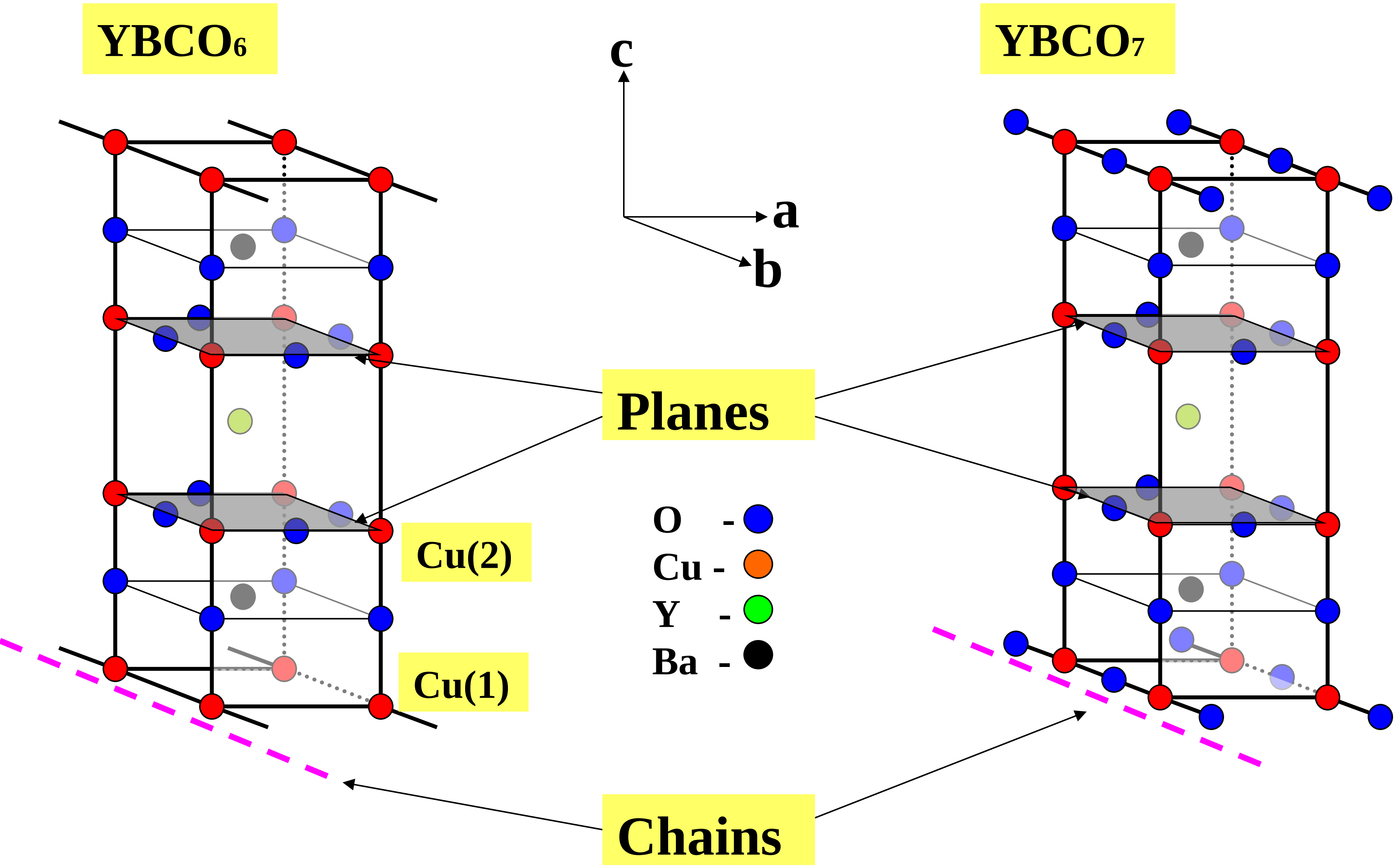
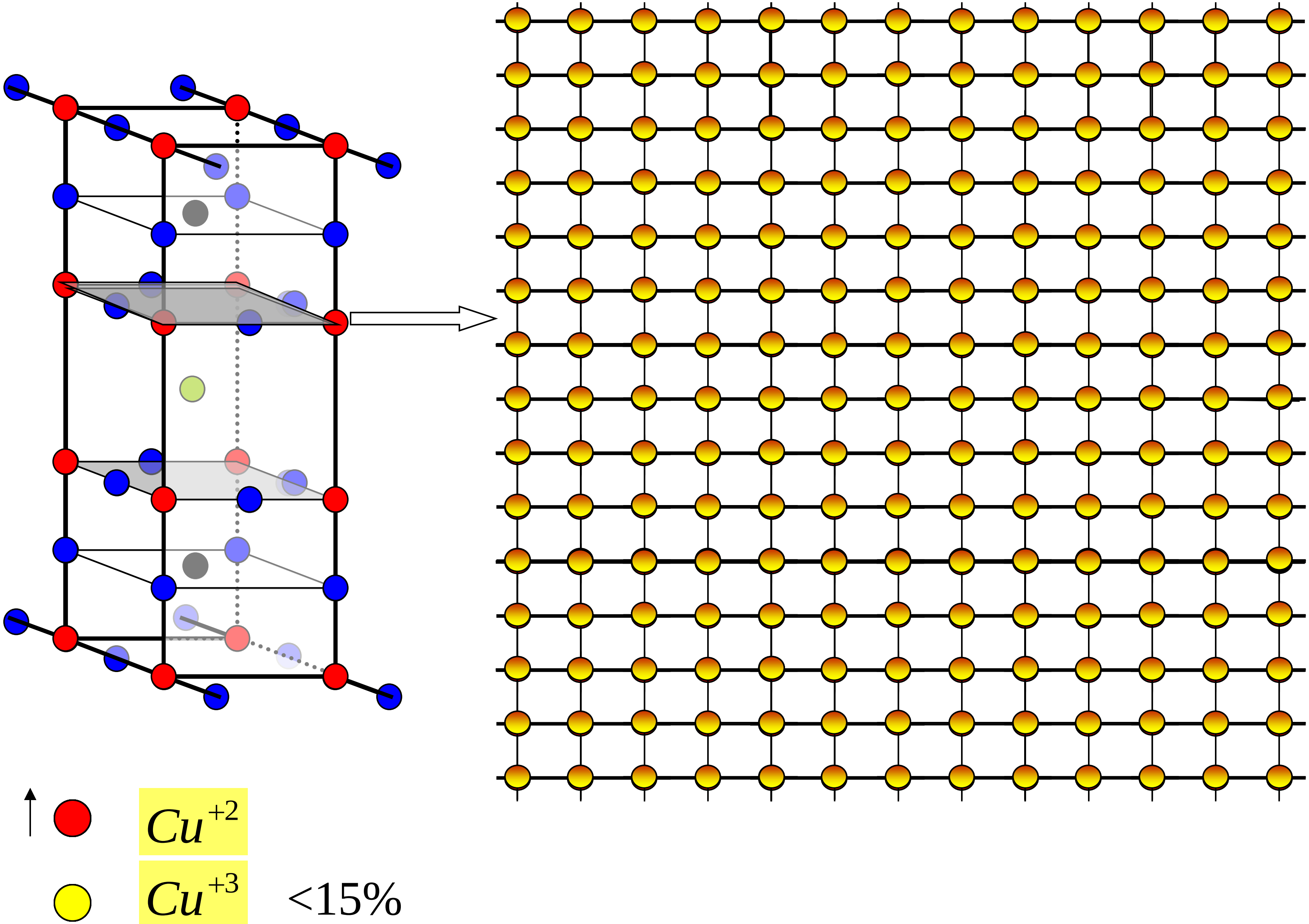
Development of a nuclear quadrupole based technique for measuring charge homogeneity, and its application for YBCO

Outline:

- What is charge homogeneity, and why is it interesting?
- Current experimental methods for measuring charge homogeneity, and their drawbacks.
- A new idea to tackle the problem.
- Experimental results
- Conclusions

