de Haas-van Alphen frequencies calculated from band structure data

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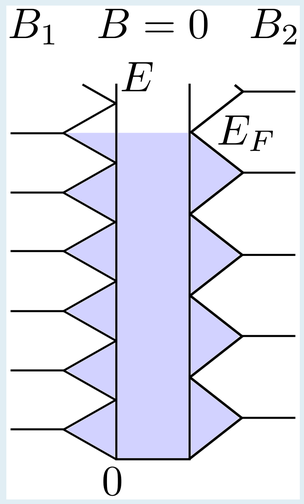
De Haas-van Alphen effect: Theory

- electron orbits in a magnetic field are quantized
- semiclassical Ansatz by Onsager and Lifshitz: $\oint d\vec{r} \cdot \left(\hbar\vec{k} + e\vec{A}\right) = 2\pi\hbar(n+\gamma)$
- orbit area in k-space is proportional to magnetic field: $S_n = (n+\gamma)2\pi eB/\hbar$
- match area of orbits n and $n-1$: $S(\frac{1}{B_n} - \frac{1}{B_{n-1}}) = S \cdot \Delta\,(1/B) = 2\pi e/\hbar$
- density of states at the Fermi level oscillates as a function of $1/B$
- ρ, χ and c_V are a function of $1/B$



dHvA frequencies from electronic structure calculations

- calculate Fermi surface and corresponding dHvA frequencies from DFT or DFT+DMFT via $F = \hbar/2\pi e \cdot S$
- in DMFT maxima of the spectral function are traced and treated as quasi-bands
- obtain absolute band masses from $m^* = \frac{\hbar^2}{2\pi}\frac{dS}{dk}\frac{dk}{dE}$
- compare experiment and calculations directly

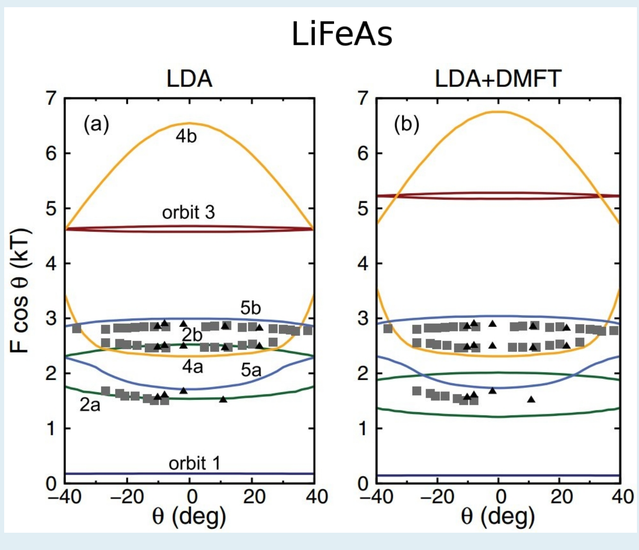
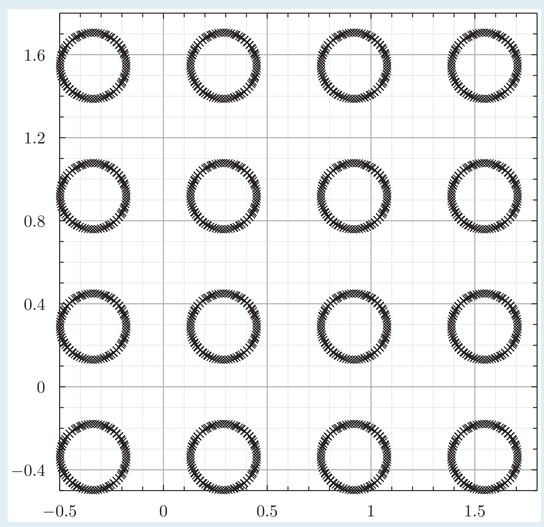


Figure: Ferber et al., PRB **85**, 094505 (2012)

The algorithm: basic ideas

- calculate electronic bands with DFT (+DMFT)
- obtain reciprocal unit cell (e.g. using XCrysDen)
- 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, Comp. Phys. Comm. **183**, 324–332 (2012)



