Calculations of de Haas van Alphen frequencies: an ab initio approach

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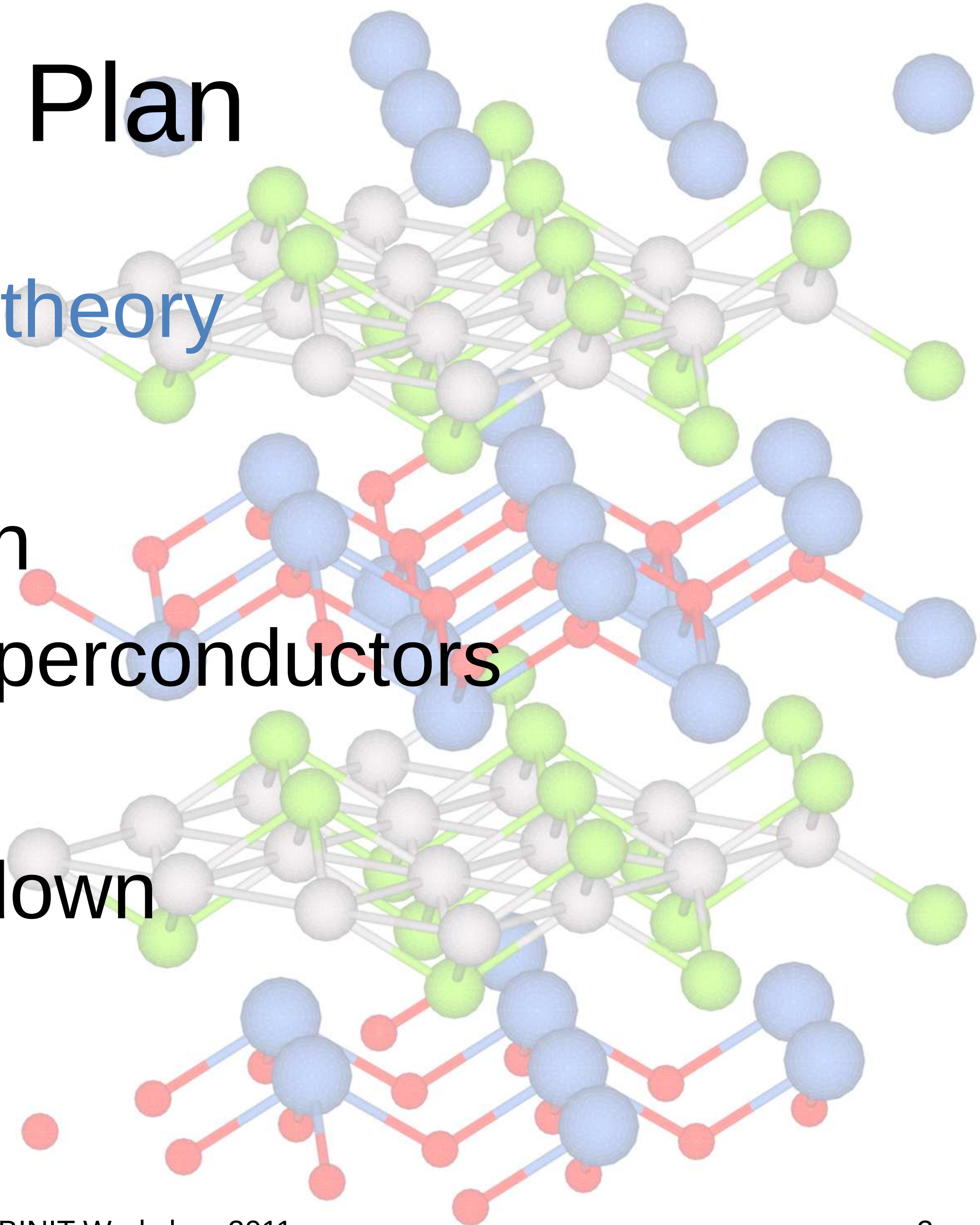
RQMP

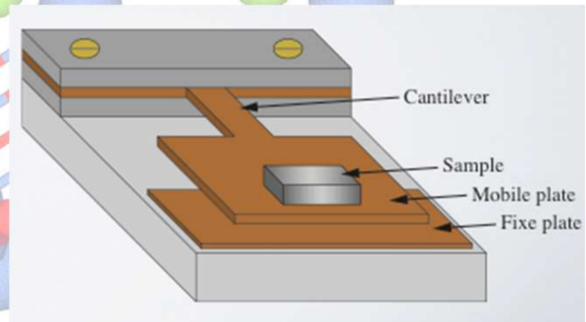
Plan

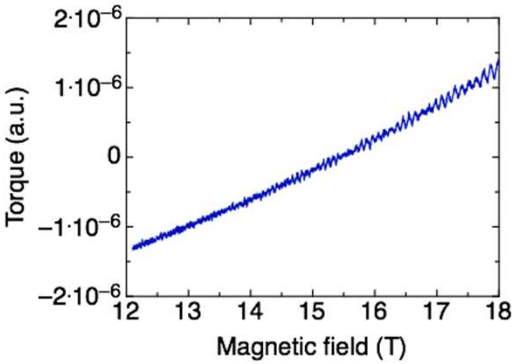


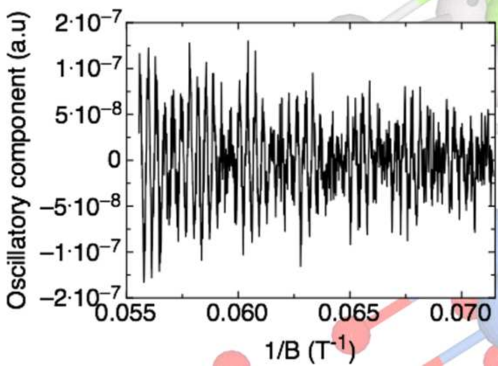
- Reminder of the theory
- MLWF
- Code explanation
- Iron pnictides superconductors
- Results
- Magnetic Breakdown

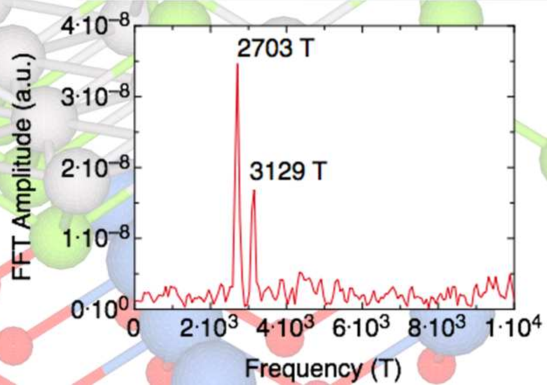
Experiment

- Sample in a magnetic field
- Torque on the cantilever measures the sample's magnetization
- Oscillations are important!









See *Condensed Matter Physics*, M.P. Marder, 2000

Semi-classical equations

- Bohr-Sommerfeld quantization

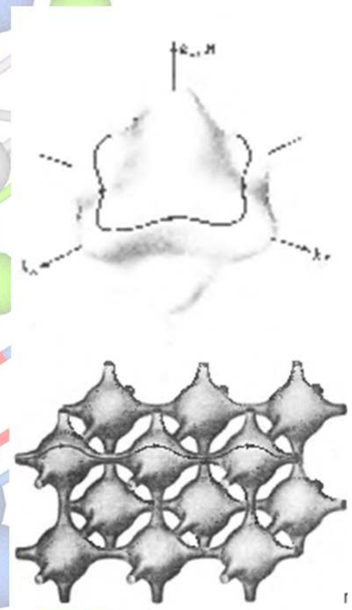
Constant

Integer

Orbit area

$$2\pi j = \Gamma + \frac{\hbar c}{eB} A$$

$$F = \left(\Delta \frac{1}{B}\right)^{-1} = \frac{c\hbar}{2\pi e} A$$



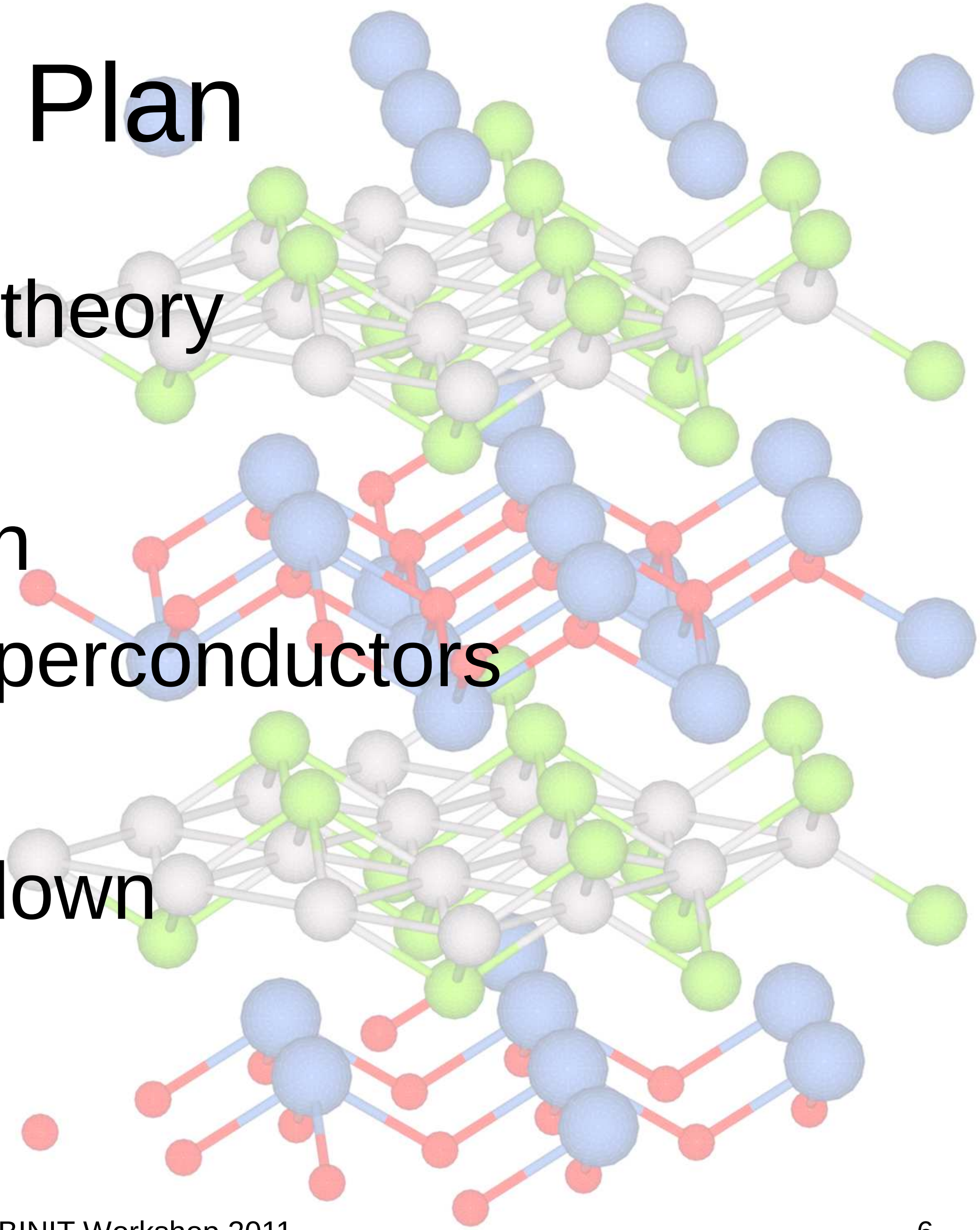
Ashcroft & Mermin, *Solid State Physics* (1976)

- Frequencies are a measure of the Fermi surface!
- Only extrema contribute.

Precision

- Typical ab initio calculation for copper: 6x6x6 k-points
- Too few points to calculate the area of a cross-section precisely
- We need interpolation.
- No need to sample all the Brillouin zone: we only need information on a plane normal to the magnetic field.

Plan



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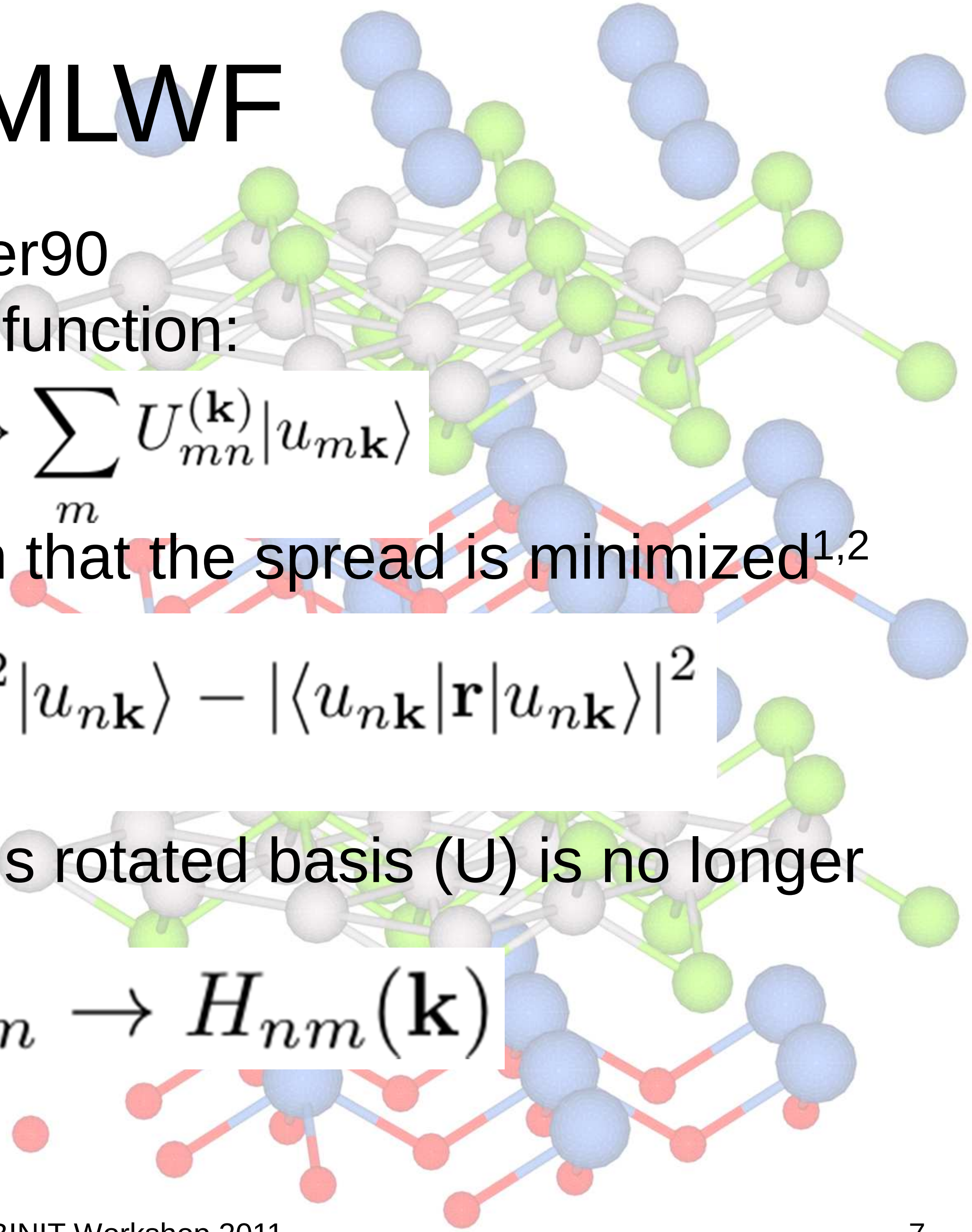
MLWF