$Y_1Ba_2Cu_3O_{7-\delta}$




Cu^{+2}
Cu^{+3}
<15%

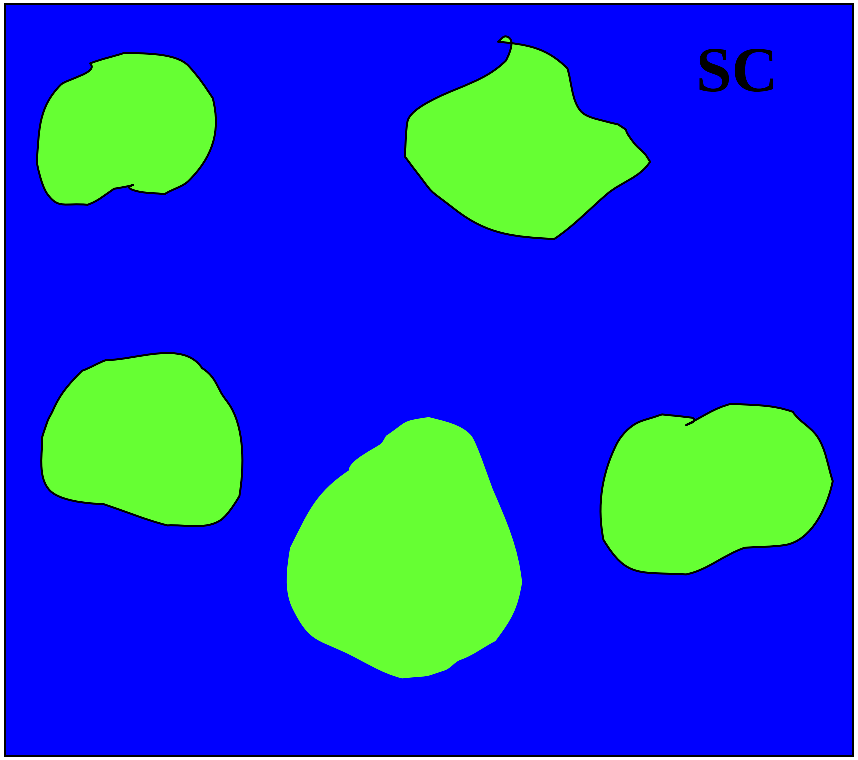
Motivation - Stripes

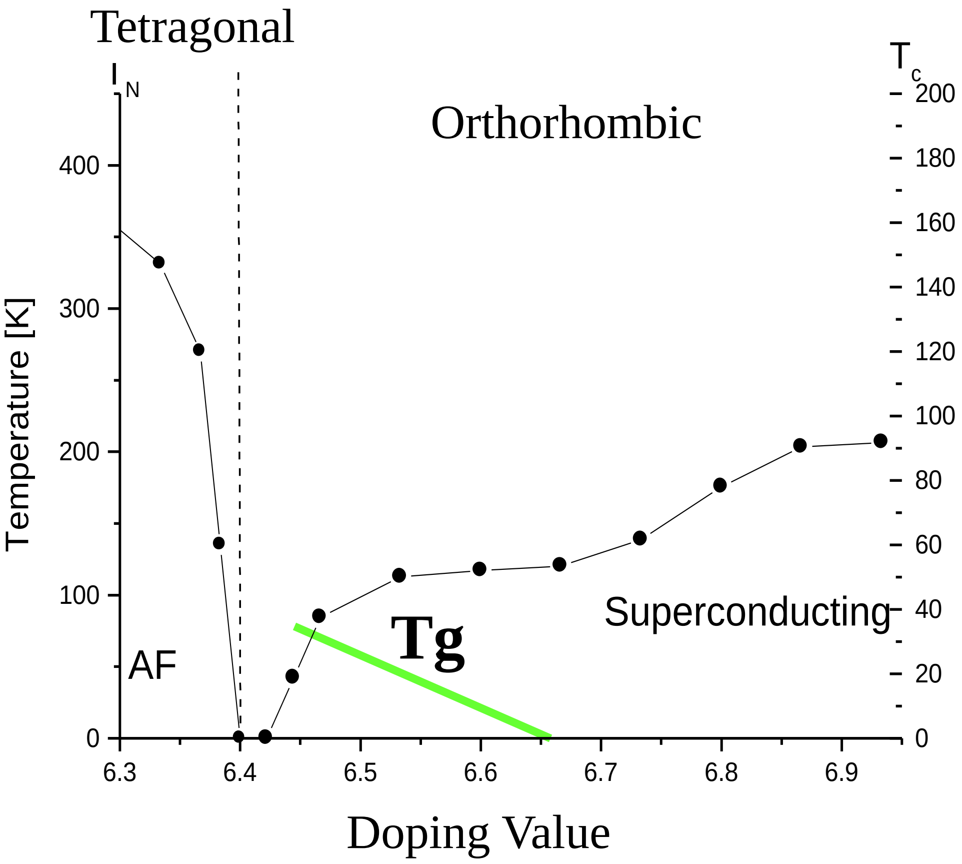
- The stripes theory claims that one dimensional charge structures in the planes play a crucial role in the mechanism of superconductivity.

- Higher doping $\Rightarrow$ more stripes $\Rightarrow$ inhomogeneity higher T_c

- There is **partial** experimental evidence for stripes.

Evidence for inhomogeneity using μSR





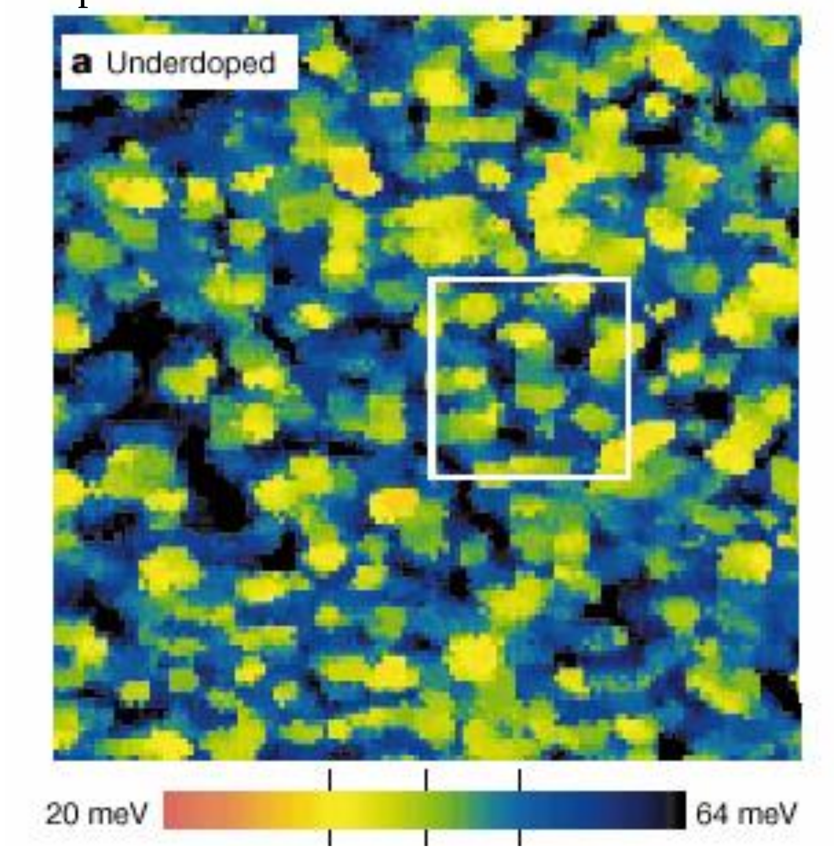
Low doping

- This result supports the presence of some magnetic structure (not necessarily in the form of stripes).
- Increasing the doping decreases the inhomogeneity.
- It looks as if the structure is a remainder of the AF phase.

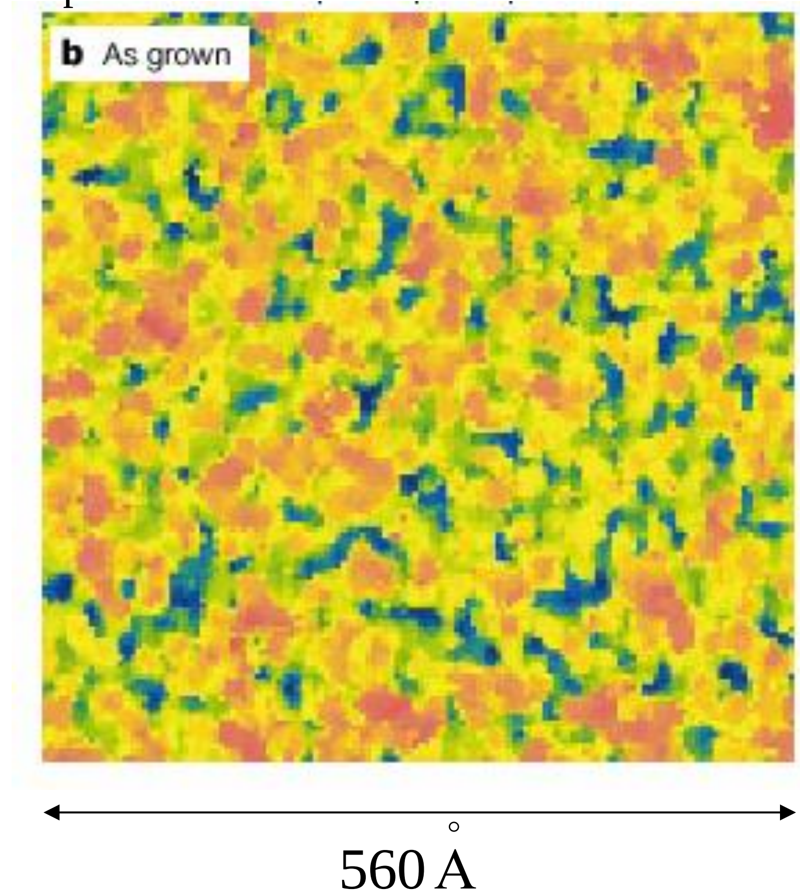
Evidence for inhomogeneity using STM

$Bi_2Sr_2CaCu_2O_{8+\delta}$

p≈0.14±0.02



p≈0.18±0.02



K.M.Lang *et al*, Nature, **415**, 412 (2002)

Surface

Summary of the introduction

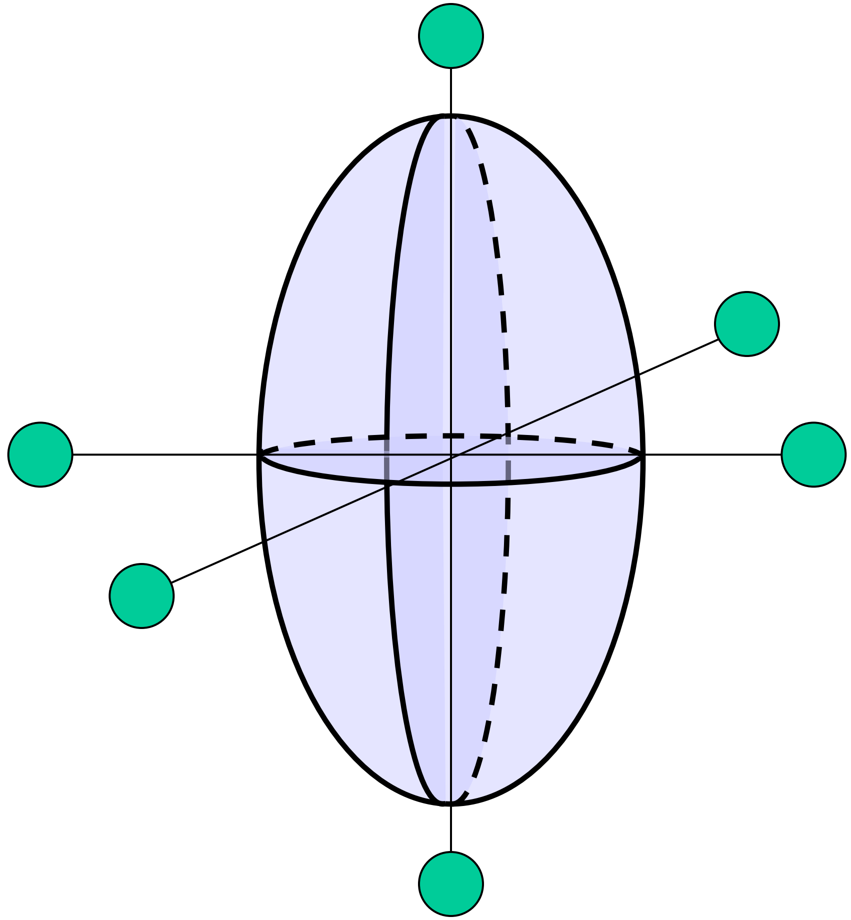
- Some theories are based on structures in the planes.
- There is **incomplete** experimental evidence for such structures.