The algorithm: super cell construction

- $\hat{z}_{\text{sc}} \parallel \vec{B}$, x-y-slices automatically contain orbits $\perp \vec{B}$
- allows tracking of orbits across multiple brillouin zones
- statistical deviations of obtained frequencies and masses give estimate of discretization errors
- cubic cell length default is $4\times$ largest reciprocal lattice vector, contains at least 64 reciprocal unit cells
- map back to reciprocal unit cell using Euler rotation and coordinate shifting
- trilinear or tricubic interpolation ($2 \cdot 10^4 \rightarrow 8 \cdot 10^6$ k-points)

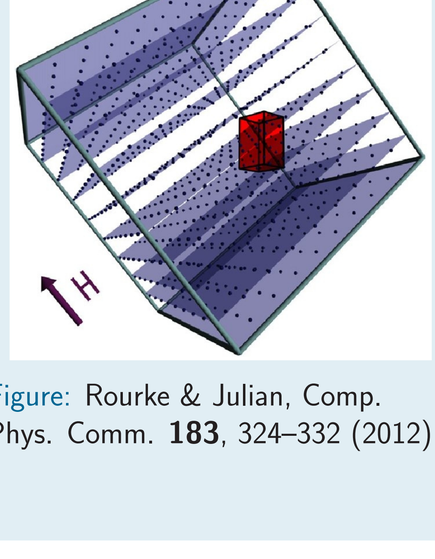


Figure: Rourke & Julian, Comp. Phys. Comm. **183**, 324–332 (2012)

The algorithm: Fermi surface detection

- stepping algorithm on slices finds Fermi surface
- FS-point ordering is crucial for calculating the area
- FS is interpolated linearly between neighbouring points
- energy slopes are recorded on-the-fly

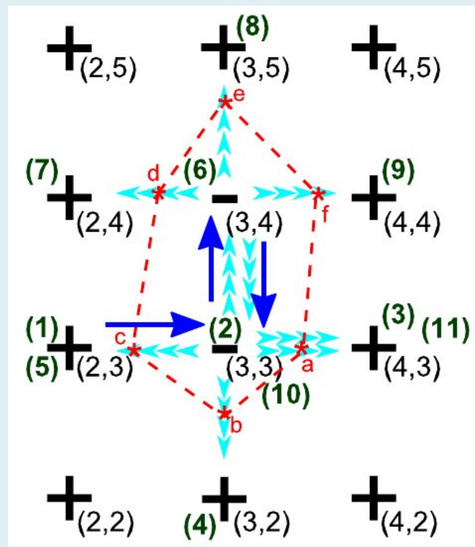
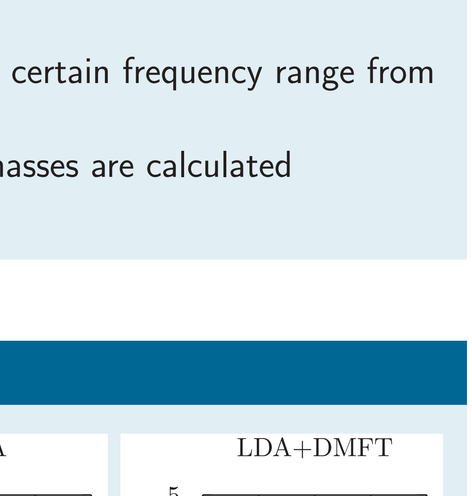


Figure: Rourke & Julian, Comp. Phys. Comm. **183**, 324–332 (2012)

The algorithm: orbit to sheet matching

- Fermi surface sheets are reconstructed from orbits on adjacent slices
- matching is done if average, minimum and maximum coordinates of one orbit are within one (average) or two (max, min) standard deviations of the other
- if more than one candidate on a slice, weighting function is calculated and orbit with minimum deviation is matched



The algorithm: evaluation

- extremal orbits are singled out from sheets
- average coordinates are transformed back to reciprocal unit cell
- frequencies and effective masses are calculated for extremal orbits
- orbits are grouped with respect to average coordinates allowing a certain range of deviations
- orbits in a group are averaged if they are in a certain frequency range from one another
- standard deviations for frequency and band masses are calculated
- output is saved to a file

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)

Summary

- dHvA frequencies can be calculated automatically
- independent of crystal structure
- successfully tested on real materials
- run time of about ten seconds per band and angle yields good results
- code is free software and hosted on GitHub: `https://github.com/danielguterding/dhva`

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