- From Abinit -> Wannier90
- Generalized Wannier function:

$$|u_{n\mathbf{k}}\rangle \rightarrow \sum_m U_{mn}^{(\mathbf{k})} |u_{m\mathbf{k}}\rangle$$

- With $U^{(k)}$ defined such that the spread is minimized[1,2]

$$\sum_n \sum_{\mathbf{k}} \langle u_{n\mathbf{k}} | r^2 | u_{n\mathbf{k}} \rangle - |\langle u_{n\mathbf{k}} | \mathbf{r} | u_{n\mathbf{k}} \rangle|^2$$

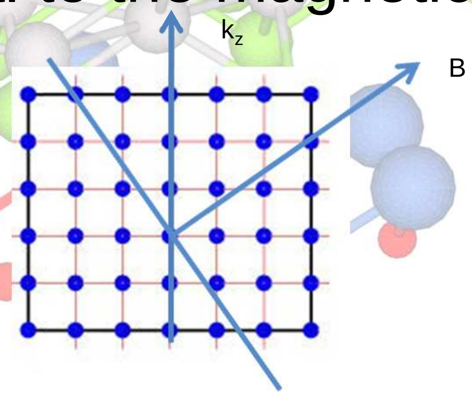
- The Hamiltonian in this rotated basis (U) is no longer diagonal:

$$\epsilon_{n\mathbf{k}} \delta_{nm} \rightarrow H_{nm}(\mathbf{k})$$

1. Marzari N. and Vanderbilt D., PRB **56**, 12847 (1997)
2. Souza I., Marzari N. and Vanderbilt D., PRB **65**, 035109 (2001)

MLWF (2)

- Fourier transform : $$H(\mathbf{k}) \rightarrow H(\mathbf{R})$$
- Since the basis is localized, H(**R**) converges to zero quickly.
- Can be interpolated on an arbitrary point in k-space (called **q**): $$H(\mathbf{R}) \rightarrow H(\mathbf{q})$$
- This method is used to calculate the band energies (eigenvalues of H(q) on a plane normal to the magnetic field)

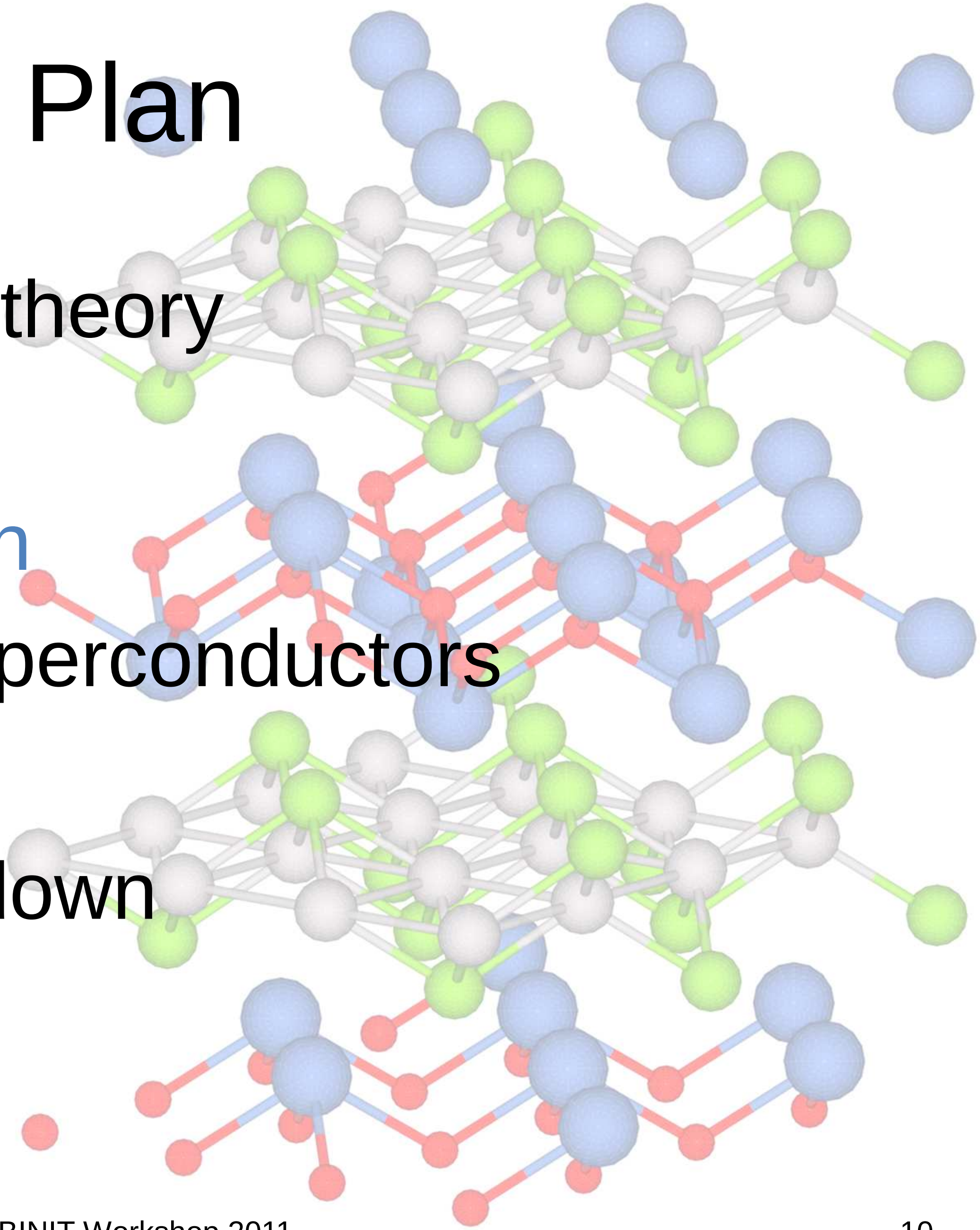


Getting a faster interpolation

$$H(\mathbf{q}) = \sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}} H(\mathbf{R})$$

- Number of R = number of k-points in the ABINIT calculations
- Size of the Hamiltonian = number of Wannier functions
  - Tuned by rejecting low (and high) energy state
- Careful about reproducing correctly the FS

Plan



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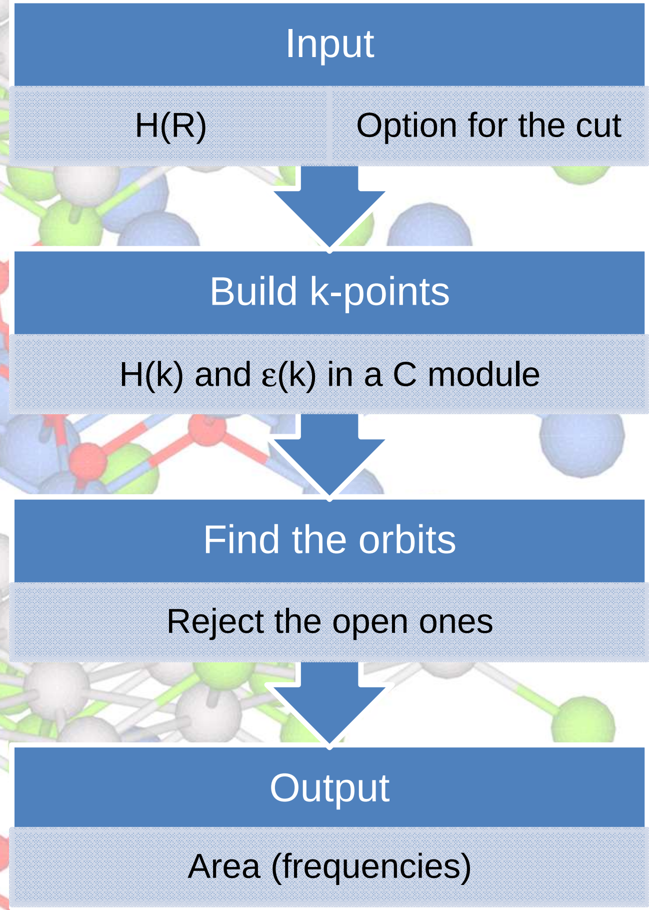
Code: dHvA.py

- Input:
  - H(**R**) from Wannier90
  - Direction for the magnetic field
  - Option for the Fermi surface slice
- Output:
  - Energy of the plane
  - Possible orbits (open and close)
  - dHvA frequencies (area of closed orbits)
- Going further:
  - Relative intensity of the signal
  - Effective mass



Slicing the Fermi surface

- Periodic boundary conditions:
  - Finds all the possible orbits
  - Force a specific direction for B
  - Unable to calculate efficiently the area of a specific orbit (too much useless information)

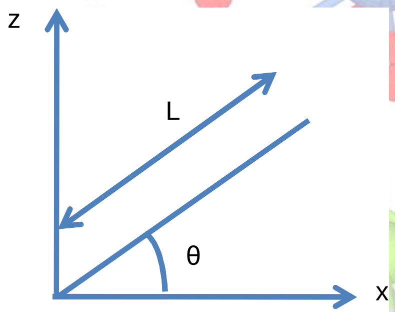
- ‘Manual’ choice
  - Manually choose the direction of the magnetic field, the size and origin of the plane
  - Cannot find an orbit (need to know its position)
  - Much more accurate (useless information is cut out)

Periodic boundary condition: example BCT crystal

- For a magnetic field in the [cosθ 0 sinθ] direction

$$(\mathbf{a}_1\ \mathbf{a}_2\ \mathbf{a}_3) = \begin{pmatrix} -a/2 & a/2 & a/2 \\ a/2 & -a/2 & a/2 \\ c/2 & c/2 & -c/2 \end{pmatrix} \qquad (\mathbf{b}_1\ \mathbf{b}_2\ \mathbf{b}_3) = \begin{pmatrix} 0 & \tilde{a}/2 & \tilde{a}/2 \\ \tilde{a}/2 & 0 & \tilde{a}/2 \\ \tilde{c}/2 & \tilde{c}/2 & 0 \end{pmatrix}$$

- For y direction, take a segment of length ã
- For x&z:



$$(L\cos\theta\ 0\ L\sin\theta) = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$$

$$\tan\theta = \frac{\tilde{c}}{\tilde{a}}\frac{n_1+n_3}{n_3-n_1} = \frac{a}{c}\frac{p}{q}$$

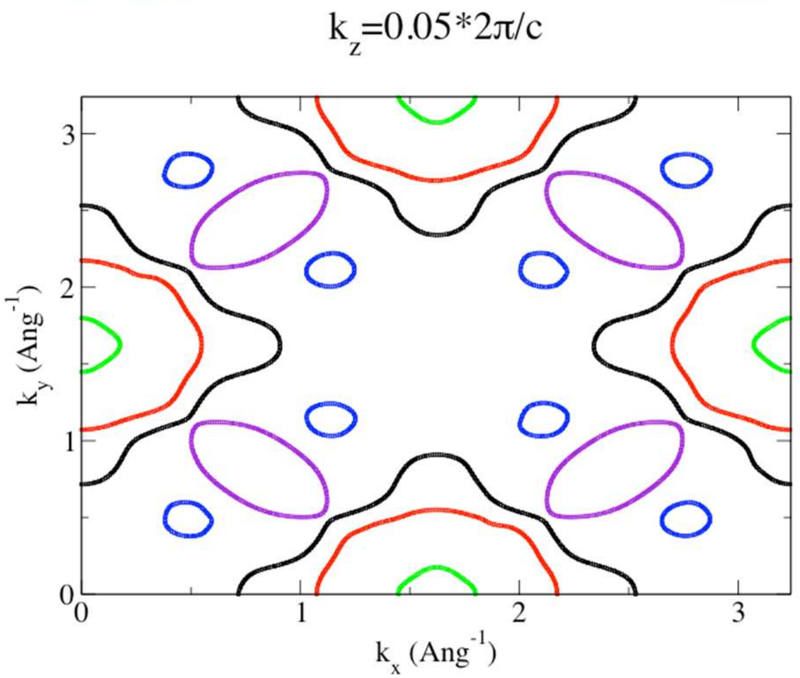
H(q) and diagonalize

- Calculate H(q) for every point on the plane
- Done in a C module: more efficient
- Only interested in a limited set of bands (do not store those not crossing the Fermi level)
- Suppose that each band can be treated separately (disconnected pieces of the FS)

Finding the orbit

- For a given band, find all the points where the energy changes sign (0 is the Fermi level)
- Connect the dots
- Calculate the area
- Converge!