Solution

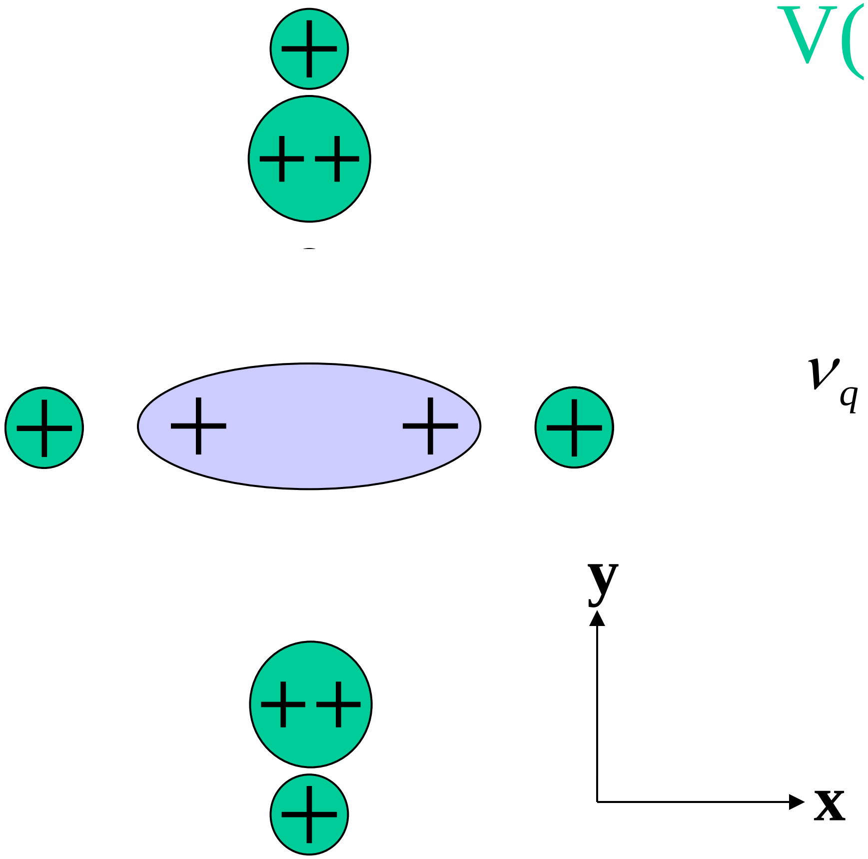
A new technique, based on the nuclear quadrupole interaction.

Outline:

- ✓ Motivation: what is charge homogeneity, and why is it interesting?
- ✓ What is the experimental evidence for homogeneity , and what are the drawbacks?
- Our new idea how to deal with this problem.
- Results
- Conclusions



Electric quadrupole interaction



$$V(\mathbf{r}) \Longrightarrow V_{ij} = \frac{\partial^2 V}{\partial r_i \partial r_j}$$

$$V_{xx} + V_{yy} + V_{zz} = 0$$

$$\nu_q \propto V_{zz} \qquad \eta = \frac{V_{xx} - V_{yy}}{V_{zz}} \Rightarrow 0 \le |\eta| \le 1$$

$$V_{ij} = \nu_q \begin{bmatrix} -\frac{1-\eta}{2} & 0 & 0 \\ 0 & -\frac{1+\eta}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\Downarrow$$

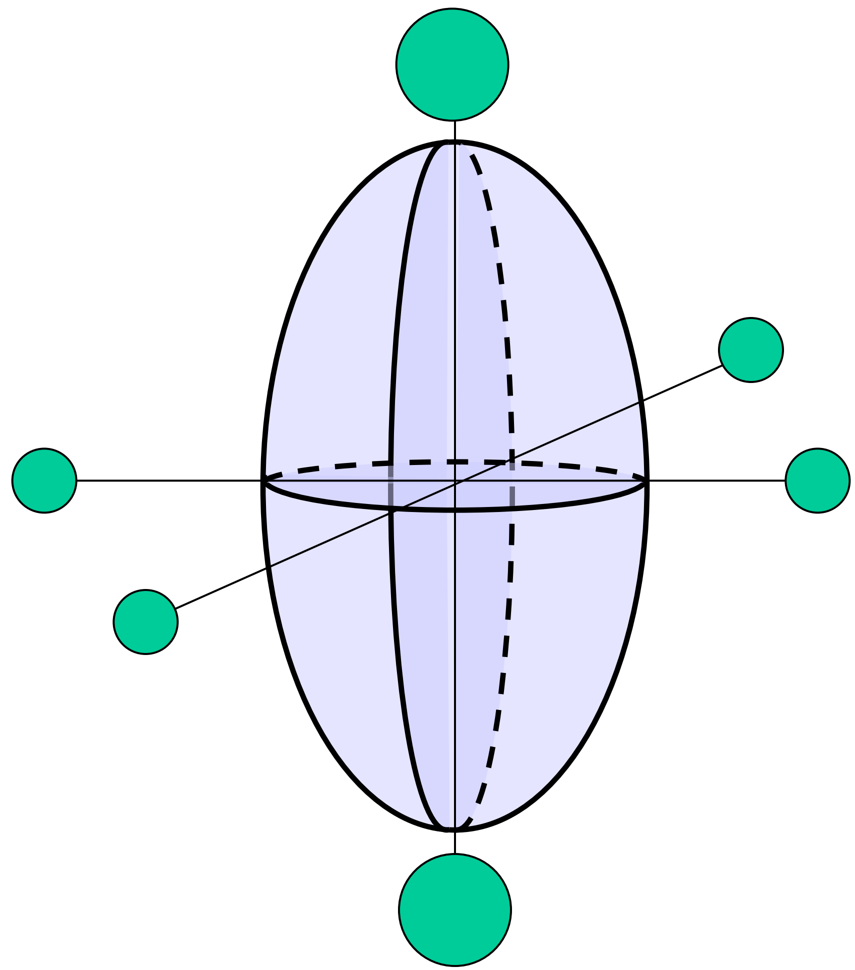
Nucleus $I_x^2 \quad I_y^2 \quad I_z^2$ $\Longrightarrow$

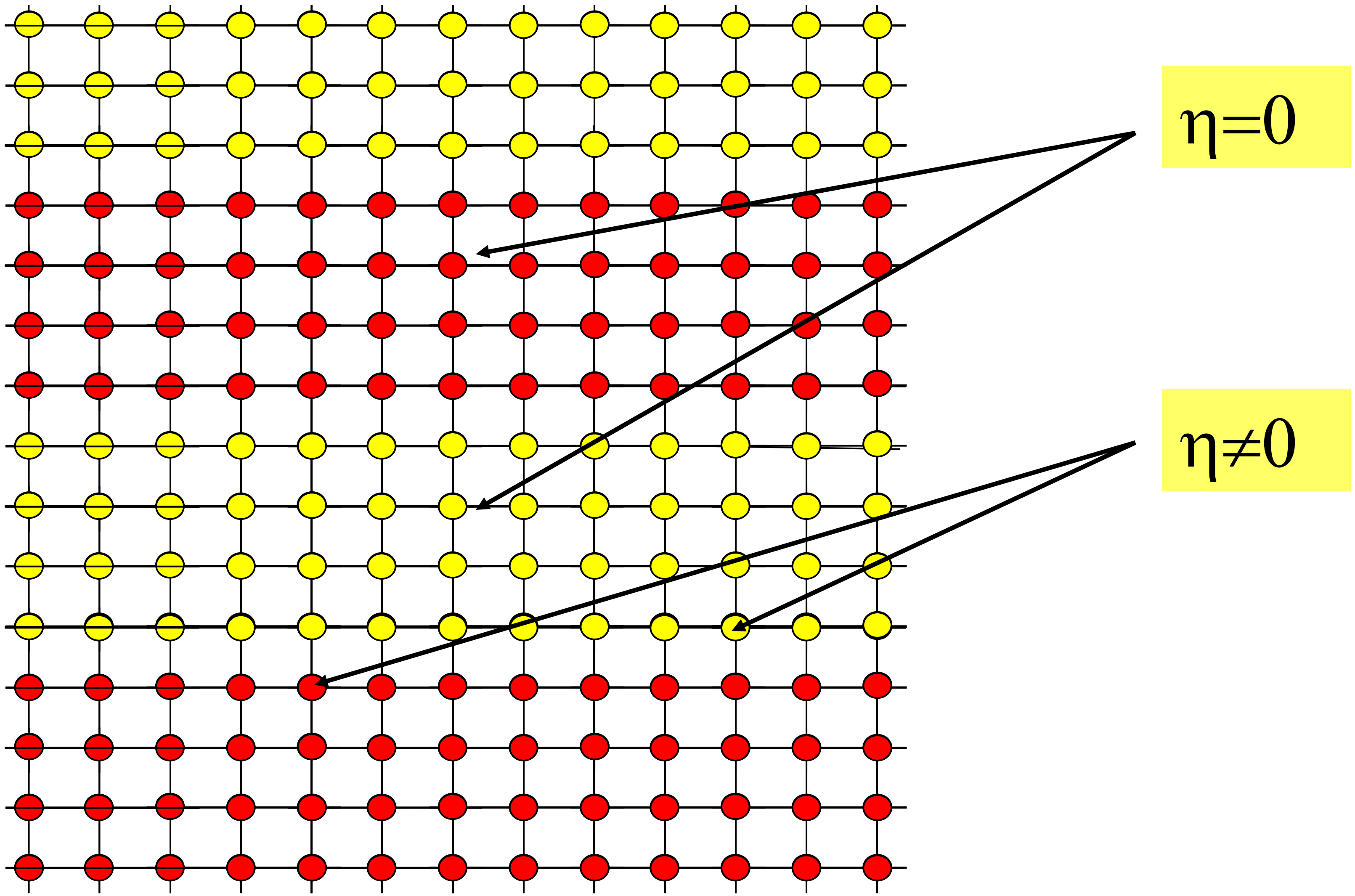
$$\hat{H}_q = \frac{\hbar \nu_q}{6}\left[3\hat{I}_z^2 - \hat{I}^2 + \eta(\hat{I}_x^2 - \hat{I}_y^2)\right]$$

