Extraction of de Haas-van Alphen frequencies from electronic structure calculations

Daniel Guterding

June 7, 2013

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 $1/B$

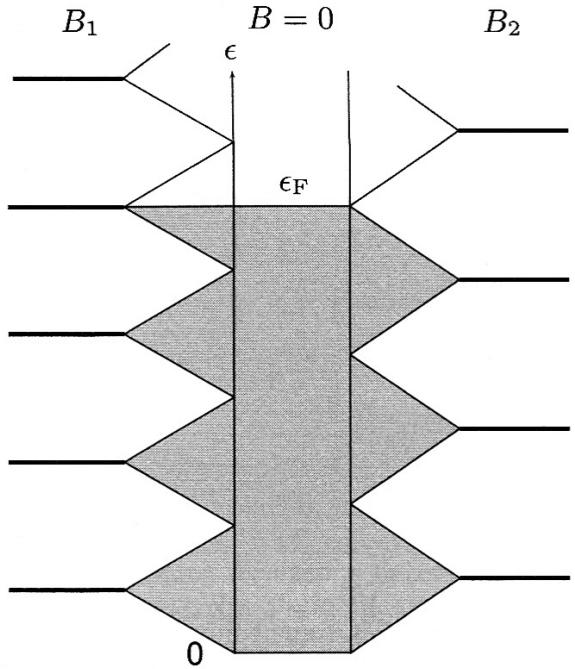


Figure : Kittel: Festkörperphysik

De Haas-van Alphen effect: Experiment

- temperatures $T < 1\,K$ and pure samples needed for well defined Landau levels
- oscillation frequencies F obtained from Fourier transformation
- amplitude $A_{osc}(T)$ and effective mass m^* related via Lifshitz-Kosevich formula