$LaFe_2P_2$: B=[001]



Shifting the plane

- Shift the origin of the plane
- Find the extremum: these are the dHvA frequencies
- Intensity (finite difference):

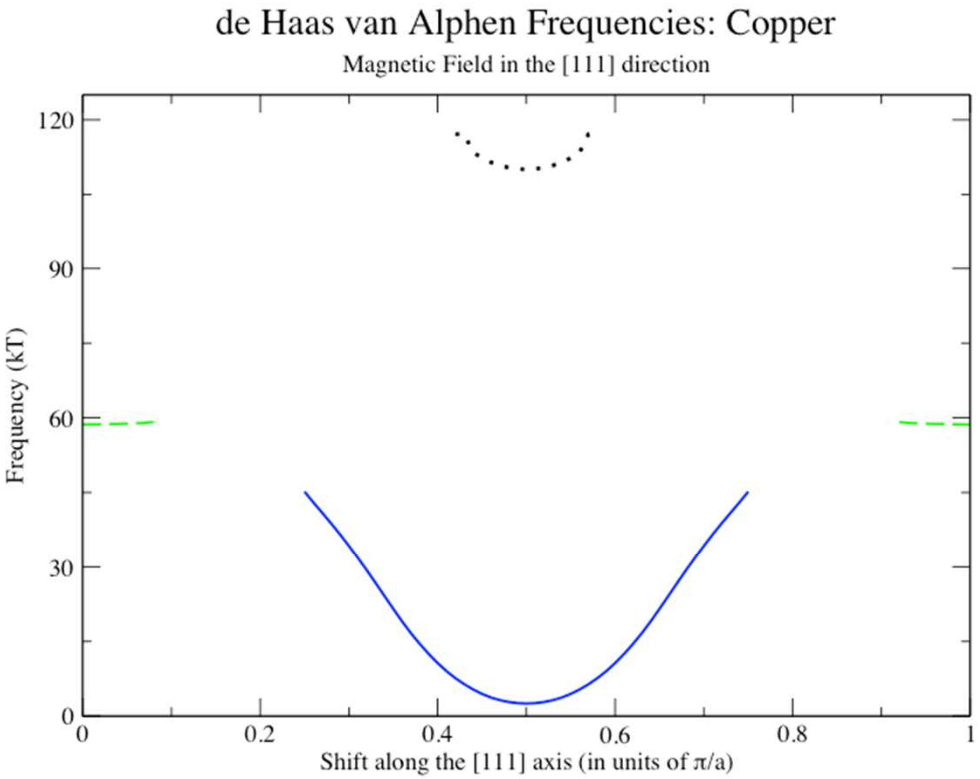
$$I \propto \left(\frac{\partial^2 A}{\partial k_B^2}\right)^{-1/2}$$

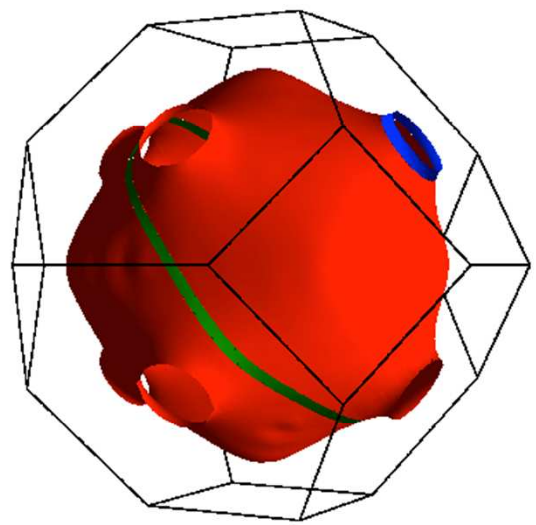
- Effective cyclotron mass (finite difference):

$$m^* = \frac{\hbar^2}{2\pi}\left(\frac{\partial A}{\partial E_F}\right)$$

Test case: copper

- For a magnetic field in the [111] direction





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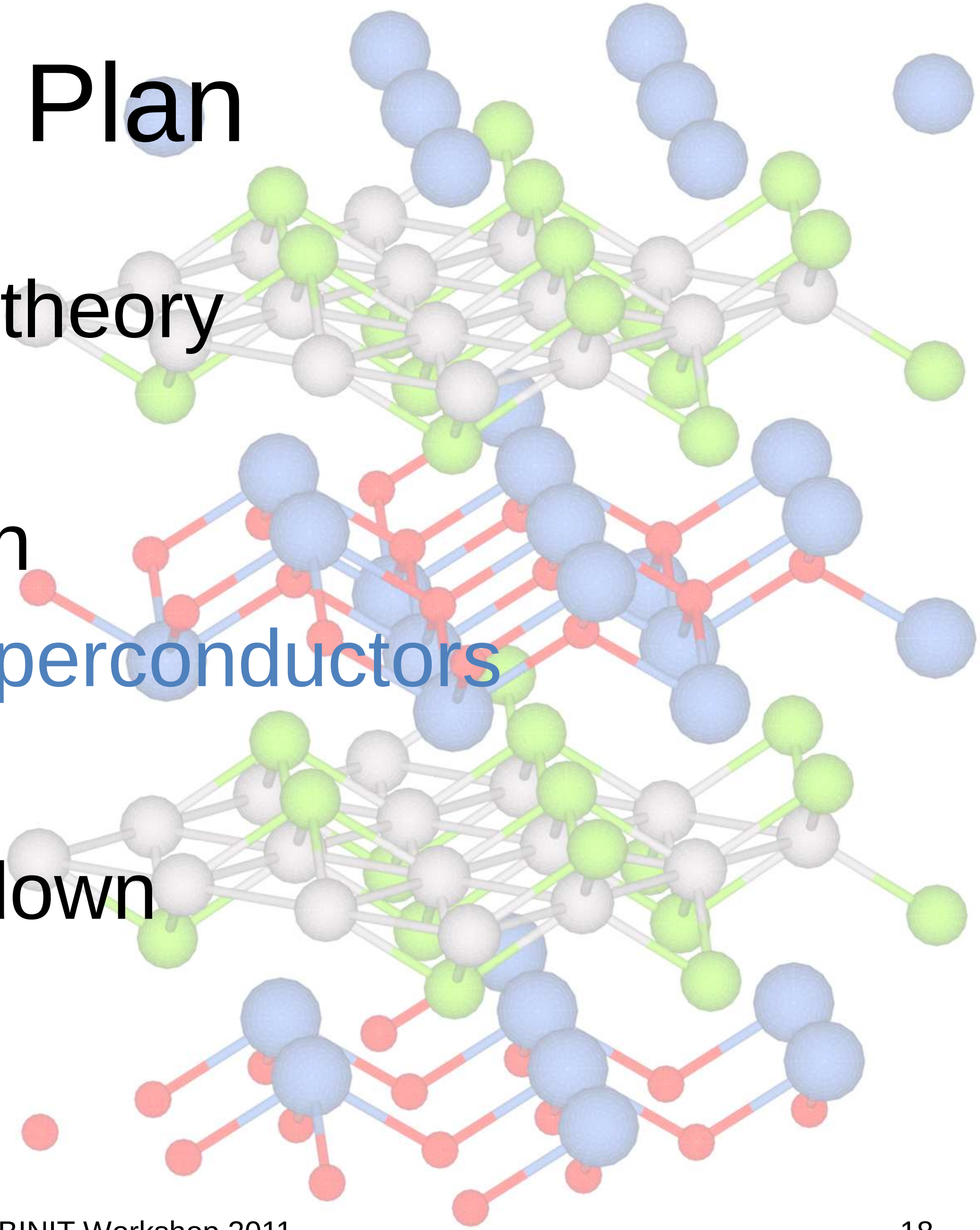

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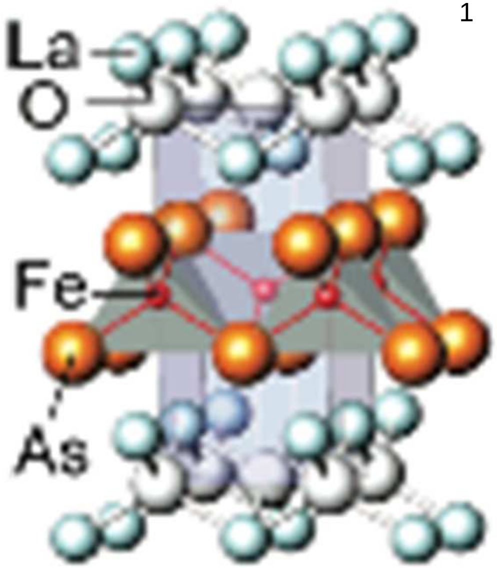
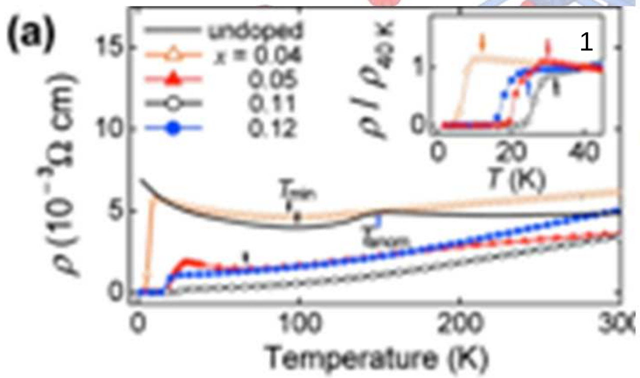
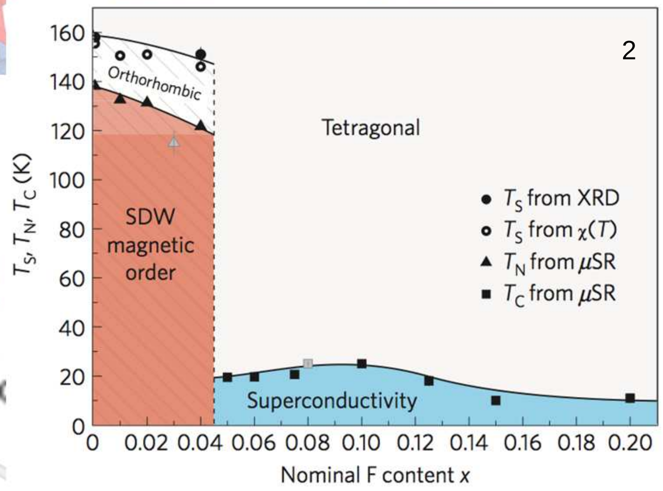
All You Need To Know About Iron Pnictide Superconductor But Were Too Afraid To Ask

$LaO_{1-x}F_xFeAs$

1







1. Kamihara Y., JACS **130**, 3296 (2008)
2. Luetkens H., Nature Materials **8**, 305 (2009)
3. Damascelli A. RMP **75**, 473 (2003)

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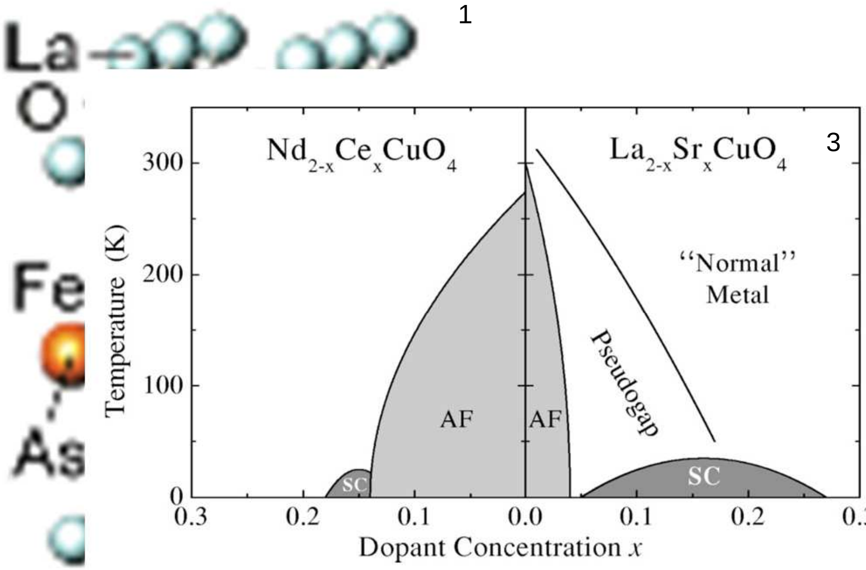
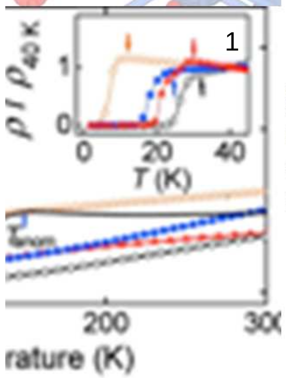
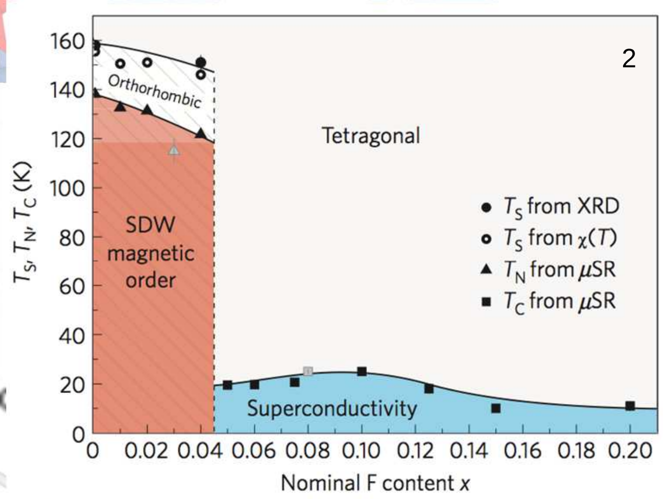
$LaO_{1-x}F_xFeAs$







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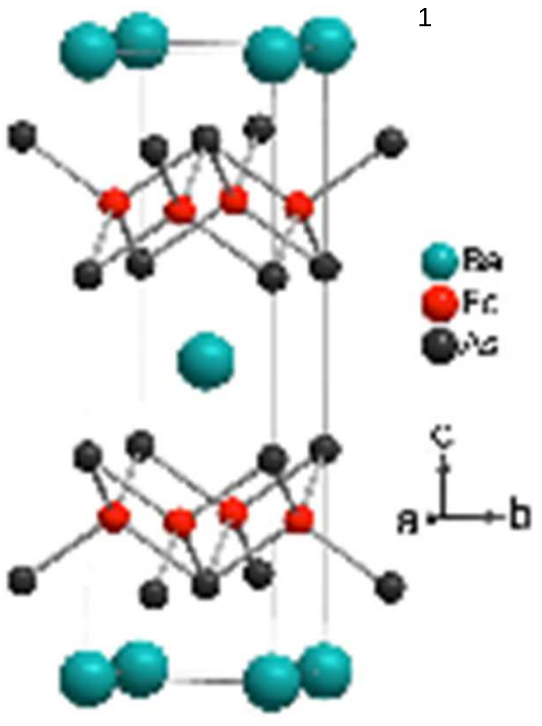
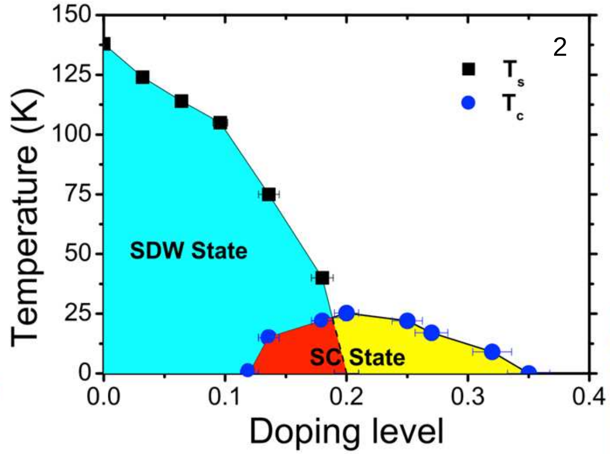
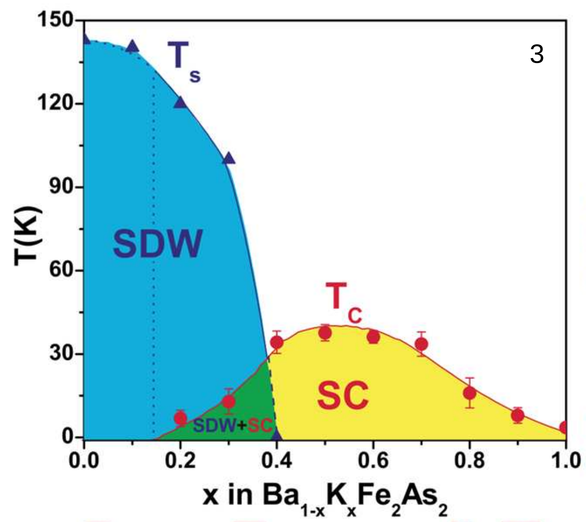
$BaFe_2As_2$