- The quadrupole interaction is sensitive to the symmetry of the charge distribution, and can be a useful tool for our purpose.
- η determines the homogeneity of the charge distribution:

  $\eta=0$ – Homogenous charge distribution

  $\eta=1$ – Inhomogenous charge distribution



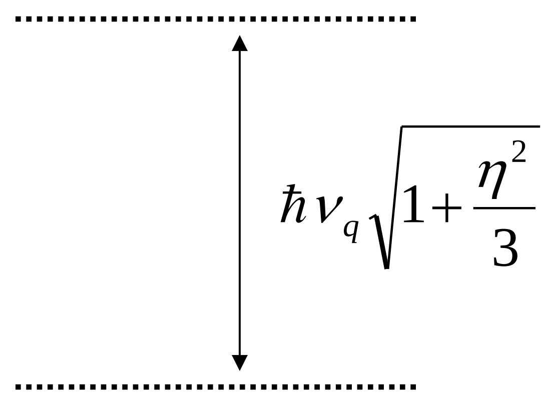


η=0
η≠0

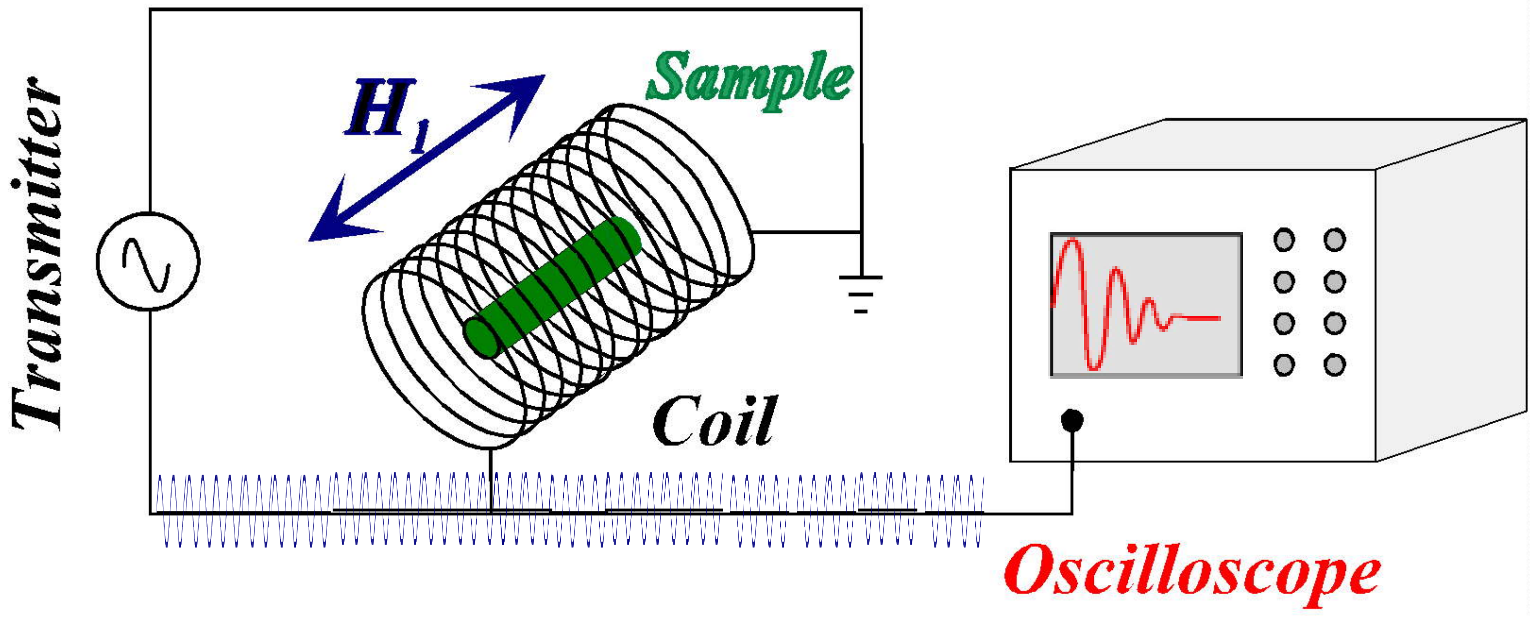
The NQR Hamiltonian for spin 3/2

$$\hat{H}_q = \frac{\hbar \nu_q \sqrt{3}}{6} \begin{bmatrix} \sqrt{3} & 0 & \eta & 0 \\ 0 & -\sqrt{3} & 0 & \eta \\ \eta & 0 & -\sqrt{3} & 0 \\ 0 & \eta & 0 & \sqrt{3} \end{bmatrix}$$

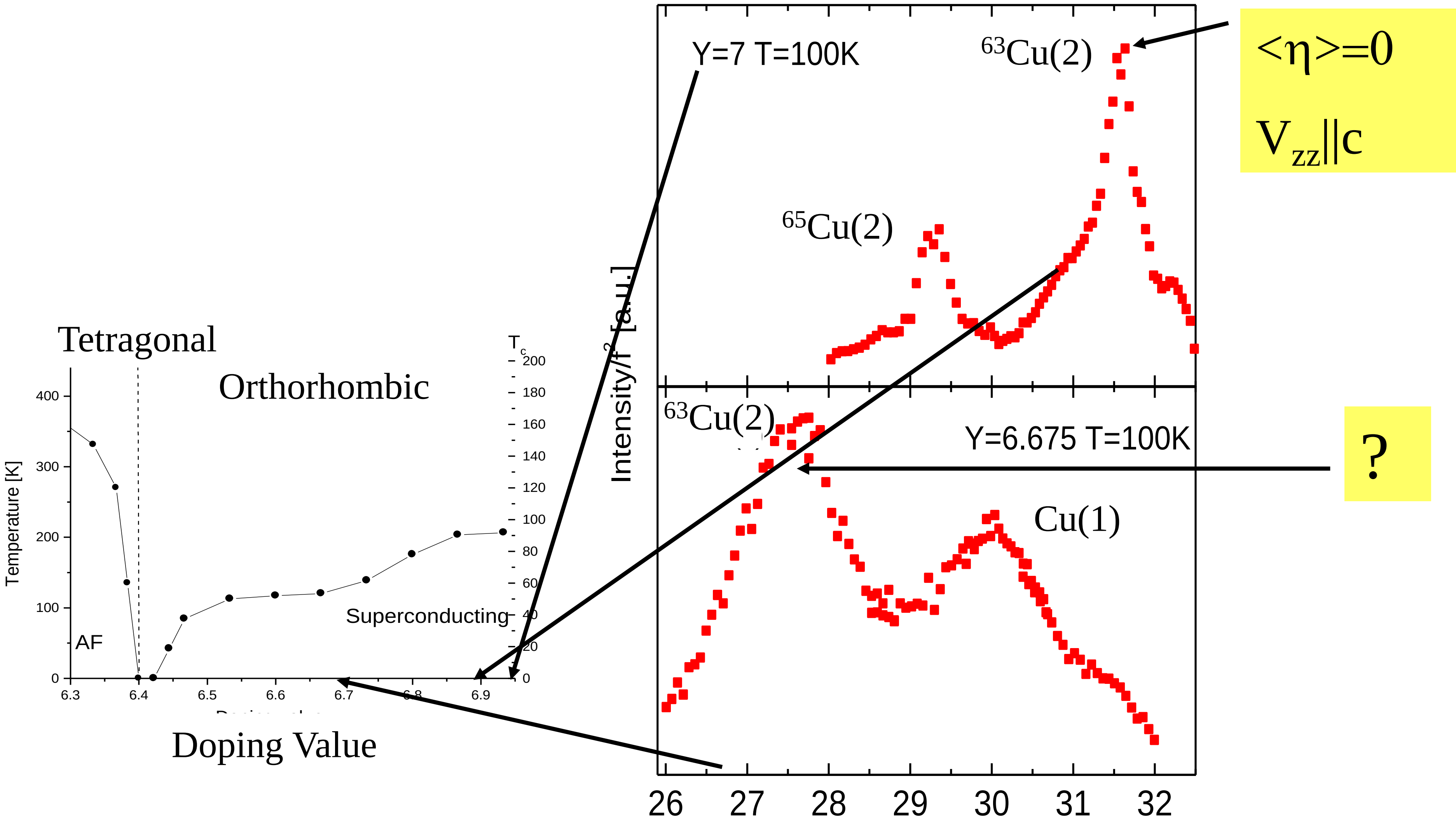
$$\hat{H}_q = \frac{\hbar \nu_q}{2} \sqrt{1 + \frac{\eta^2}{3}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$