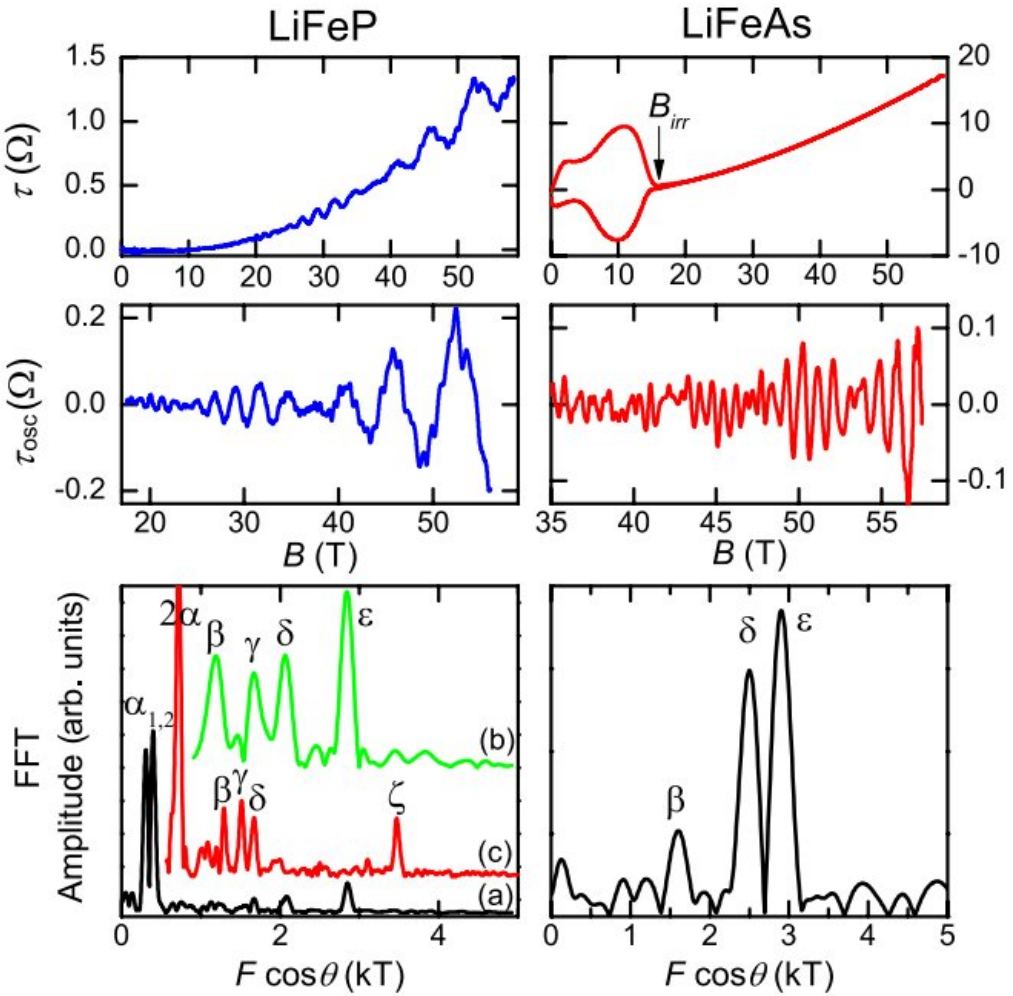


Figure : Putzke et al., PRL 108, 047002

Motivation:
dHvA frequencies from electronic structure calculations

- calculate Fermi surface and corresponding dHvA frequencies from DFT or DFT+DMFT via $F = \hbar/2\pi e \cdot S$