$BaFe_{2-x}Co_xAs_2$
Electron Doped

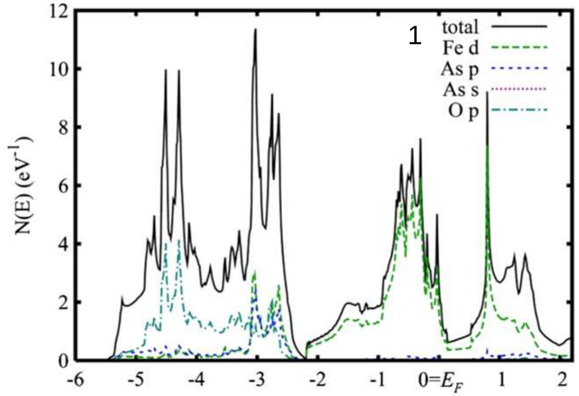


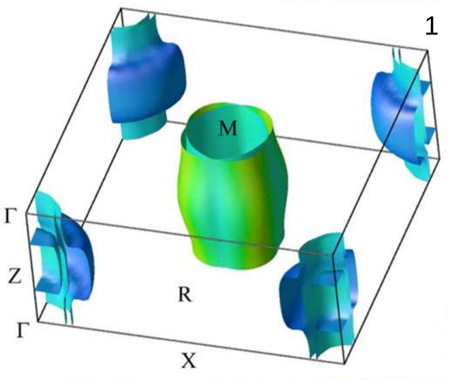
$Ba_{1-x}K_xFe_2As_2$
Hole Doped

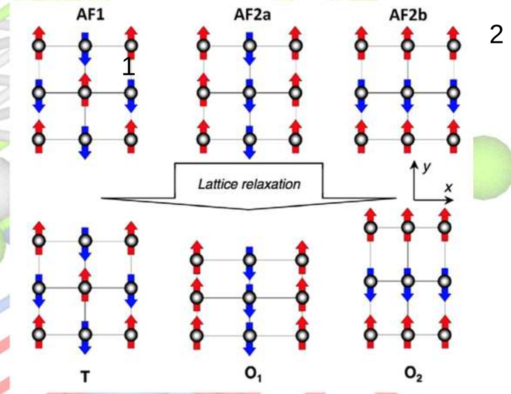
1. Rotter M., PRL **101**, 107006 (2008)
2. Wang X., New Journal of Physics **11**, 045003 (2009)
3. Chen H. EPL **85**, 17006 (2009)

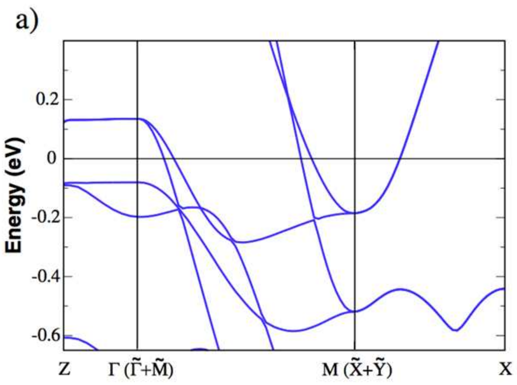
Band Structure & FS

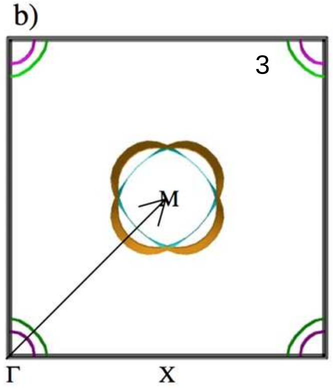
LaOFeAs: DOS







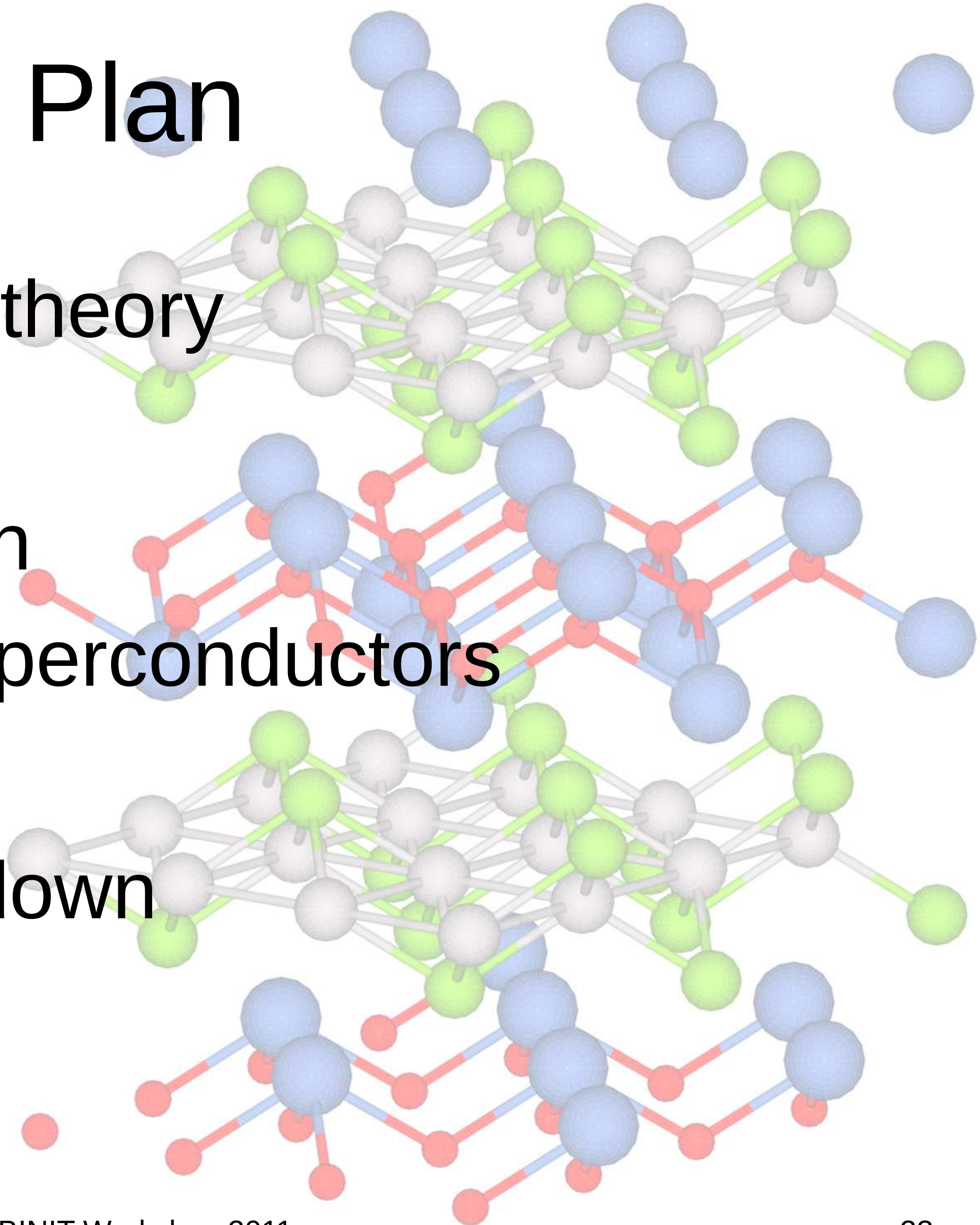




Stripe order (SDW)
$s_{\pm}$ model for superconducting gap

1. Singh D., PRL **100**, 237003 (2008)
2. Nomura T., Superconductor Science and Tech. **21**, 125028 (2008)
3. Mazin I. PRL **101**, 057003 (2008)

Plan



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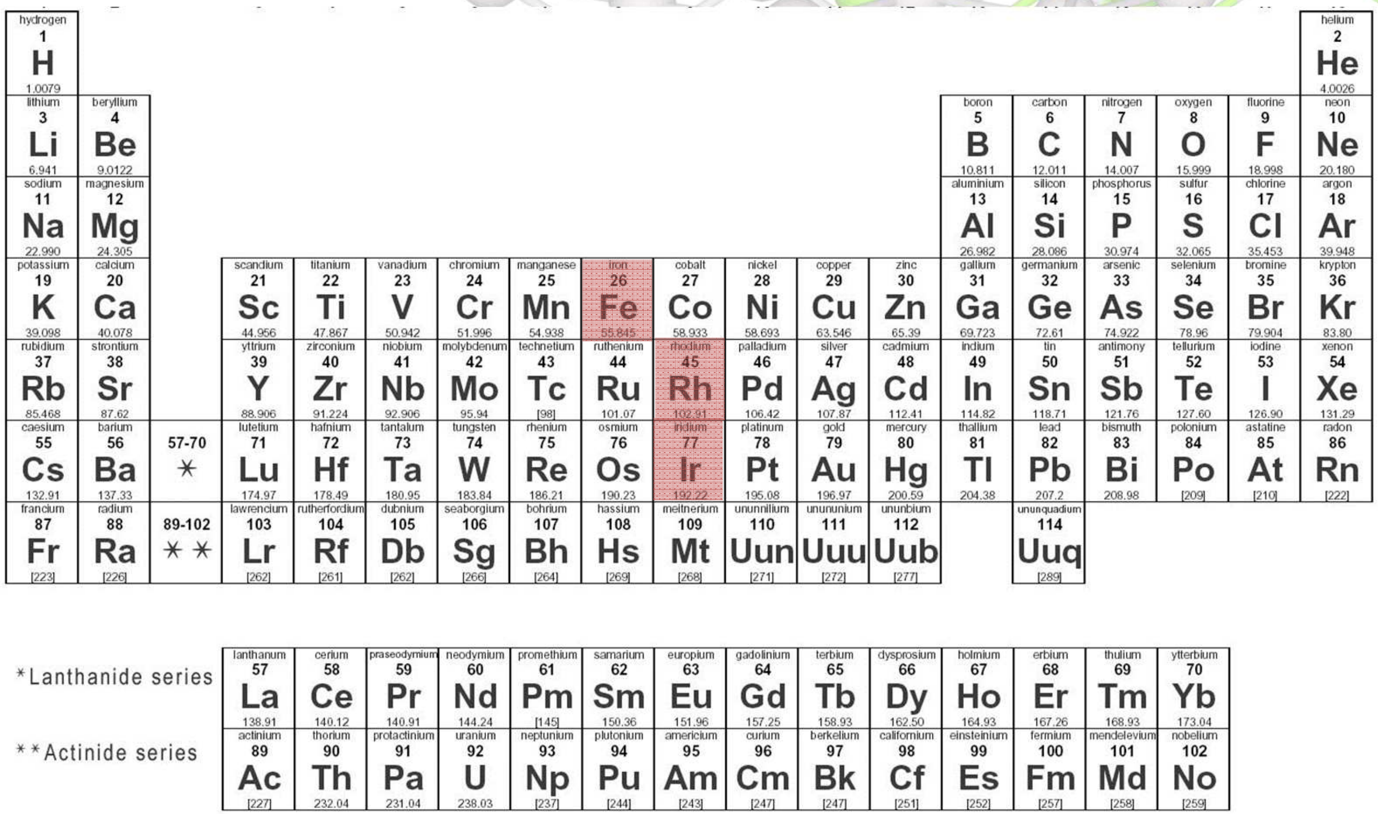
$BaRh_2P_2$ and $BaIr_2P_2$

- We substitute iron ($BaFe_2P_2$) by rhodium or iridium.