NQR experimental setup

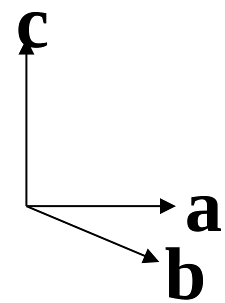


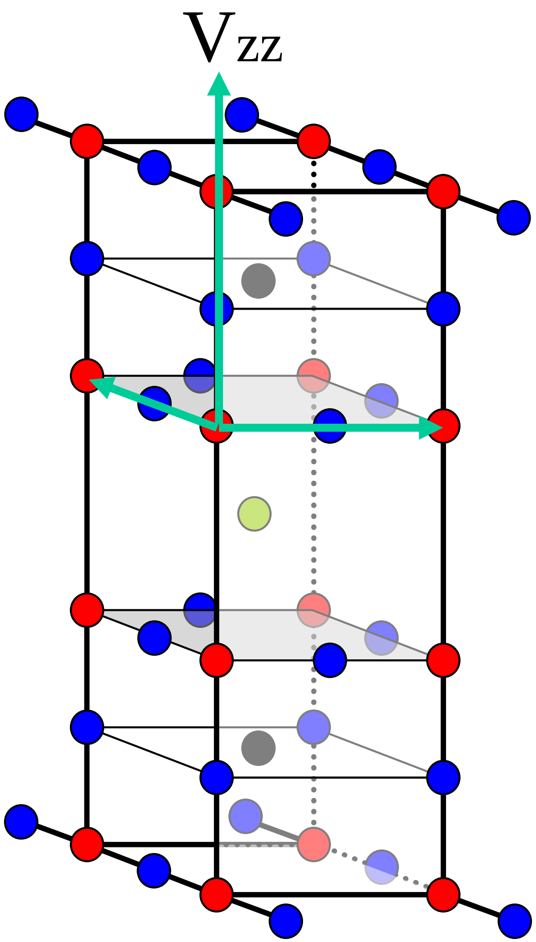
NQR Spectrum of YBCO

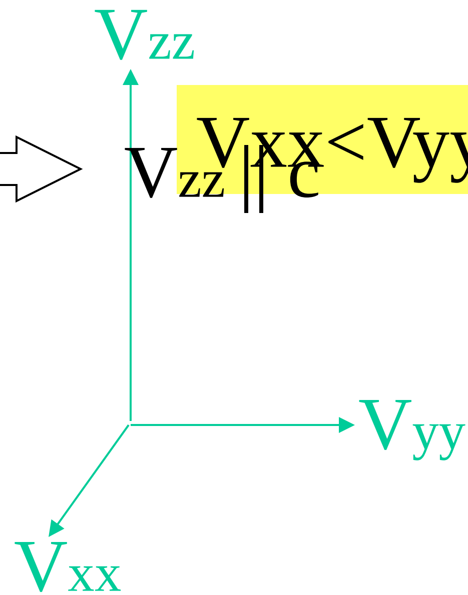


<η> is known only for optimal doping

The EFG tensor for Cu(2) in $YBCO_7$



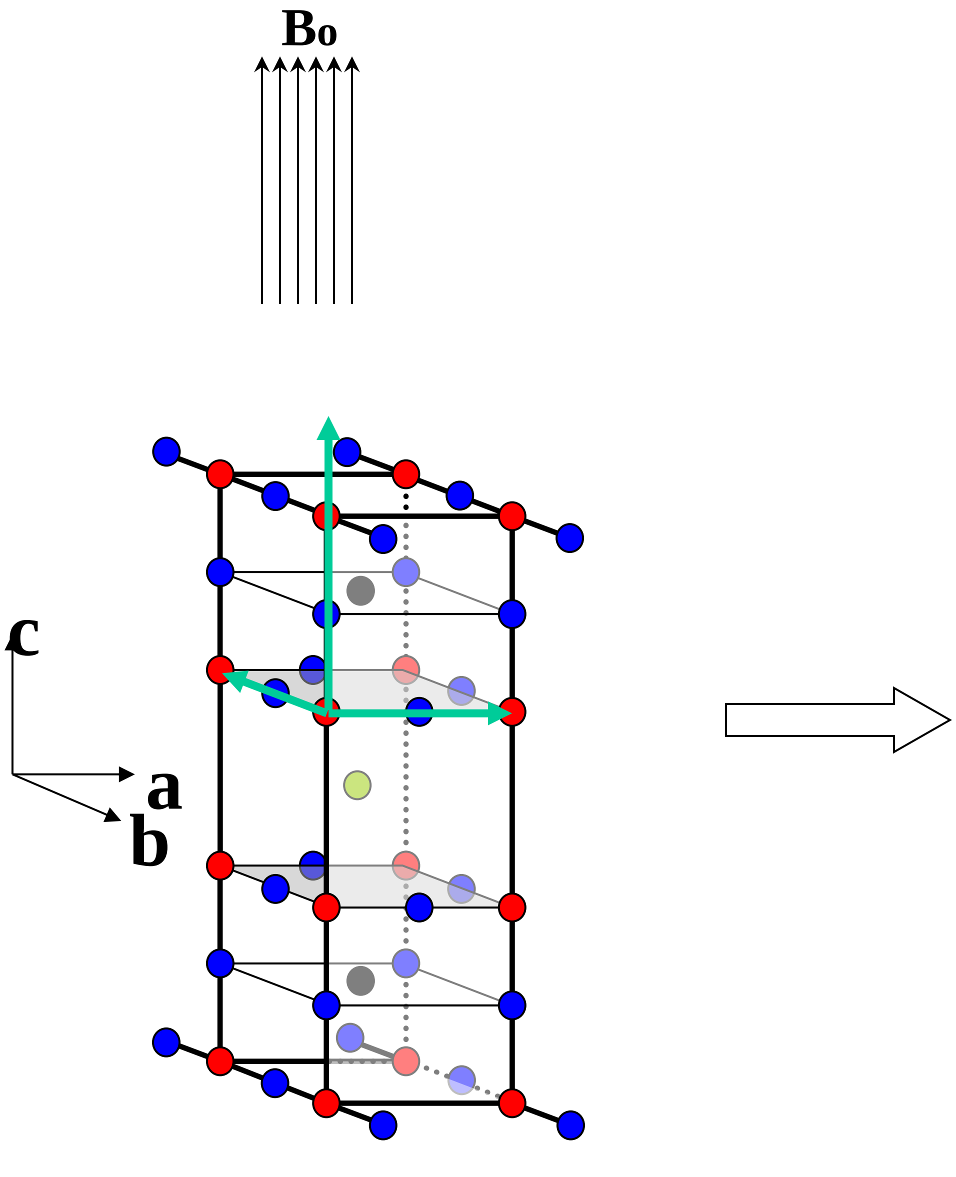




$V_{xx}<V_{yy}<V_{zz}$

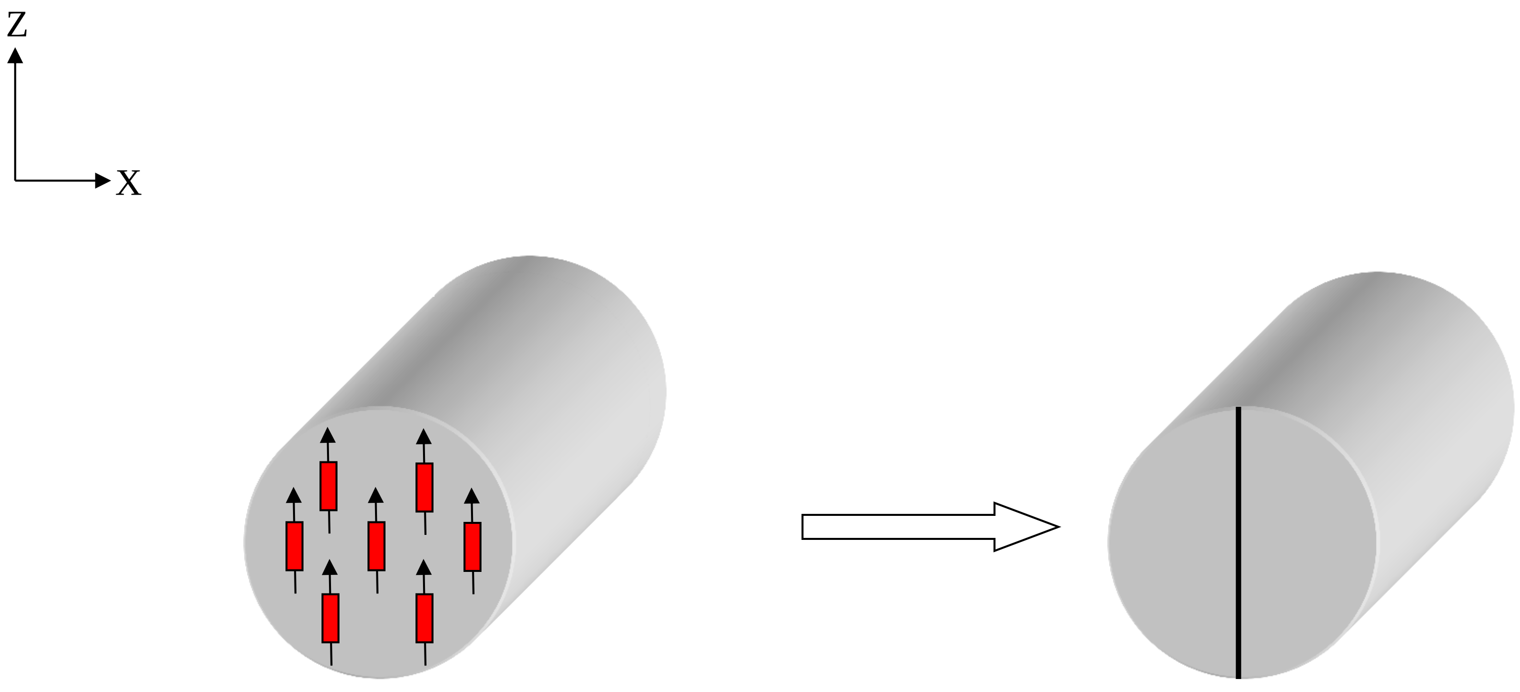
$V_{zz} \parallel c$

YBCO in a magnetic field