- obtain effective masses from $m^* = \frac{\hbar^2}{2\pi} \frac{dS}{dk} \frac{dk}{dE}$
- compare experiment and calculations directly

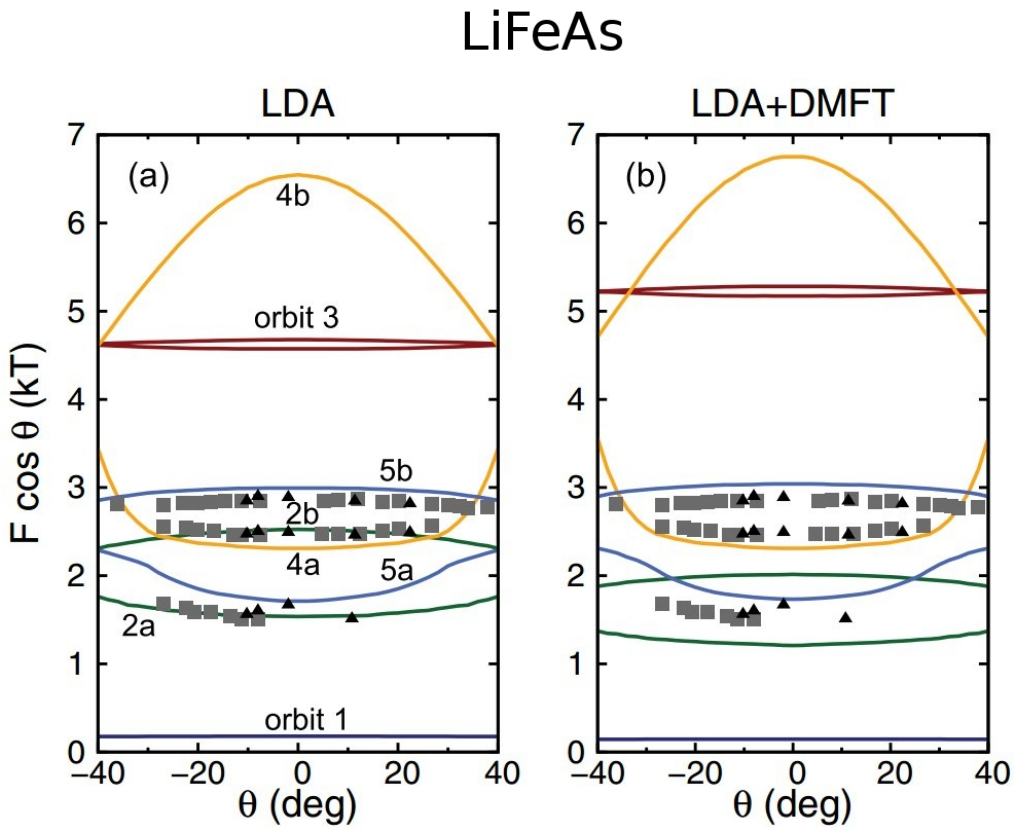
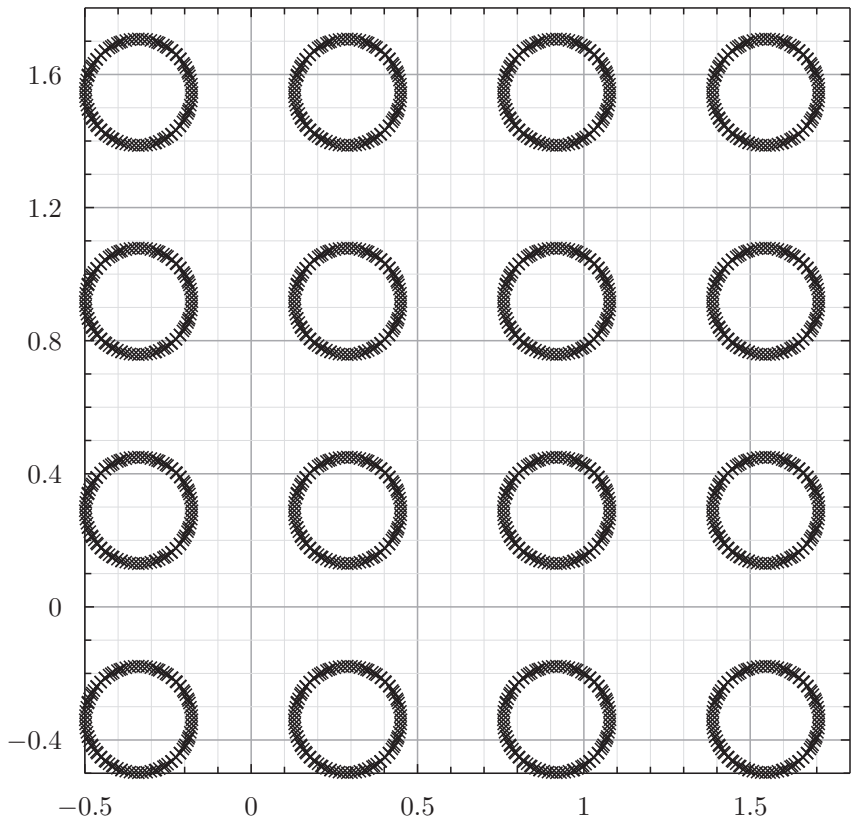