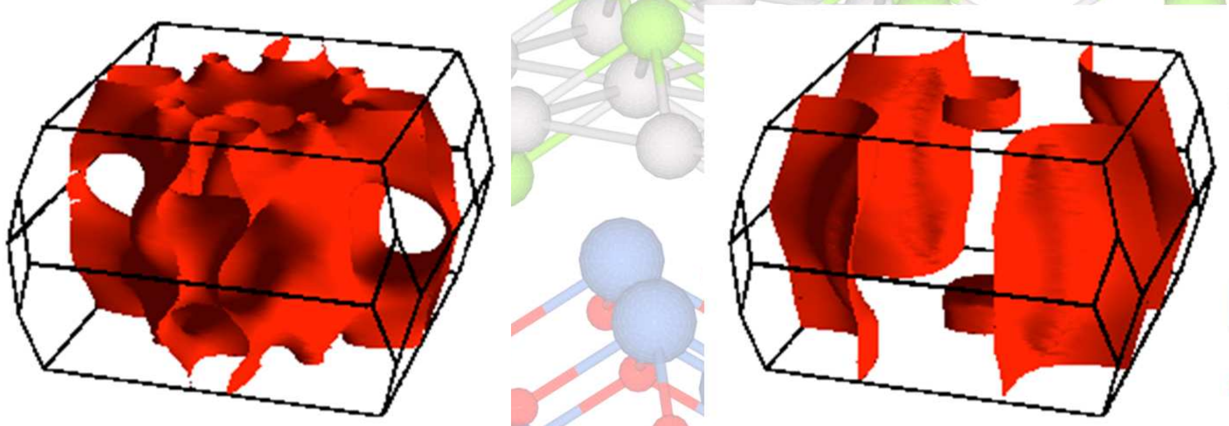


hydrogen 1 **H** 1.0079																		helium 2 **He** 4.0026
lithium 3 **Li** 6.941	beryllium 4 **Be** 9.0122												boron 5 **B** 10.811	carbon 6 **C** 12.011	nitrogen 7 **N** 14.007	oxygen 8 **O** 15.999	fluorine 9 **F** 18.998	neon 10 **Ne** 20.180
sodium 11 **Na** 22.990	magnesium 12 **Mg** 24.305												aluminium 13 **Al** 26.982	silicon 14 **Si** 28.086	phosphorus 15 **P** 30.974	sulfur 16 **S** 32.065	chlorine 17 **Cl** 35.453	argon 18 **Ar** 39.948
potassium 19 **K** 39.098	calcium 20 **Ca** 40.078		scandium 21 **Sc** 44.956	titanium 22 **Ti** 47.867	vanadium 23 **V** 50.942	chromium 24 **Cr** 51.996	manganese 25 **Mn** 54.938	iron 26 **Fe** 55.845	cobalt 27 **Co** 58.933	nickel 28 **Ni** 58.693	copper 29 **Cu** 63.546	zinc 30 **Zn** 65.39	gallium 31 **Ga** 69.723	germanium 32 **Ge** 72.61	arsenic 33 **As** 74.922	selenium 34 **Se** 78.96	bromine 35 **Br** 79.904	krypton 36 **Kr** 83.80
rubidium 37 **Rb** 85.468	strontium 38 **Sr** 87.62		yttrium 39 **Y** 88.906	zirconium 40 **Zr** 91.224	niobium 41 **Nb** 92.906	molybdenum 42 **Mo** 95.94	technetium 43 **Tc** [98]	ruthenium 44 **Ru** 101.07	rhodium 45 **Rh** 102.91	palladium 46 **Pd** 106.42	silver 47 **Ag** 107.87	cadmium 48 **Cd** 112.41	indium 49 **In** 114.82	tin 50 **Sn** 118.71	antimony 51 **Sb** 121.76	tellurium 52 **Te** 127.60	iodine 53 **I** 126.90	xenon 54 **Xe** 131.29
caesium 55 **Cs** 132.91	barium 56 **Ba** 137.33	57-70 *	lutetium 71 **Lu** 174.97	hafnium 72 **Hf** 178.49	tantalum 73 **Ta** 180.95	tungsten 74 **W** 183.84	rhenium 75 **Re** 186.21	osmium 76 **Os** 190.23	iridium 77 **Ir** 192.22	platinum 78 **Pt** 195.08	gold 79 **Au** 196.97	mercury 80 **Hg** 200.59	thallium 81 **Tl** 204.38	lead 82 **Pb** 207.2	bismuth 83 **Bi** 208.98	polonium 84 **Po** [209]	astatine 85 **At** [210]	radon 86 **Rn** [222]
francium 87 **Fr** [223]	radium 88 **Ra** [226]	89-102 **	lawrencium 103 **Lr** [262]	rutherfordium 104 **Rf** [261]	dubnium 105 **Db** [262]	seaborgium 106 **Sg** [266]	bohrium 107 **Bh** [264]	hassium 108 **Hs** [269]	meitnerium 109 **Mt** [268]	ununnilium 110 **Uun** [271]	unununium 111 **Uuu** [272]	ununbium 112 **Uub** [277]		ununquadium 114 **Uuq** [289]				

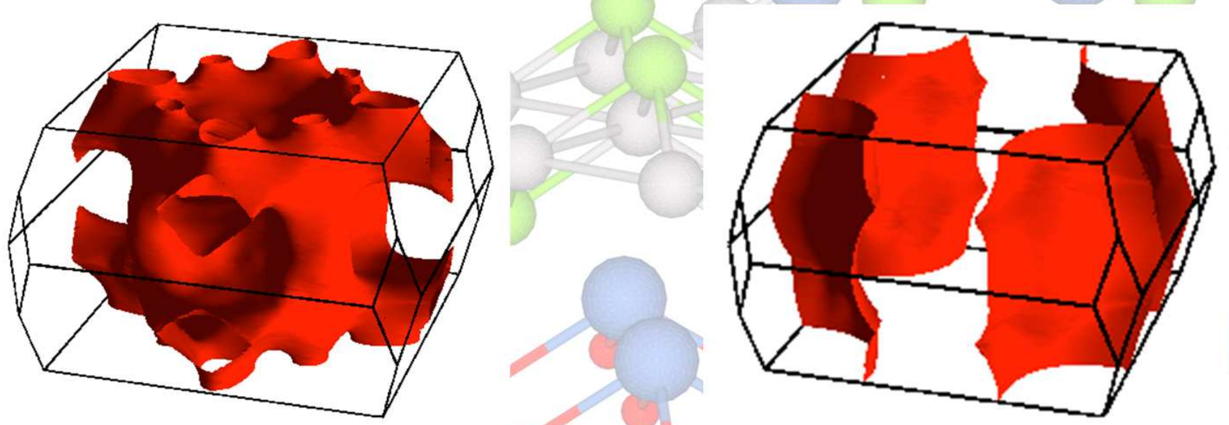
*Lanthanide series	lanthanum 57 **La** 138.91	cerium 58 **Ce** 140.12	praseodymium 59 **Pr** 140.91	neodymium 60 **Nd** 144.24	promethium 61 **Pm** [145]	samarium 62 **Sm** 150.36	europium 63 **Eu** 151.96	gadolinium 64 **Gd** 157.25	terbium 65 **Tb** 158.93	dysprosium 66 **Dy** 162.50	holmium 67 **Ho** 164.93	erbium 68 **Er** 167.26	thulium 69 **Tm** 168.93	ytterbium 70 **Yb** 173.04
**Actinide series	actinium 89 **Ac** [227]	thorium 90 **Th** 232.04	protactinium 91 **Pa** 231.04	uranium 92 **U** 238.03	neptunium 93 **Np** [237]	plutonium 94 **Pu** [244]	americium 95 **Am** [243]	curium 96 **Cm** [247]	berkelium 97 **Bk** [247]	californium 98 **Cf** [251]	einsteinium 99 **Es** [252]	fermium 100 **Fm** [257]	mendelevium 101 **Md** [258]	nobelium 102 **No** [259]

Fermi Surfaces

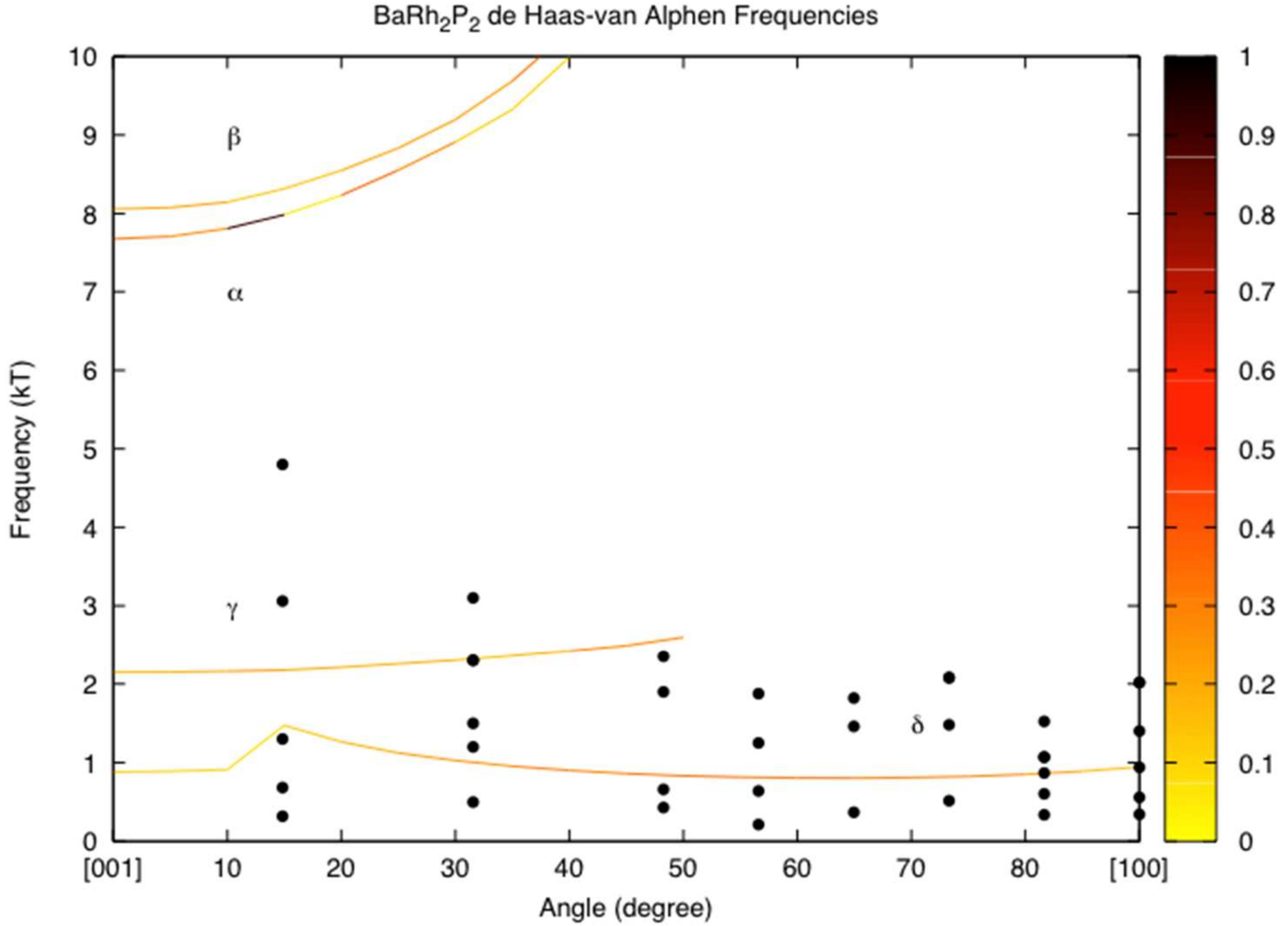
$BaRh_2P_2$

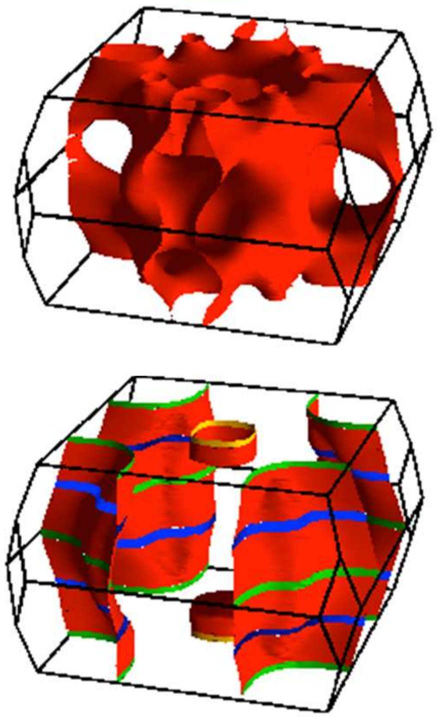


$BaIr_2P_2$



Results: $BaRh_2P_2$





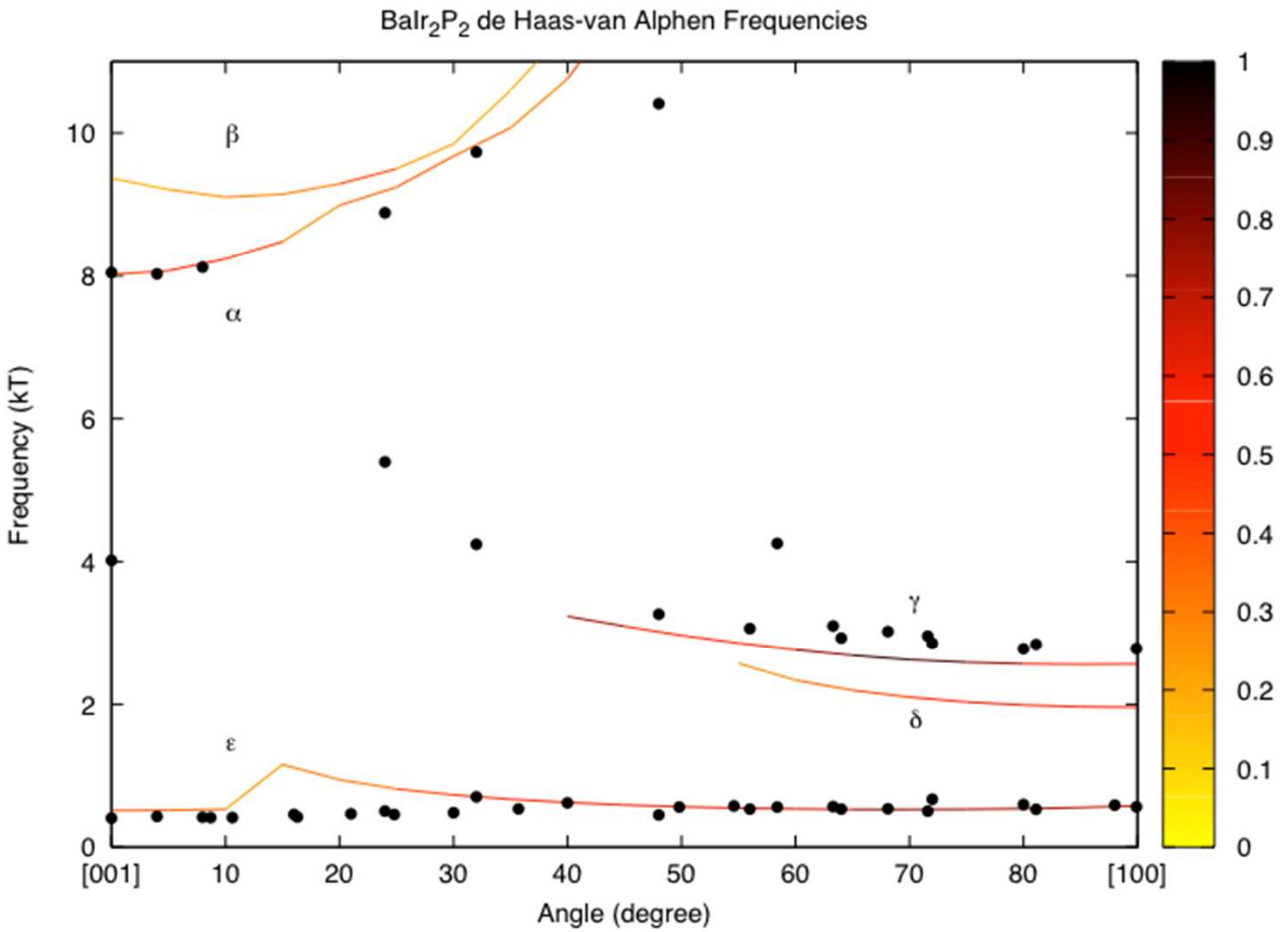
α=

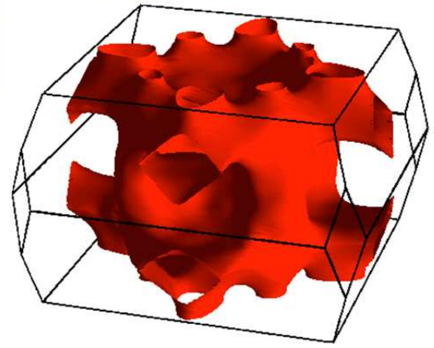
β=

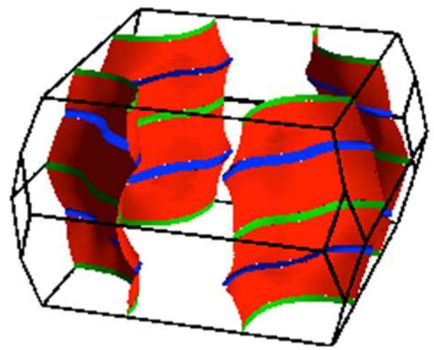
γ= not shown (first piece)