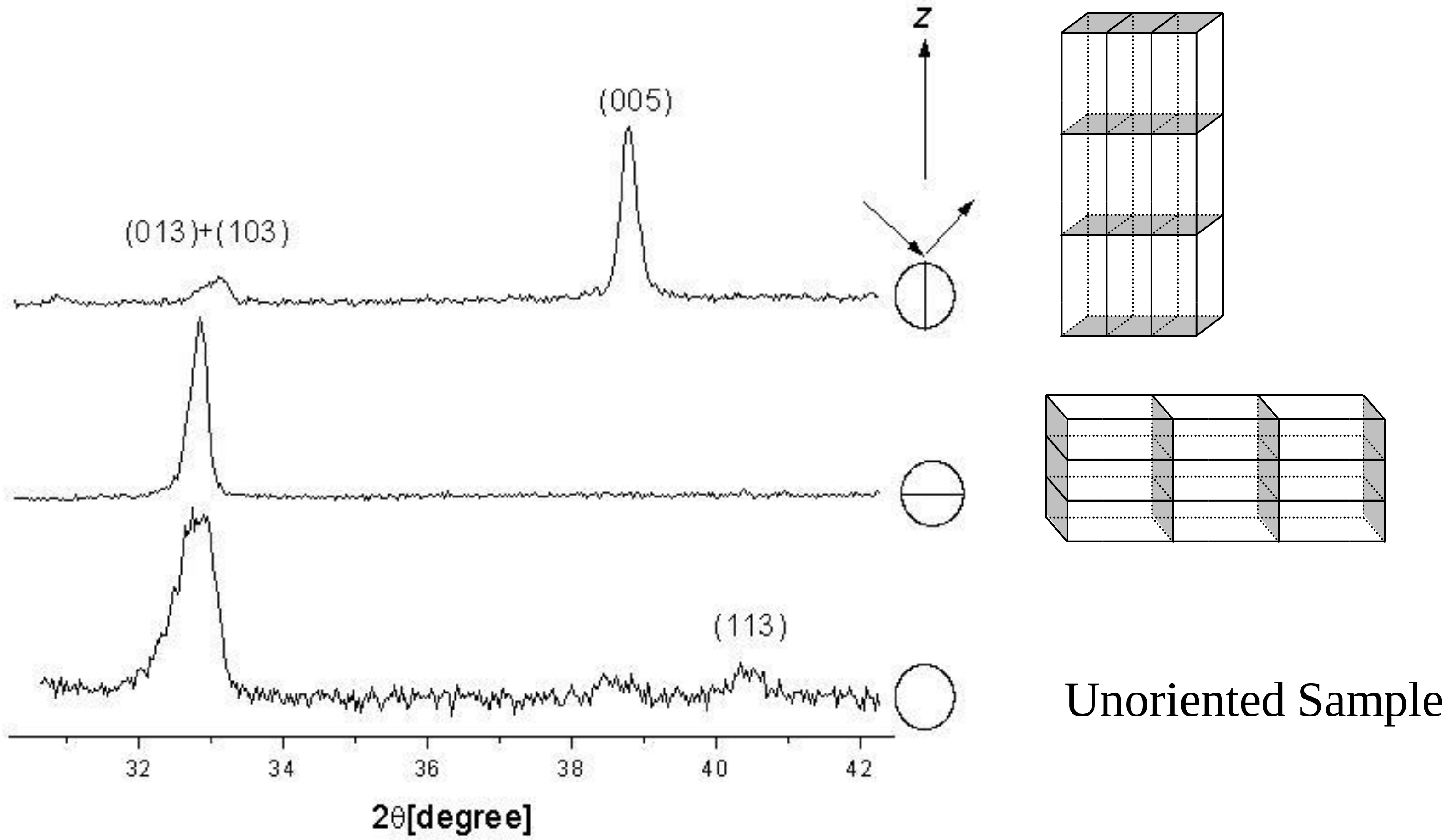
Bo || c || Vzz ≡ z

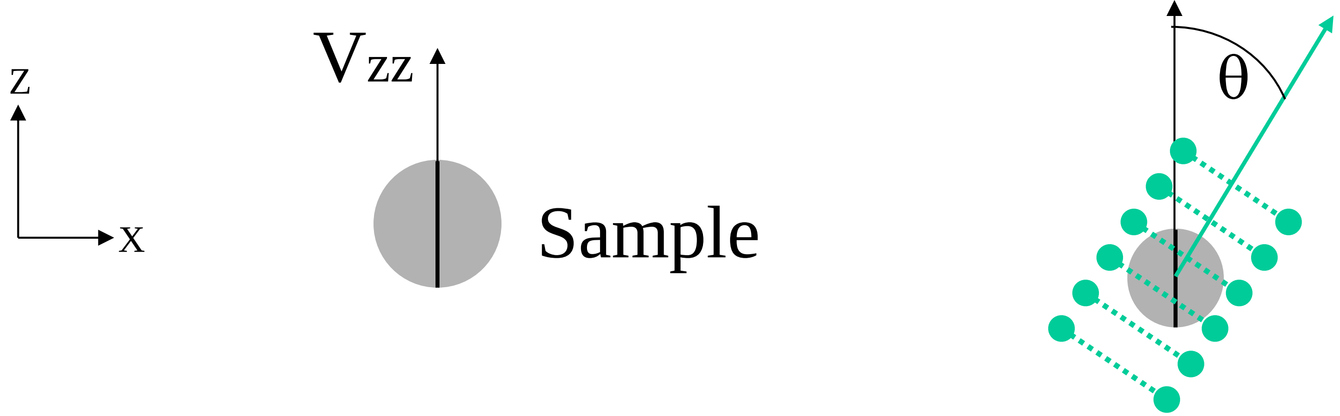
Orientation



Orientation quality

X-ray diffraction





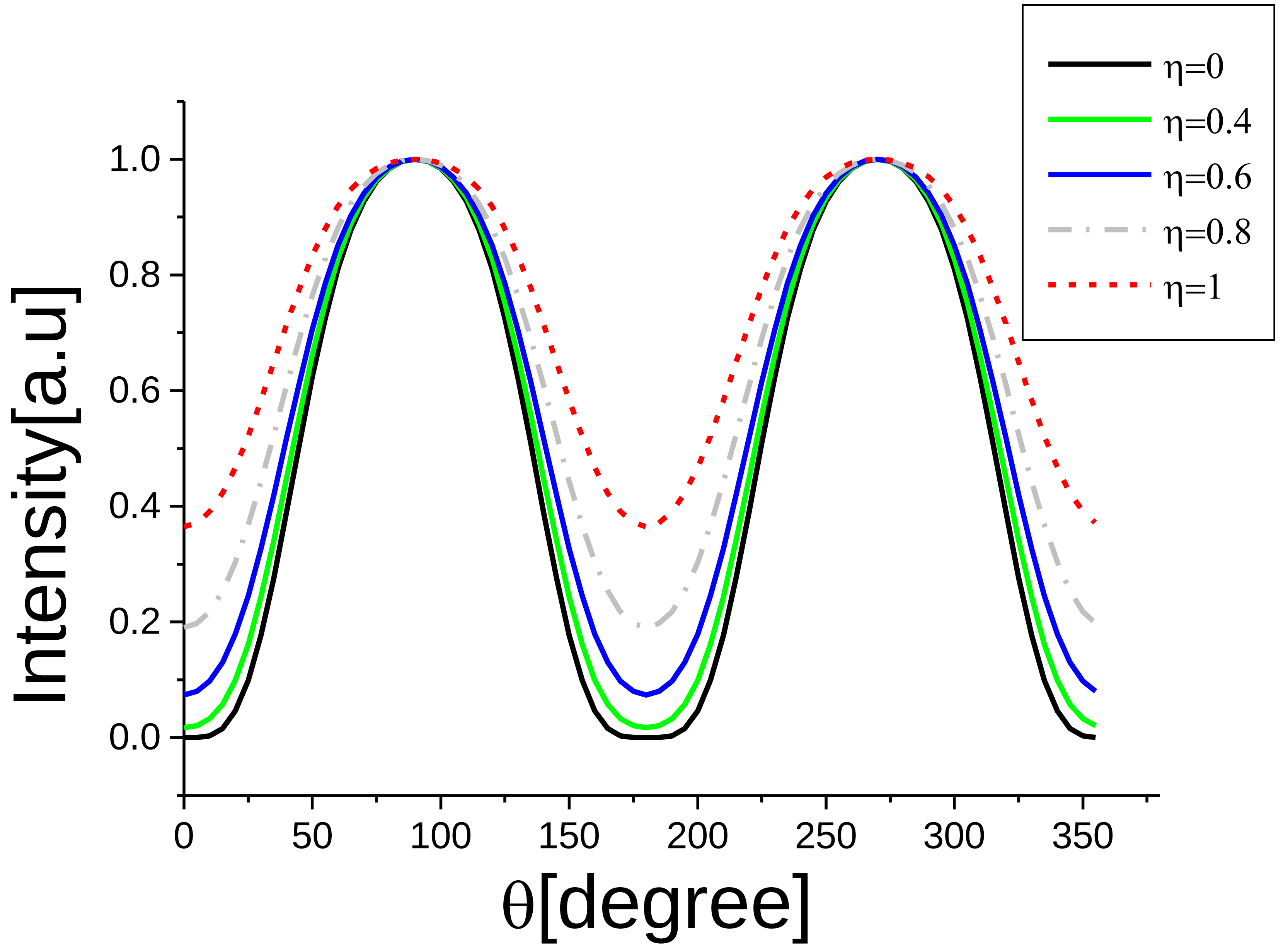
η=0

$$\frac{\hbar\nu_q}{2}\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{bmatrix} + \sqrt{3}\hbar\gamma B_1 Cos(\omega t)\begin{bmatrix}0&Sin(\theta)&0&0\\Sin(\theta)&0&0&0\\0&0&0&Sin(\theta)\\0&0&Sin(\theta)&0\end{bmatrix}$$