Figure : Ferber et al., PRB 85, 094505

The algorithm: basic ideas

1. calculate electronic bands with DFT (+ extensions)
2. obtain reciprocal unit cell (e.g. using XCrysDen)
3. construct super cell using heavy interpolation
4. find Fermi surface with stepping algorithm on slices
5. calculate frequencies and effective masses
6. match orbits to sheets
7. single out extremal orbits



The algorithm: super cell construction

- $\hat{z}_{sc} \parallel \vec{B}$, 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 is $4\times$ largest reciprocal lattice vector, contains at least 64 reciprocal unit cells
- map back to RUC using Euler rotation and coordinate shifting
- trilinear or tricubic interpolation ($2 \cdot 10^4 \rightarrow 6 \cdot 10^7$ k-points)

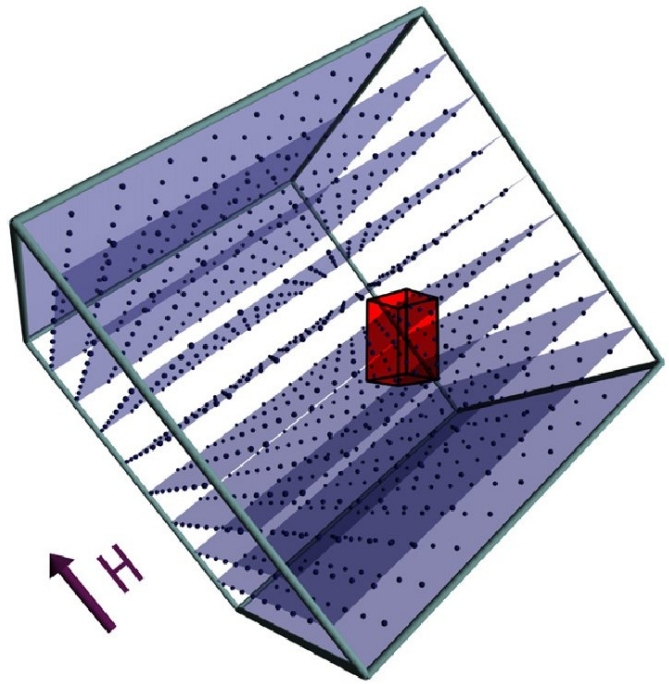


Figure : Rourke & Julian, Comp. Phys. Comm. 183, 324–332

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

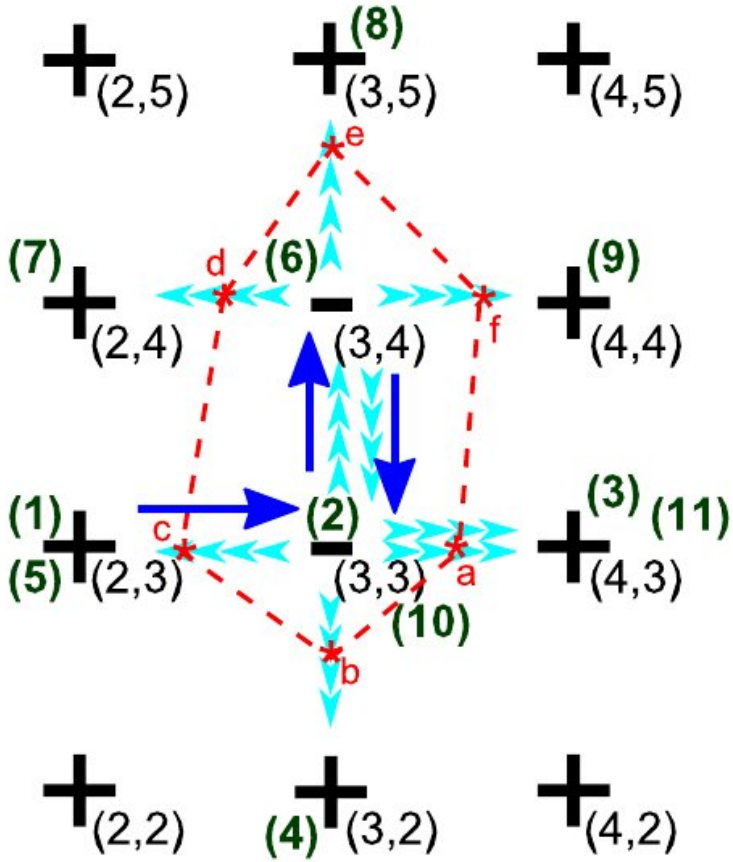
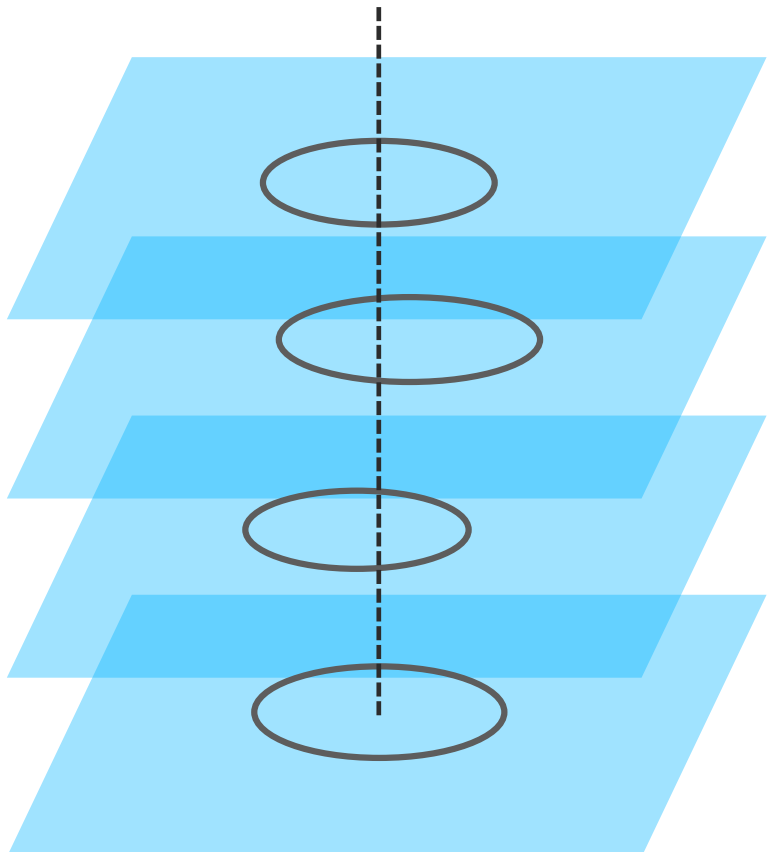