δ=

Results: $BaIr_2P_2$







α=

β=

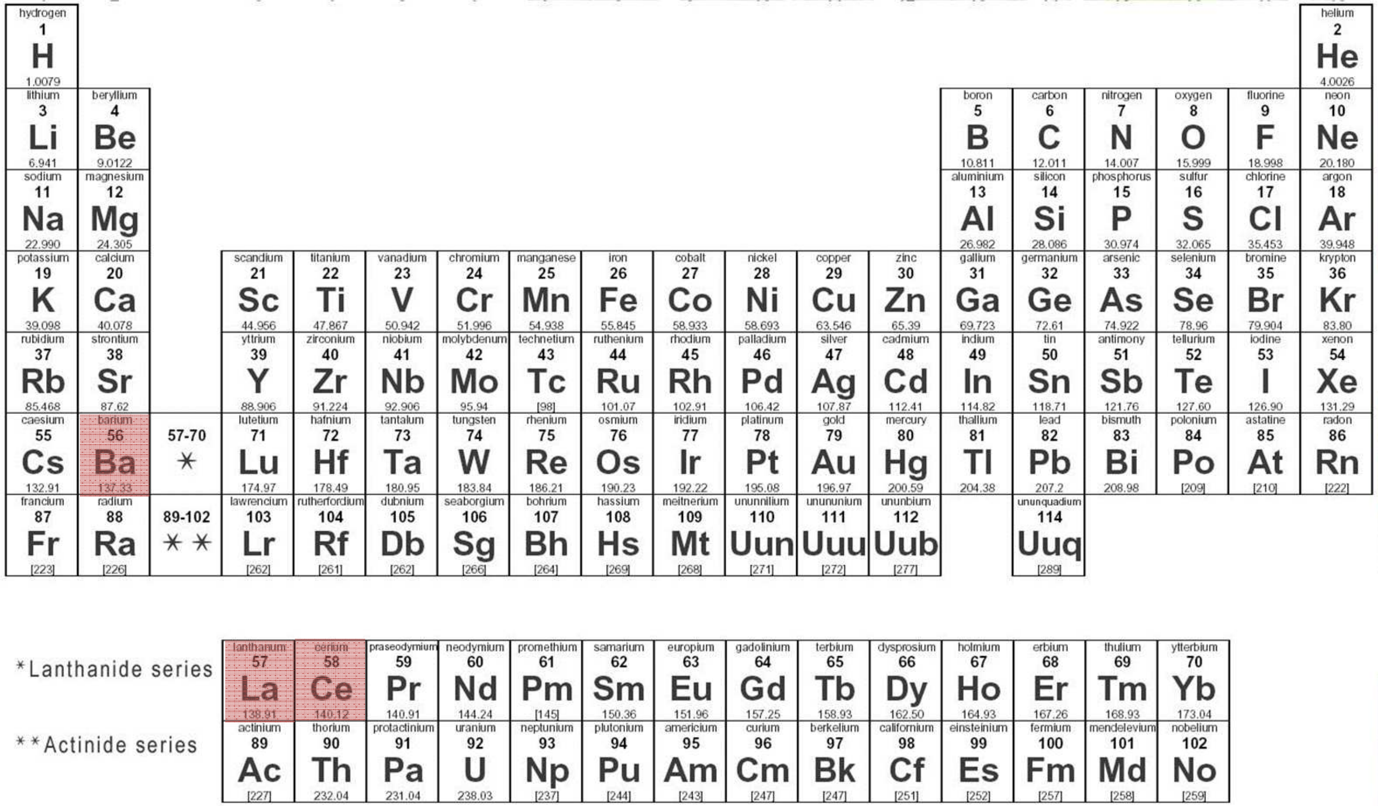
γ= not shown (first piece)

δ= not shown (first piece)

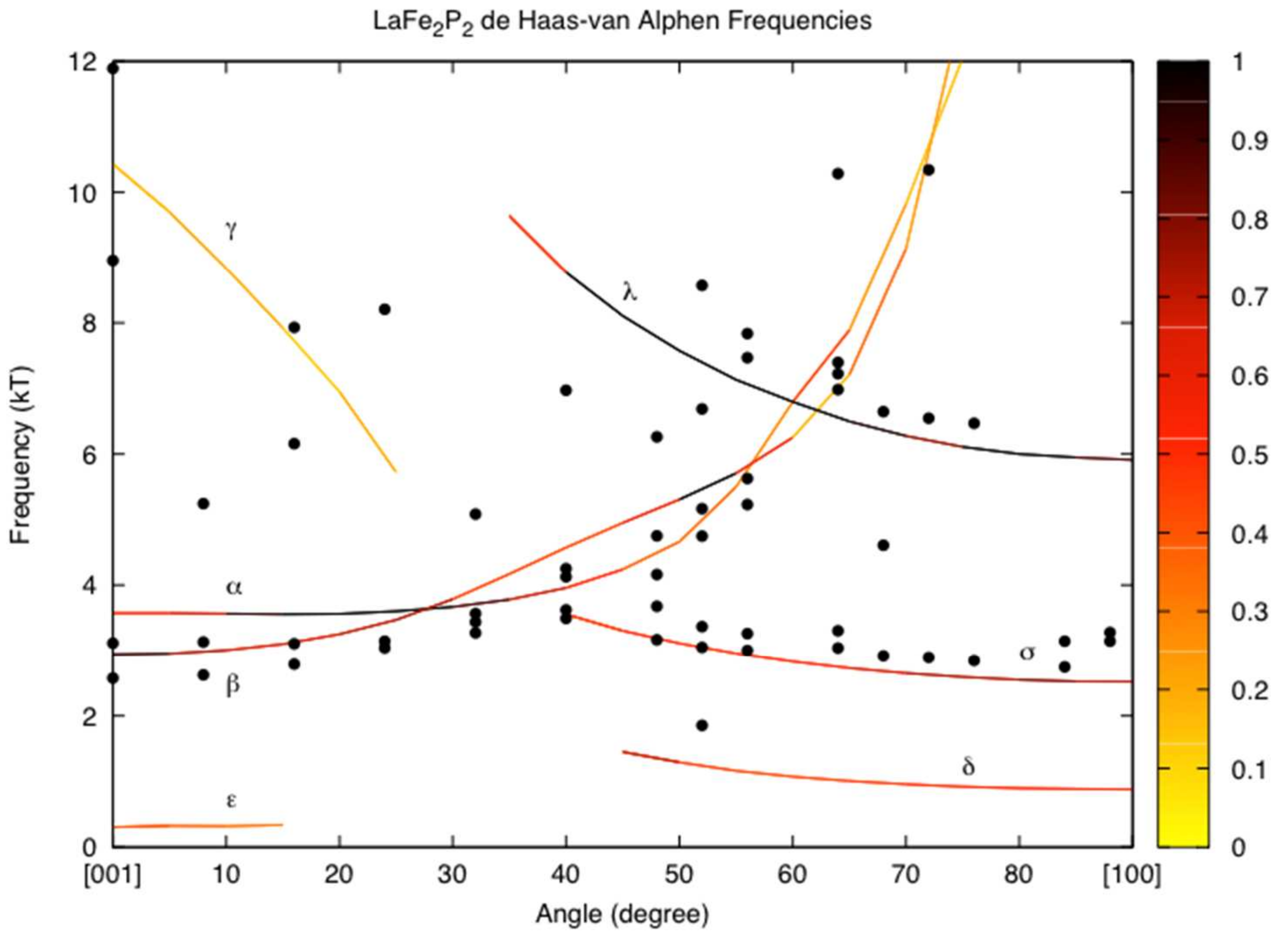
ε= not shown (first piece)