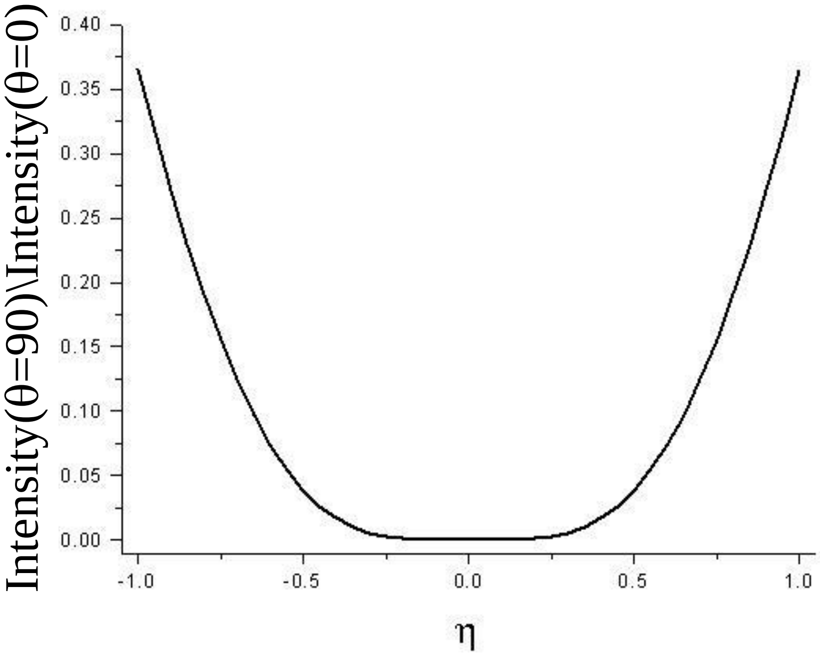
η≠0

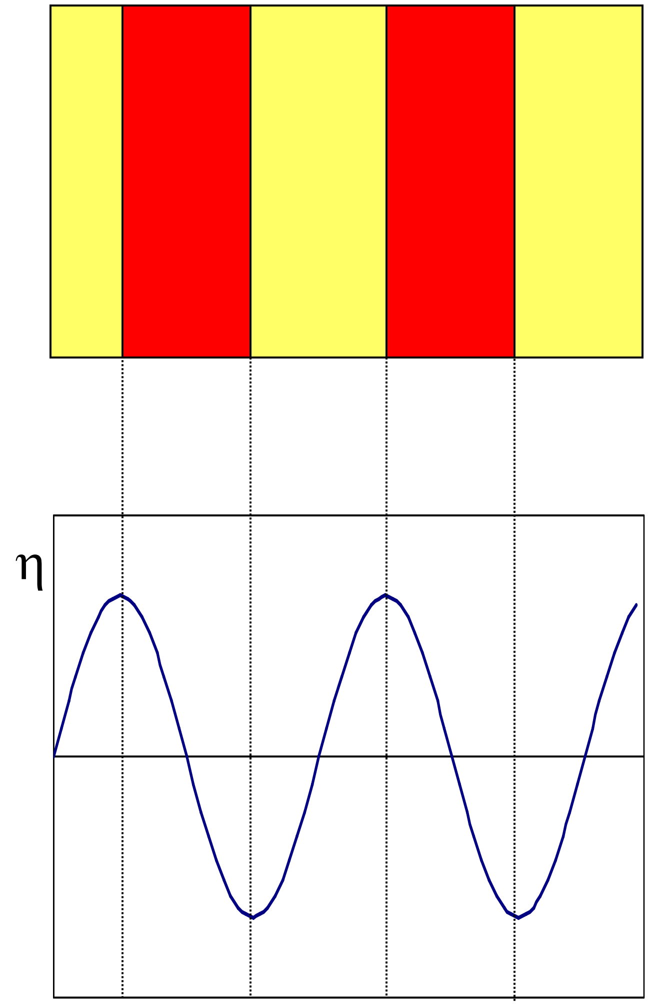
$$\frac{\hbar\nu_q}{2}\sqrt{1+\frac{\eta^2}{3}}\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{bmatrix} + 2\hbar\gamma B_1 Cos(\omega t)\begin{bmatrix}0&g_\eta Sin(\theta)&f_\eta Cos(\theta)&0\\g_\eta Sin(\theta)&0&0&f_\eta Cos(\theta)\\f_\eta Cos(\theta)&0&0&g_\eta Sin(\theta)\\0&f_\eta Cos(\theta)&g_\eta Sin(\theta)&0\end{bmatrix}$$

Echo Intensity vs. θ - Theoretical Result



Intensity (θ=90)/Intensity (θ=0)





