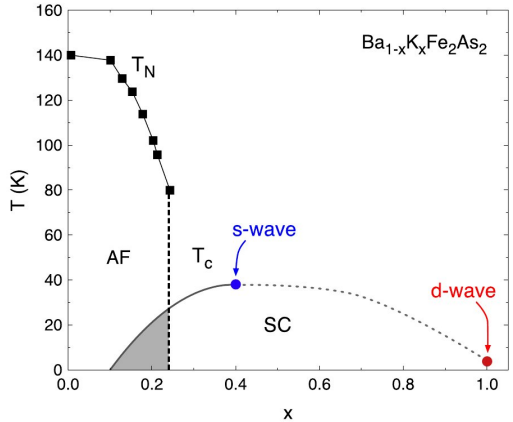


Figure: Reid et al., Supercond. Sci. Technol. **25**, 084013 (2012)

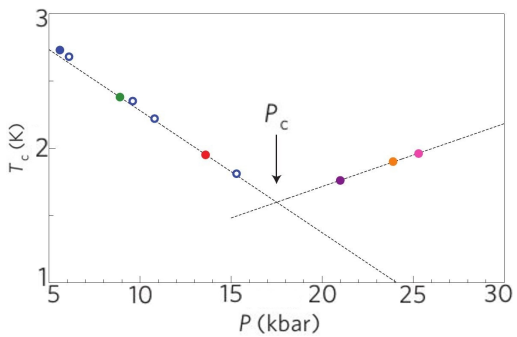


Figure: Tafti et al., Nature Physics **9**, 349 (2013)

de Haas-van Alphen effect in KFe_2As_2

- strong changes when going from DFT to DFT+DMFT
- z_{As} differs very much between available structures (Rosza & Schuster, Z. Naturforsch. B **36**, 1668 (1981); Tafti et al., arXiv:1403.0110)
- z_{As} has very strong impact on Fermi surface and dHvA frequencies
- compare orbit resolved effective masses

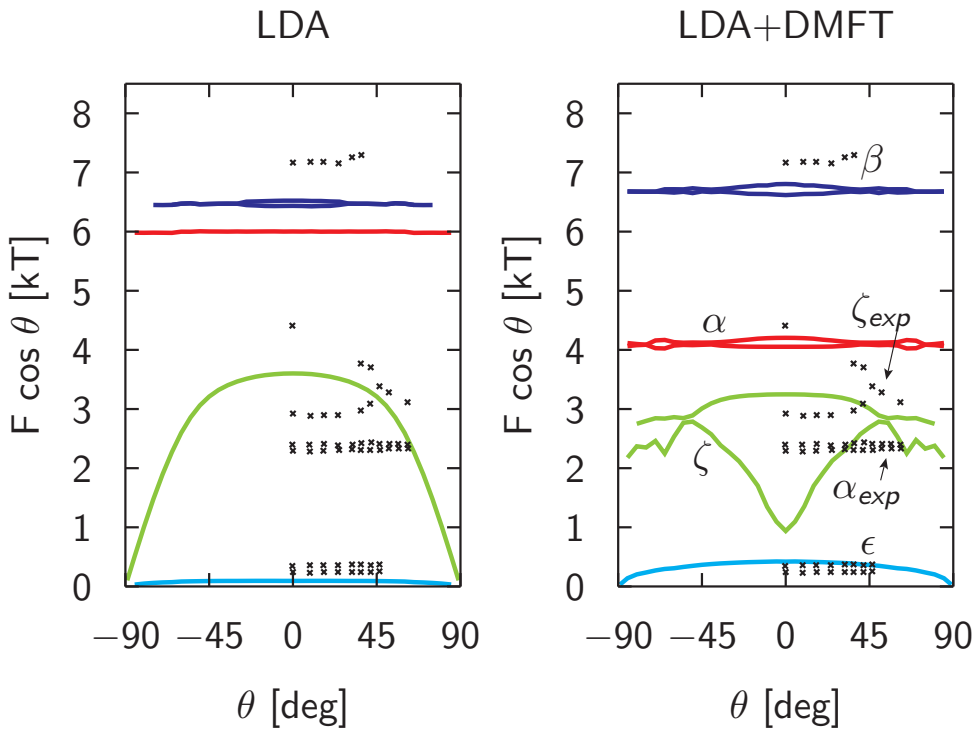


Figure: small crosses are experimental data from Terashima et al., PRB **87**, 224512 (2013)

	ϵ_Γ	ϵ_Z	α_Γ	α_Z	ζ_Γ	ζ_Z	β_Γ	β_Z
exp.	6.0	7.2	6.0	6.5	8.5	18.0	19.0	19.0
LDA+DMFT	-	5.9	3.4	4.6	2.4	5.3	8.3	8.3