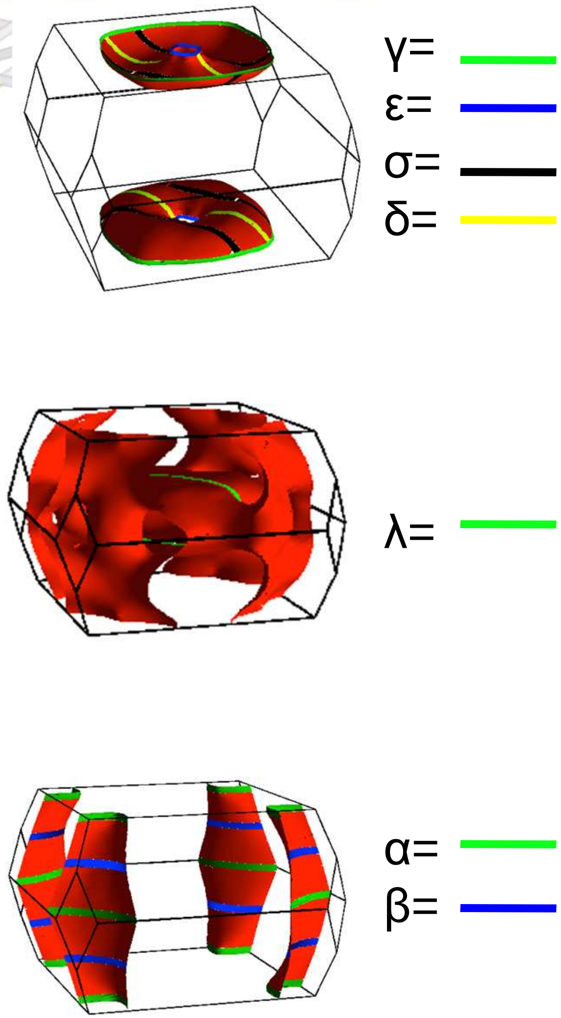
$LaFe_2P_2$ and $CeFe_2P_2$

- Changing the rare earth

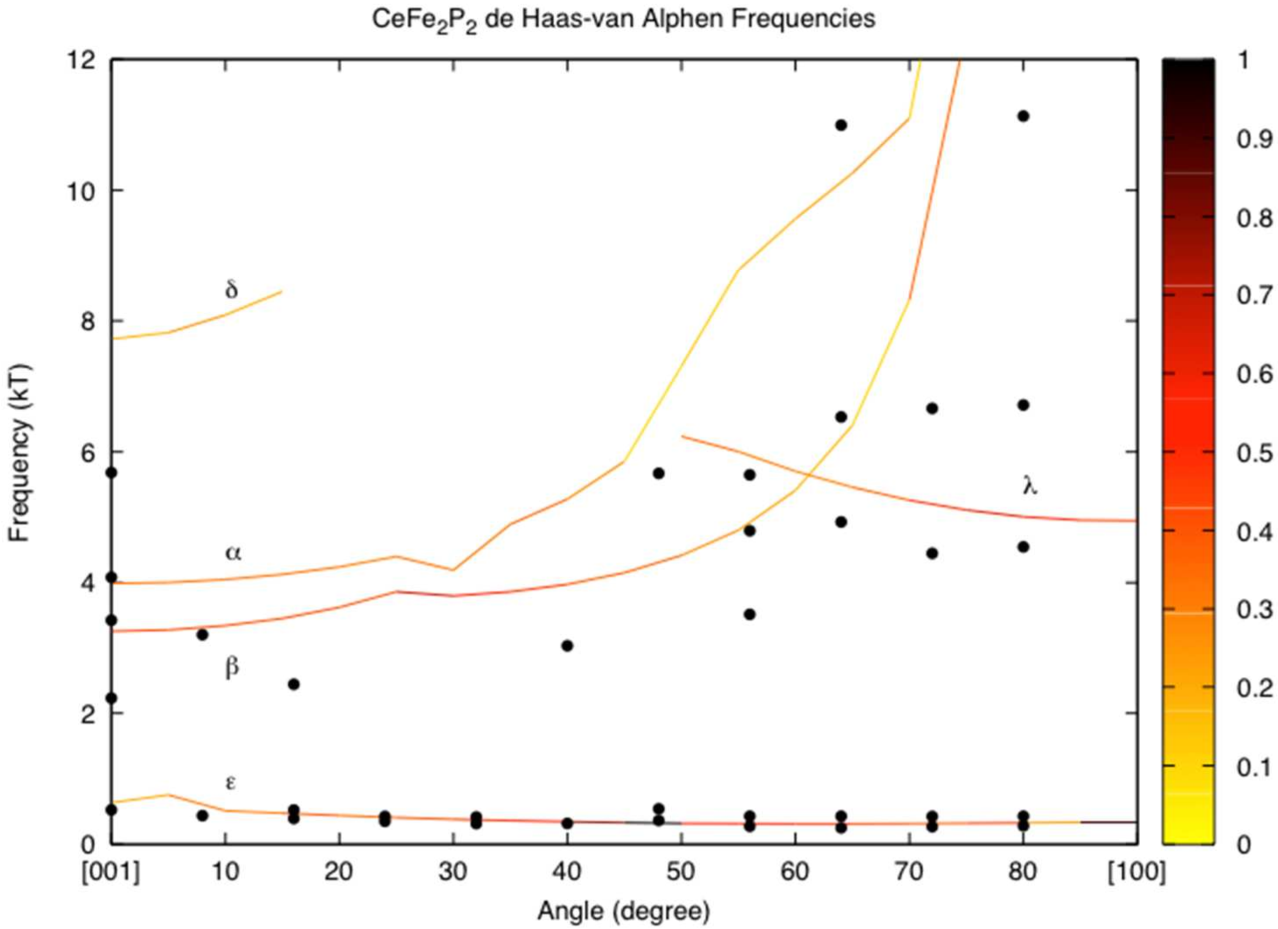


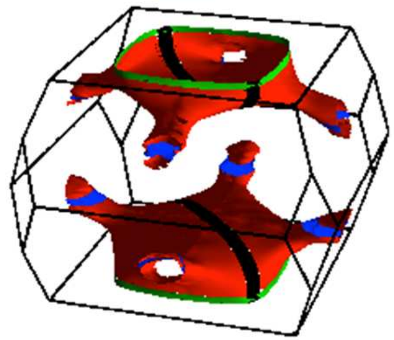
Results: $LaFe_2P_2$

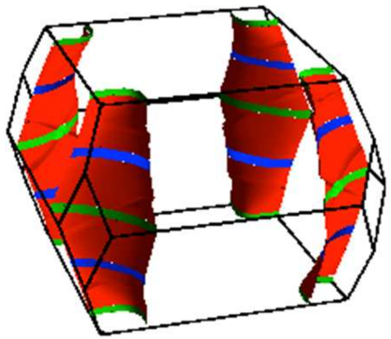




Results: $CeFe_2P_2$





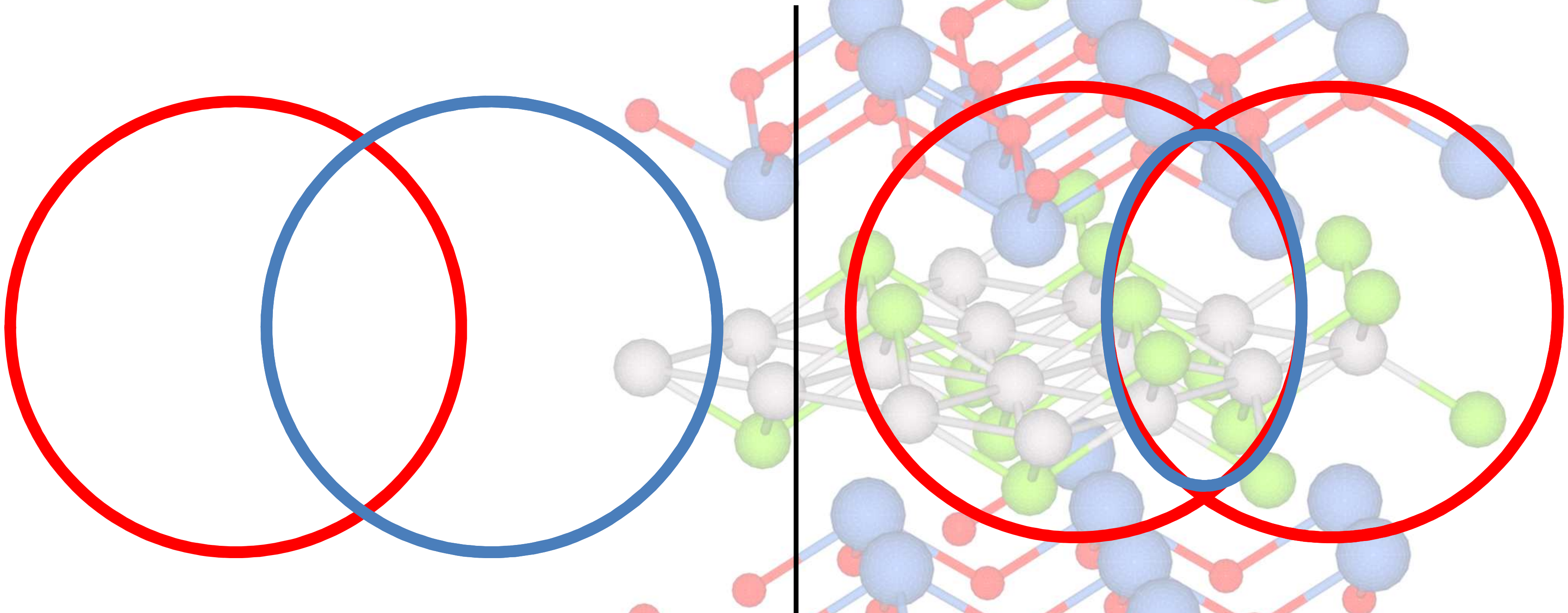


Plan

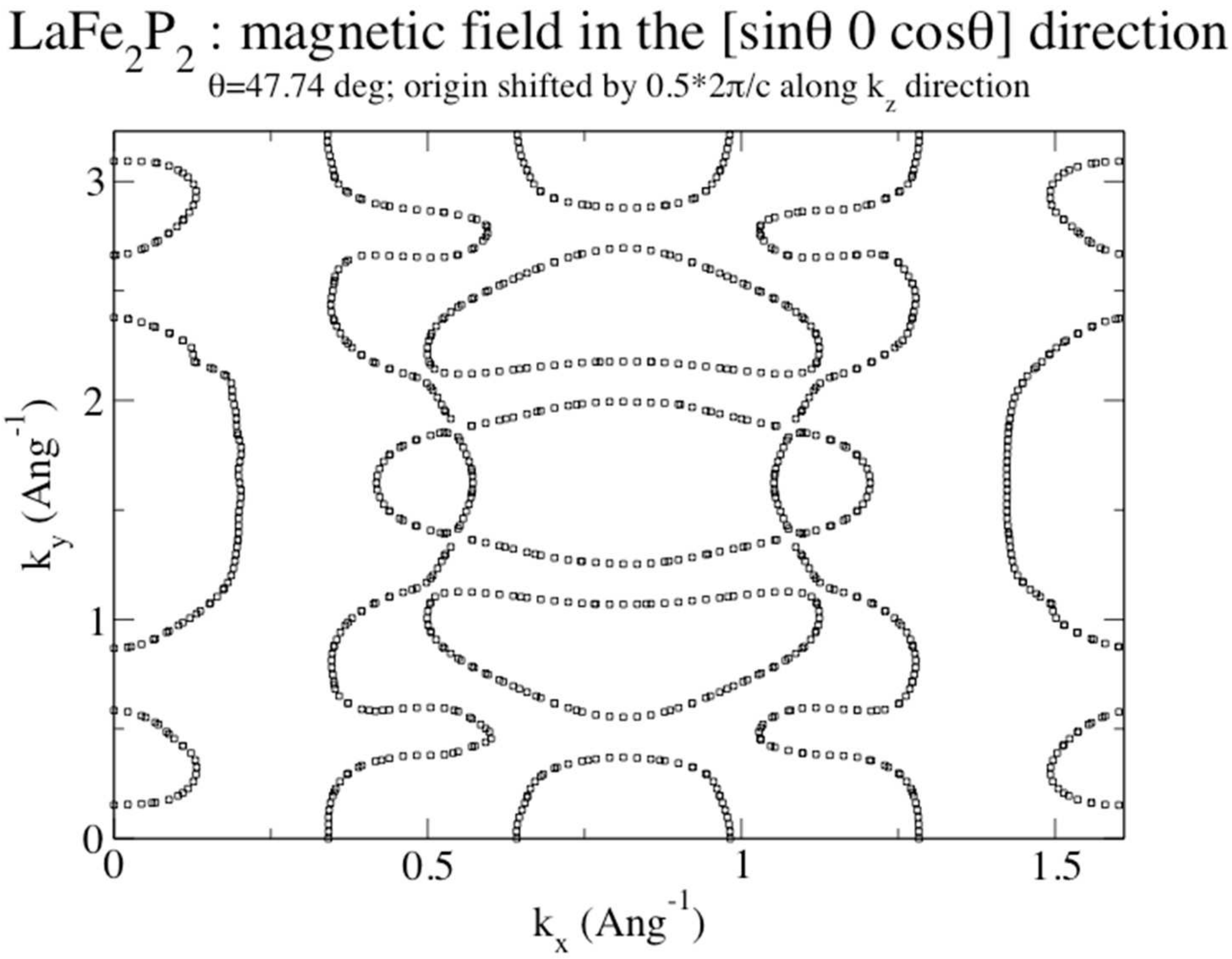
- Reminder of the theory
- MLWF
- Code explanation
- Iron pnictides superconductors
- Results
- Magnetic Breakdown

Magnetic Breakdown

- When 2 pieces of the FS are close, the orbit can change

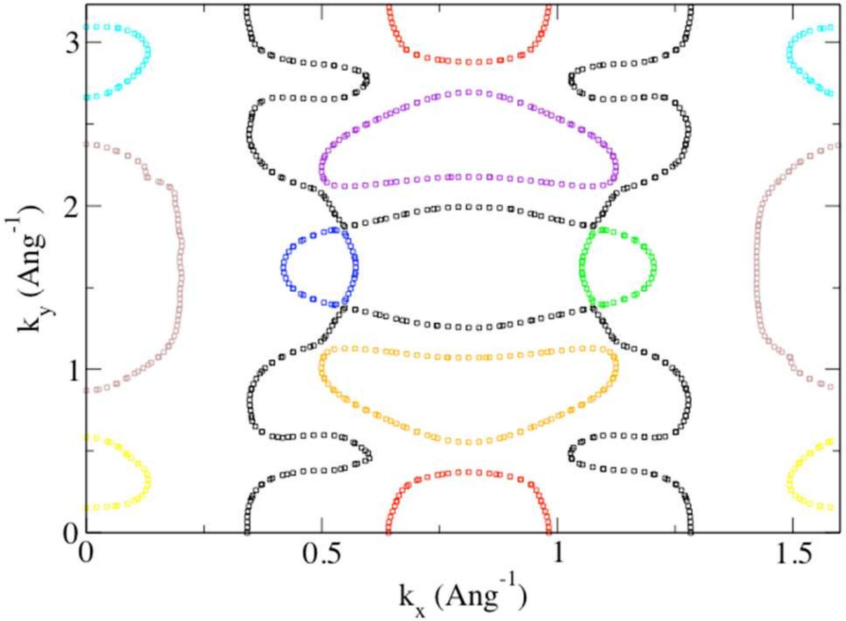


Example of MB



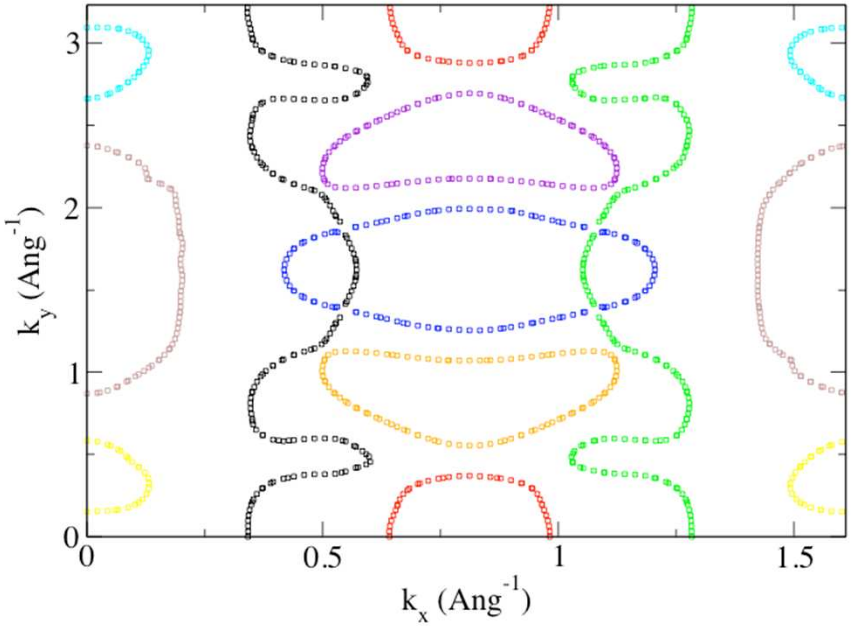
Is this possible?

$LaFe_2P_2$: magnetic field in the [sinθ 0 cosθ] direction
θ=47.74 deg; origin shifted by c/a along k_z direction



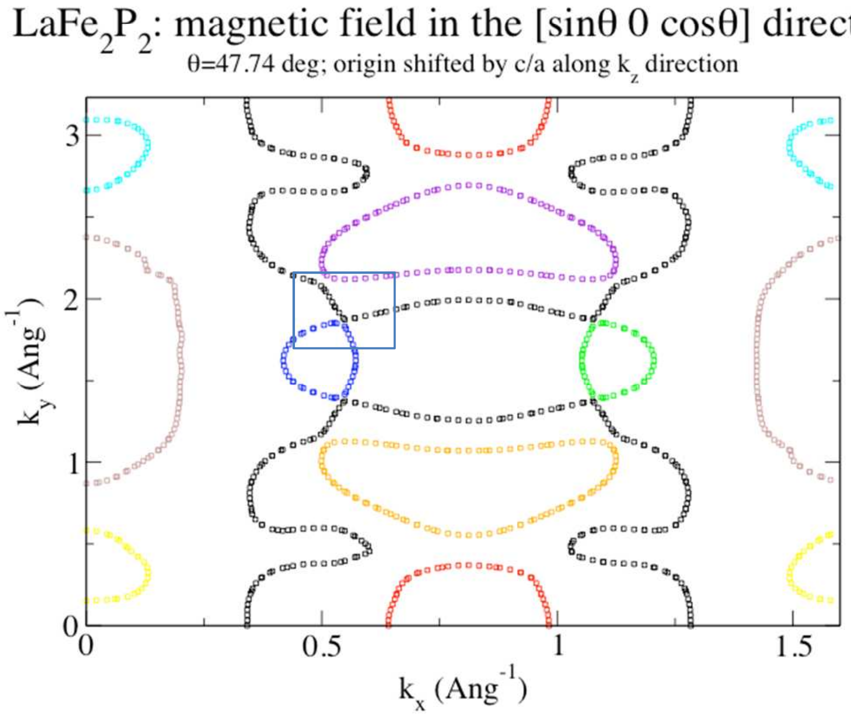
Normal connection

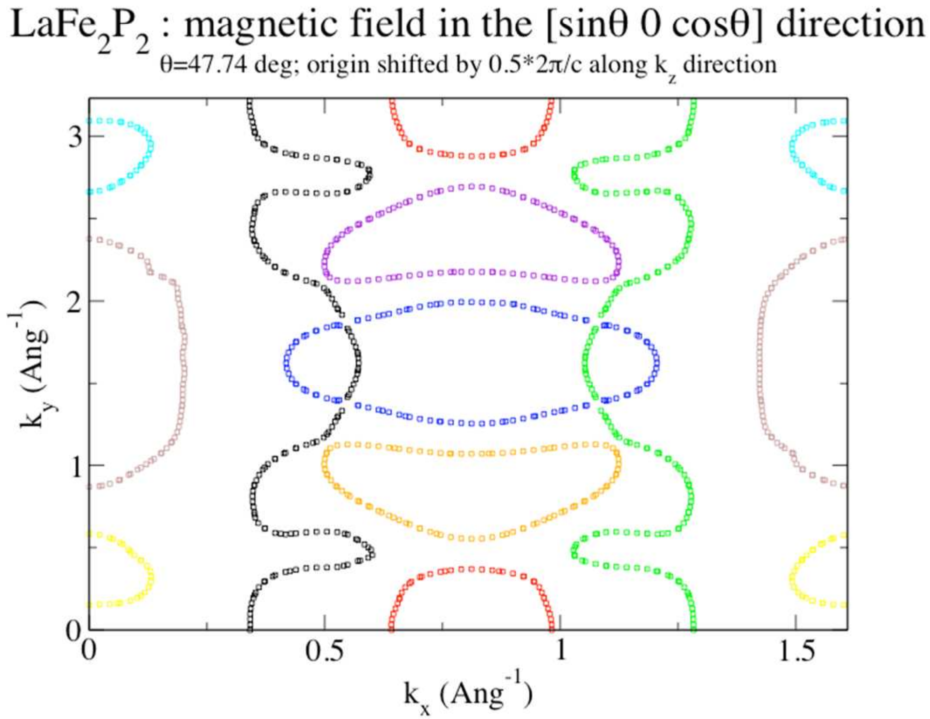
$LaFe_2P_2$: magnetic field in the [sinθ 0 cosθ] direction
θ=47.74 deg; origin shifted by 0.5*2π/c along k_z direction



Continuous orbit

Is this possible?