Figure : Rourke & Julian, Comp. Phys. Comm. 183, 324–332

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

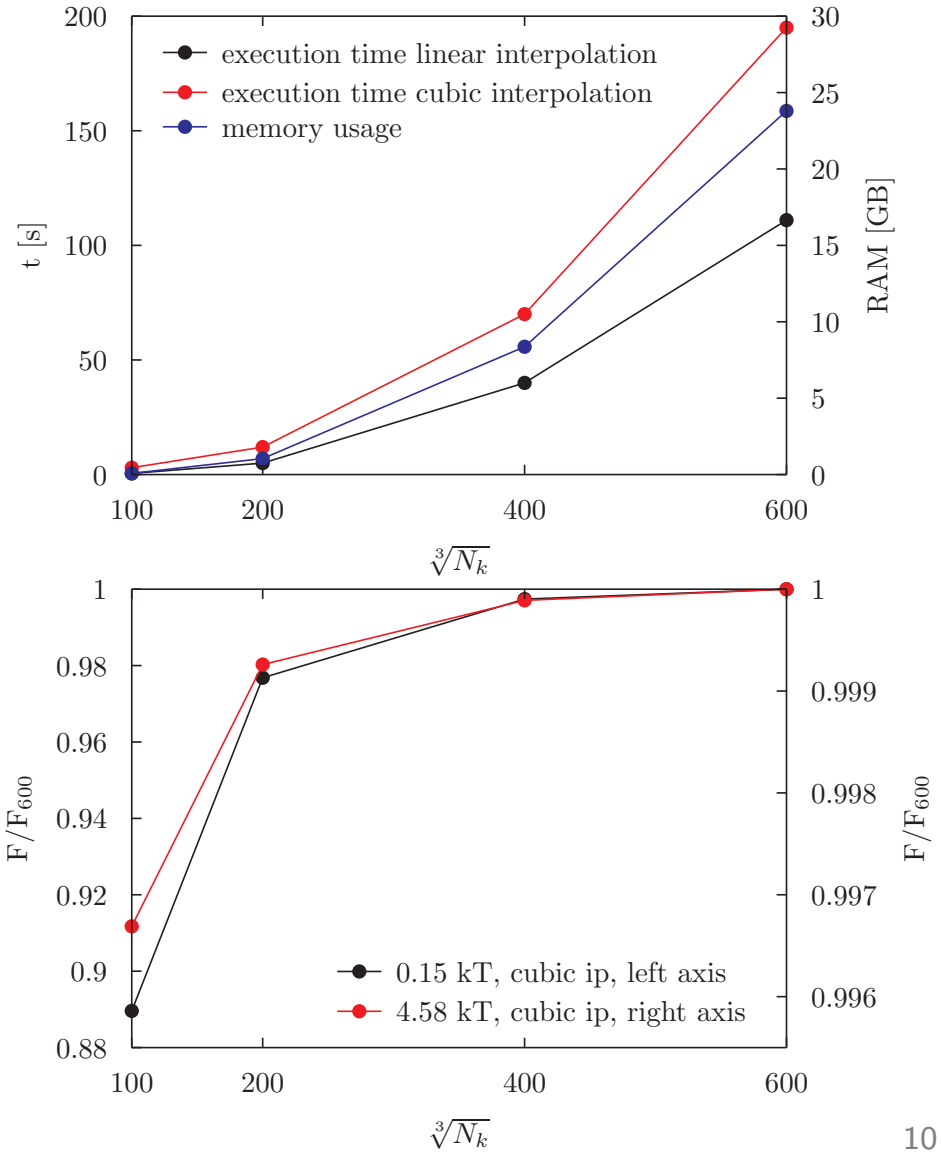


The algorithm: evaluation

- 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 effective masses are calculated
- output is saved to a file

Performance

- almost entirely dominated by interpolation algorithm
- for very high k-point numbers memory access becomes more important
- tricubic interpolation is almost as fast as trilinear
- setting with $400^3 = 64 \cdot 10^6$ k-points is converged, run time of about one minute, RAM usage of about 8 GB



Summary and outlook

Summary

- dHvA frequencies can be calculated automatically
- independent of crystal structure
- successfully tested on real materials
- run time of about one minute yields good results

Outlook

- investigate correlation effects on fermi surfaces and effective masses in iron pnictides