Summary

ab-initio calculation of de Haas-van Alphen frequencies

- dHvA frequencies can be calculated automatically
- code is free software and hosted on GitHub: `github.com/danielguterding/dhva`

Electronic structure in KFe_2As_2

- methods beyond DFT are necessary to describe electronic structure correctly
- DMFT yields good description of Fermi surface
- preprint available: **arXiv:1403.6993**

Fermi surface topology in LaFePO

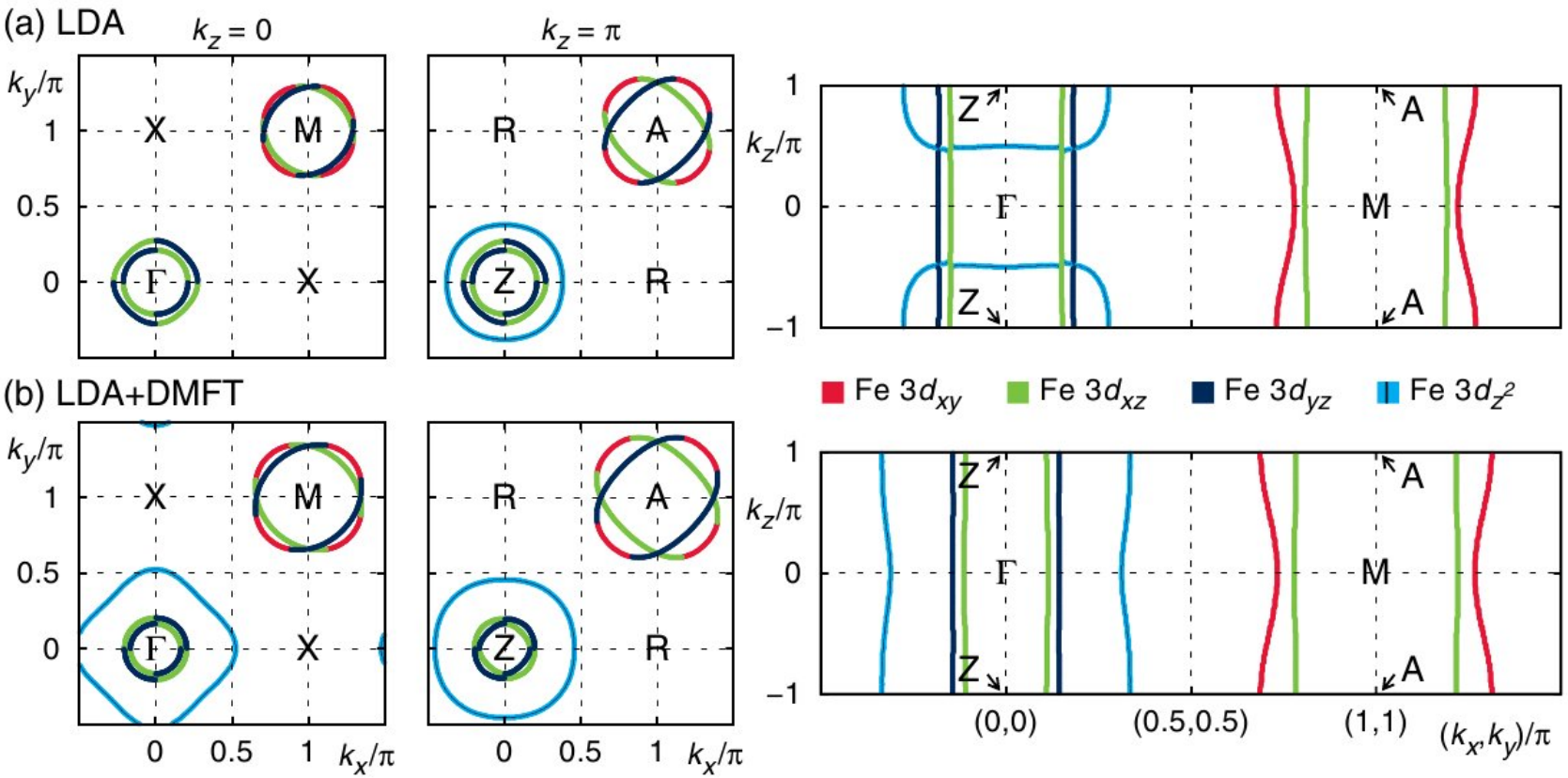


Figure: Ferber et al., PRL **109**, 236403 (2012)

Fermi surface topology in KFe_2As_2