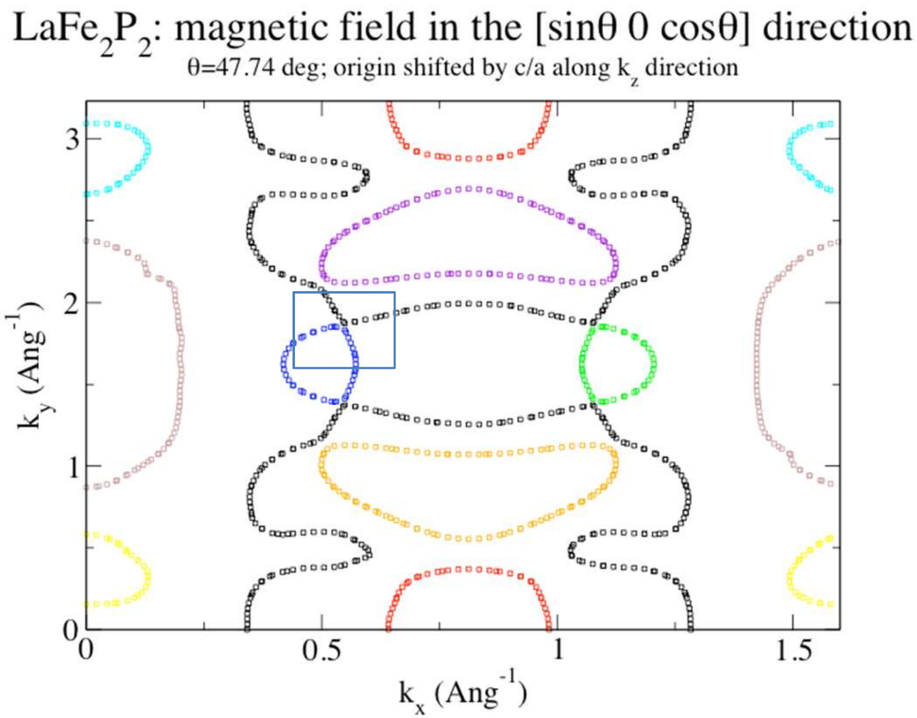




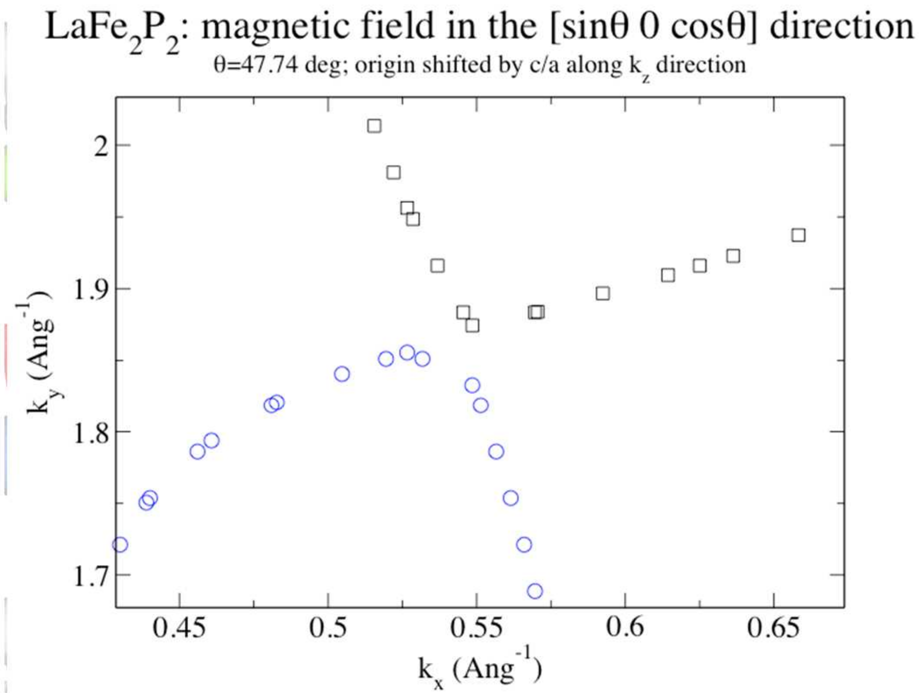
Normal connection

Continuous orbit

Is this possible?

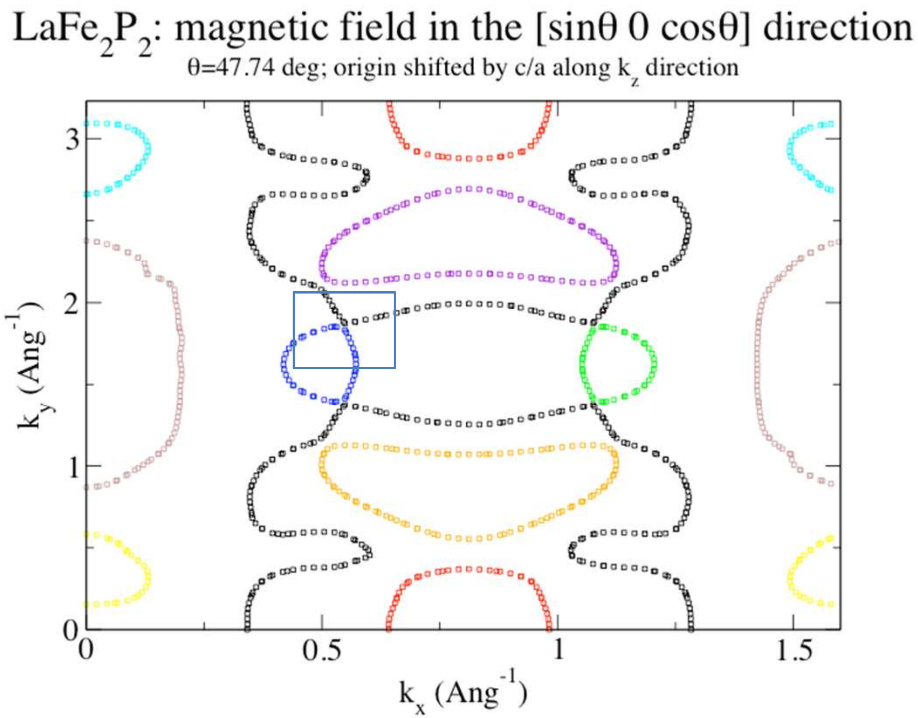


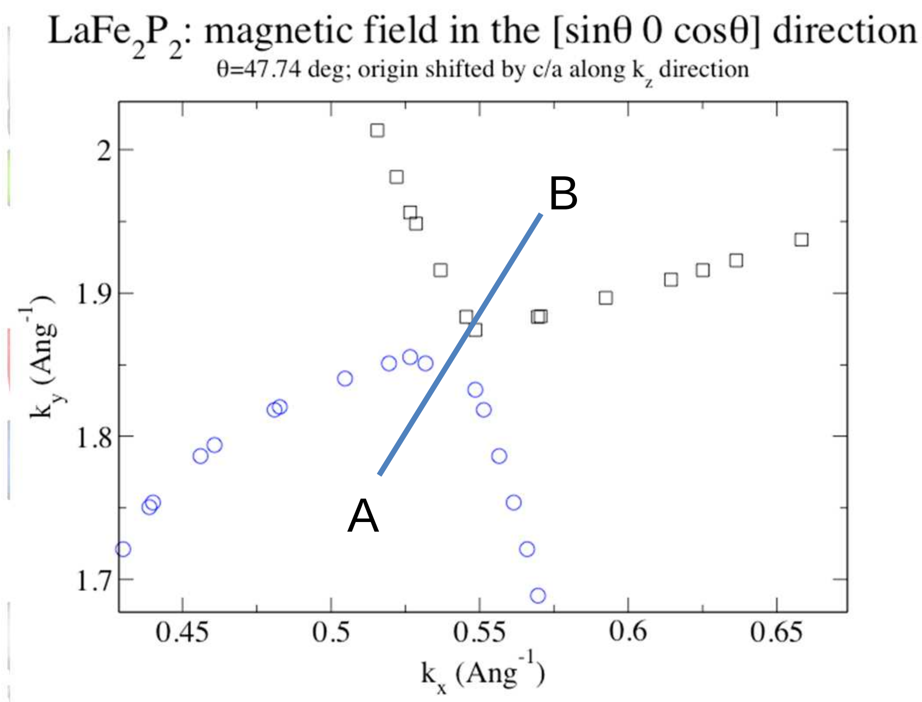
Normal connection



Zoom near the crossing

Is this possible?

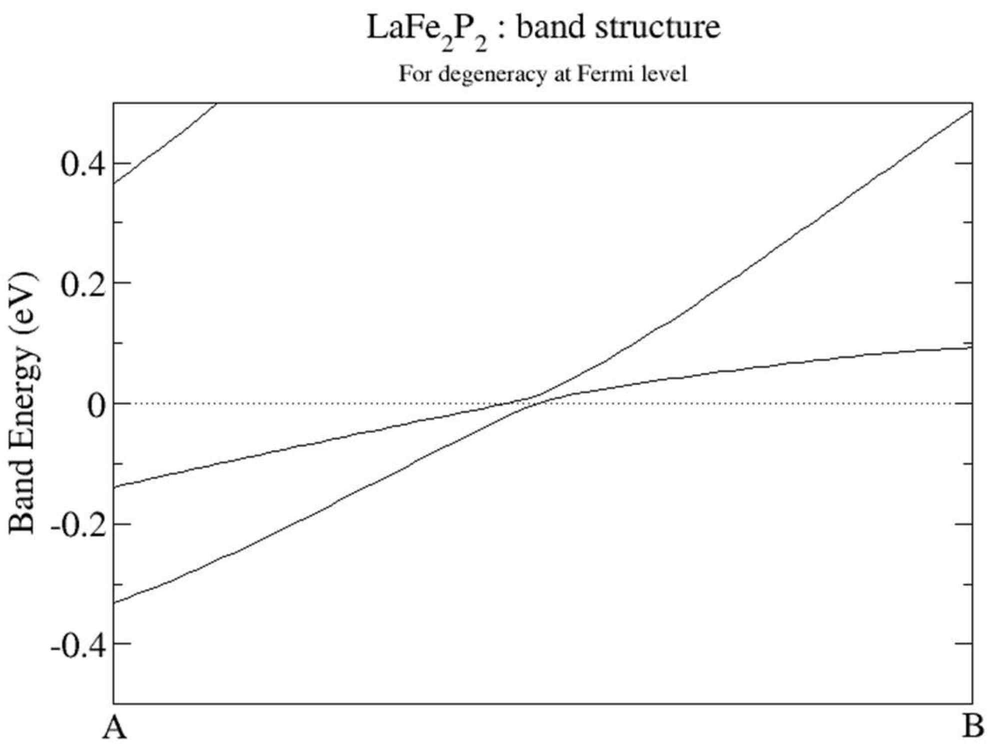




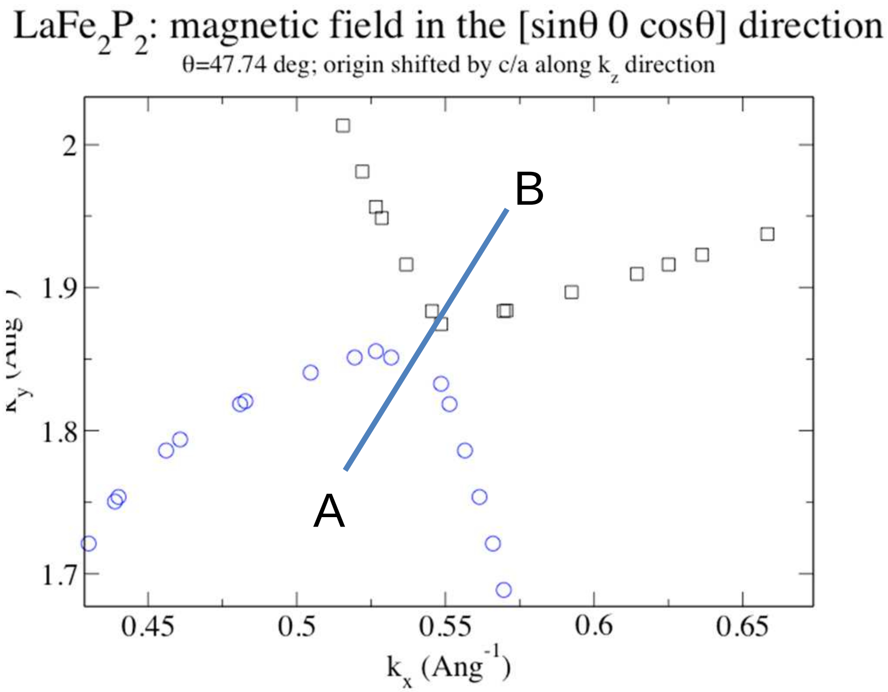
Normal connection

Zoom near the crossing

Is this possible?



Band structure near the crossing



Zoom near the crossing

Conclusion

- We presented a novel way of calculating dHvA frequencies using maximally localized Wannier function
  - Accurate
  - Low computational cost
- Results for various iron pnictides: LaFe2P2, CeFe2P2, BaRh2P2, BaIr2P2
- If 2 (or more) bands are almost degenerate at the Fermi level, the electron orbit is reconstruted (breakdown of the semi-classical equation of motion)

Acknowledgement

- Thanks to:
  - NSERC for financial support
  - RQCHP, CLUMEQ and Compute Canada for computational resources
- Collaborators (experimental part of the project):
  - Bobby Prévost, Andrea Bianchi (UdM)
  - Marek Bartkowiak (Paul Scherrer Institut-LDM, PSI, Switzerland)
  - Beate Bergk, Oleg Ignatchi, Jochen Wosnitza (Dresden High Magnetic Field Laboratory, Germany)
  - Gabriel Seyfarth (University of Geneva, Switzerland)
  - Cigdem Capan, Zachary Fisk (University of California Irvine, USA)