$\langle\eta\rangle = 0$

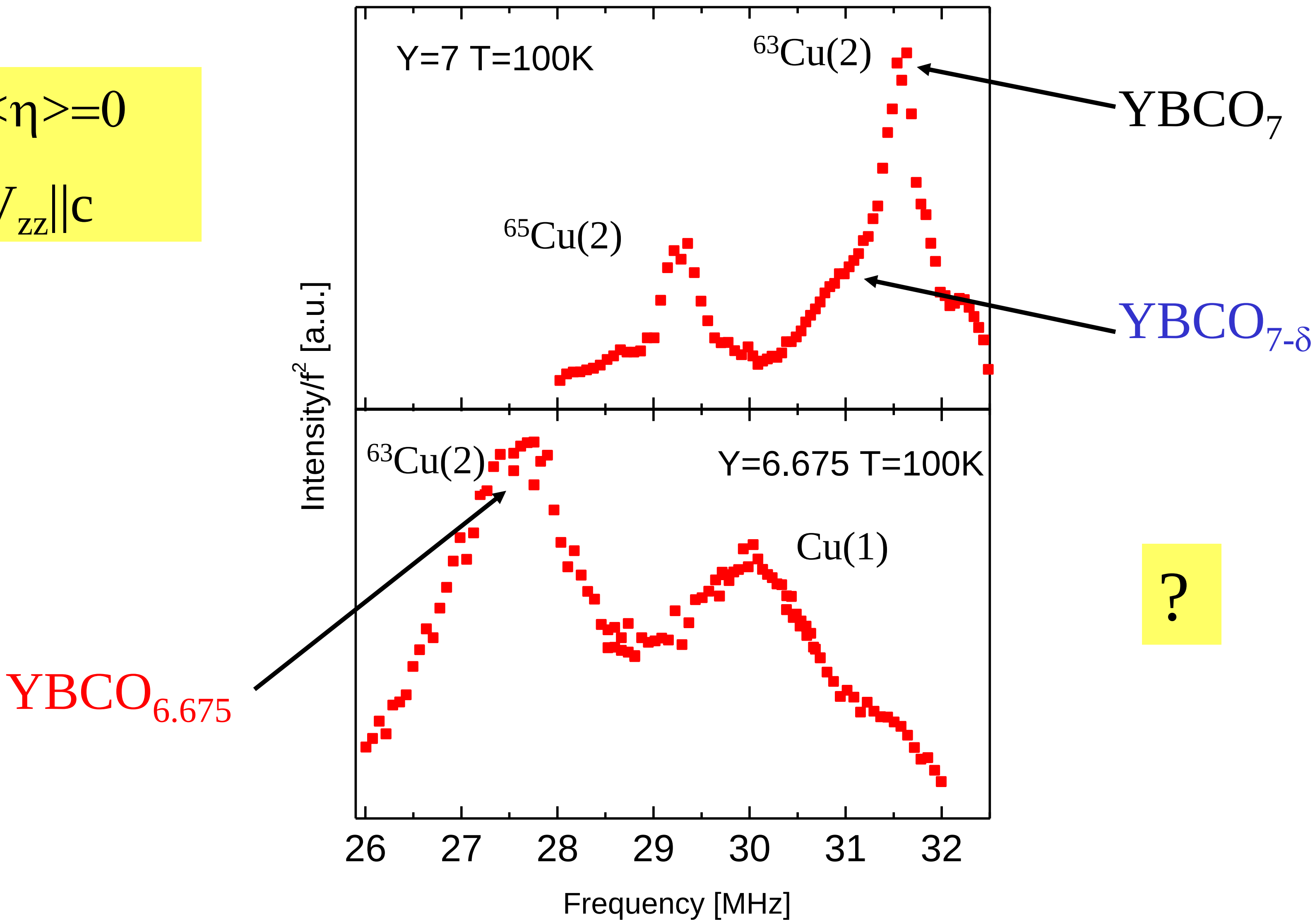
$\langle |\eta| \rangle \neq 0$

$|\eta|$

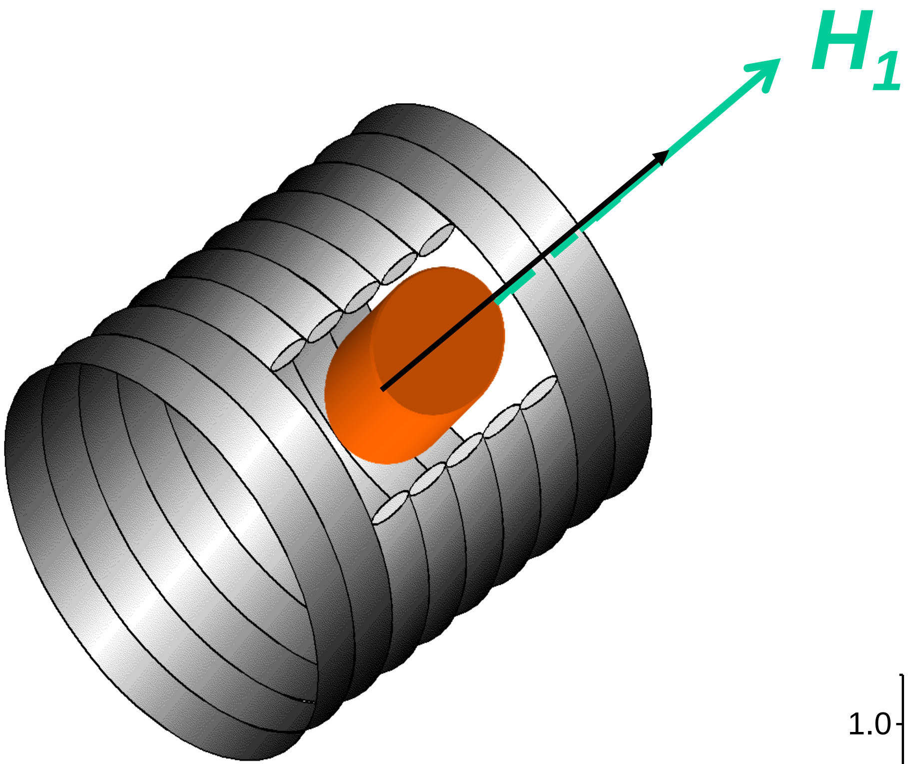
NQR Spectrum of YBCO

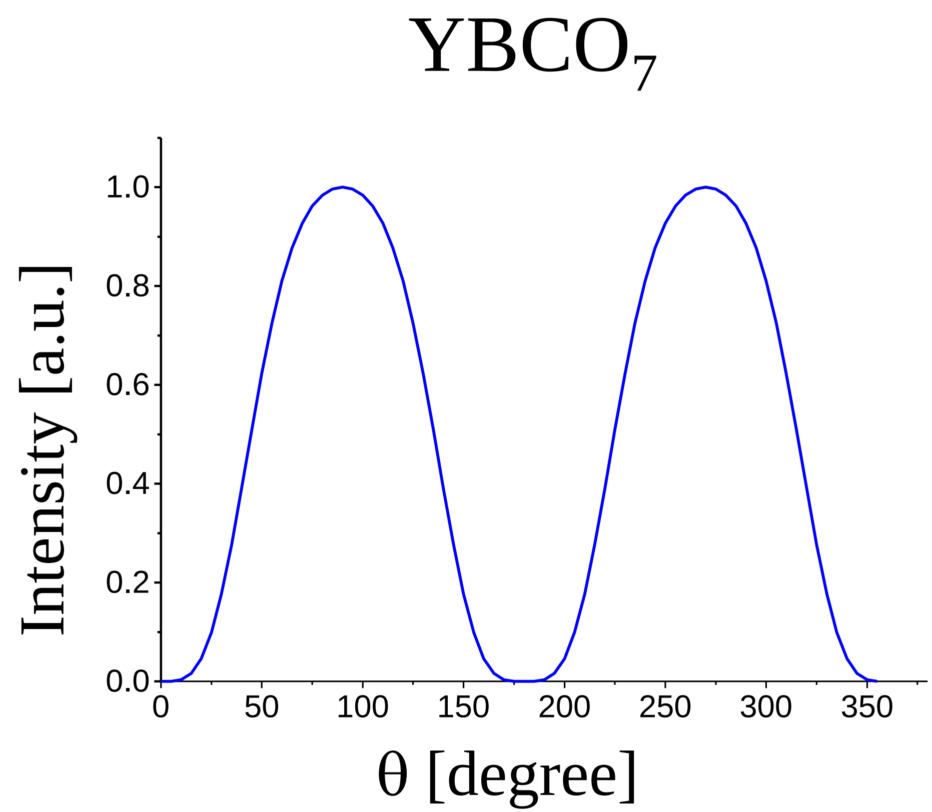
$\langle\eta\rangle=0$

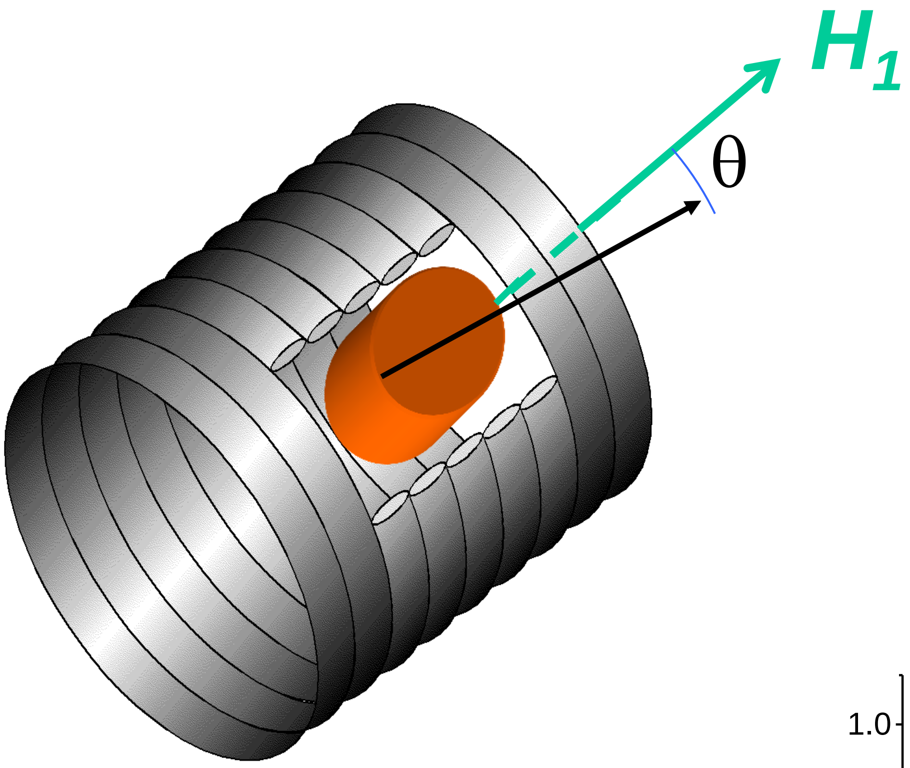
$V_{zz}||c$



?

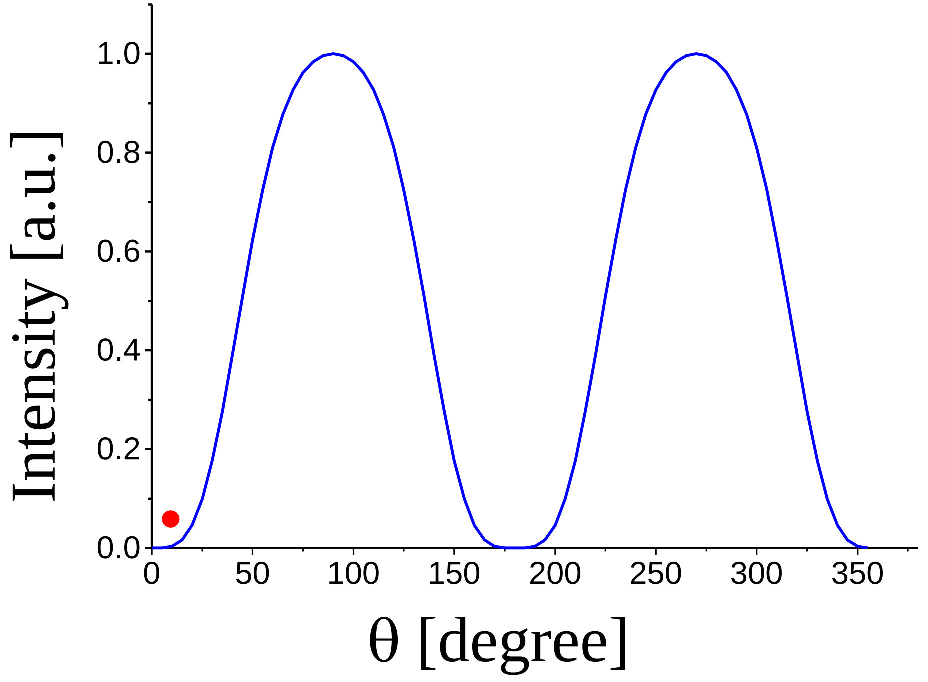

H1


YBCO7
Intensity [a.u.]
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
θ [degree]

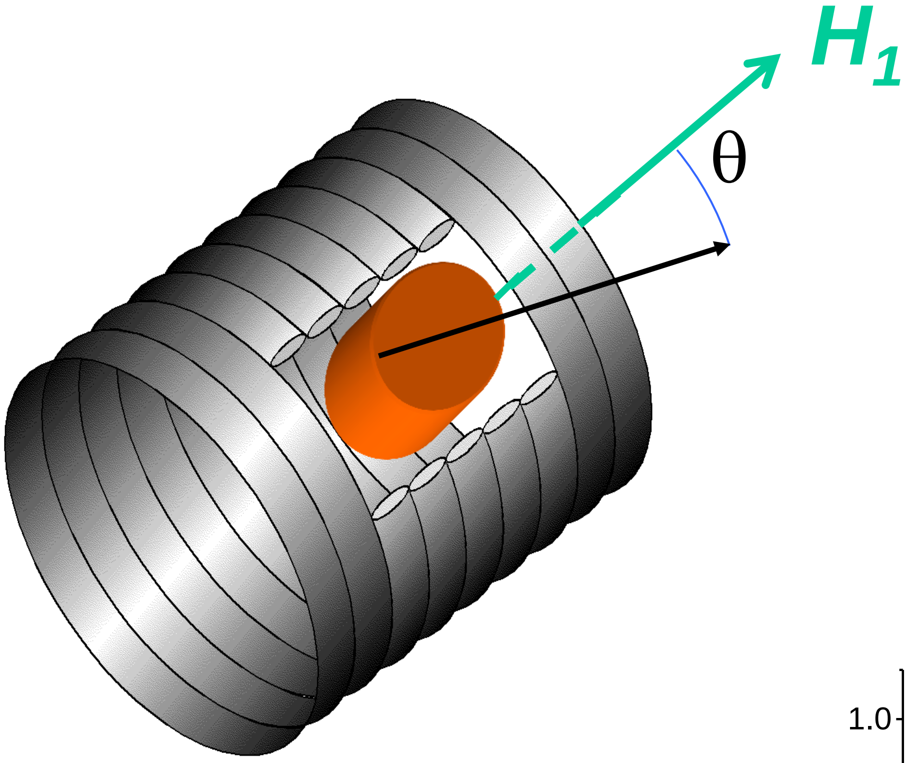


H1
θ

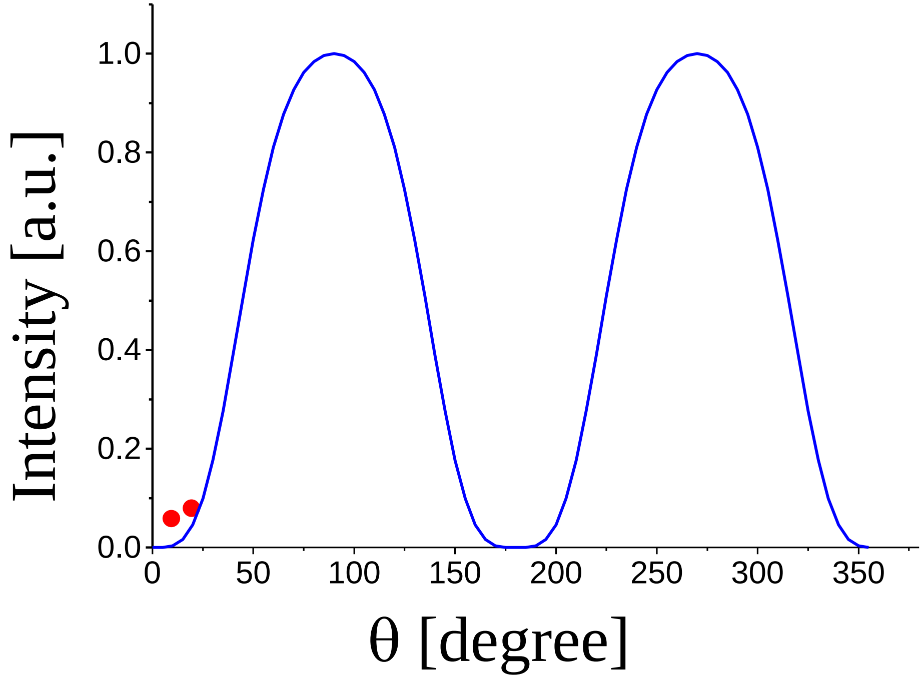
$YBCO_7$

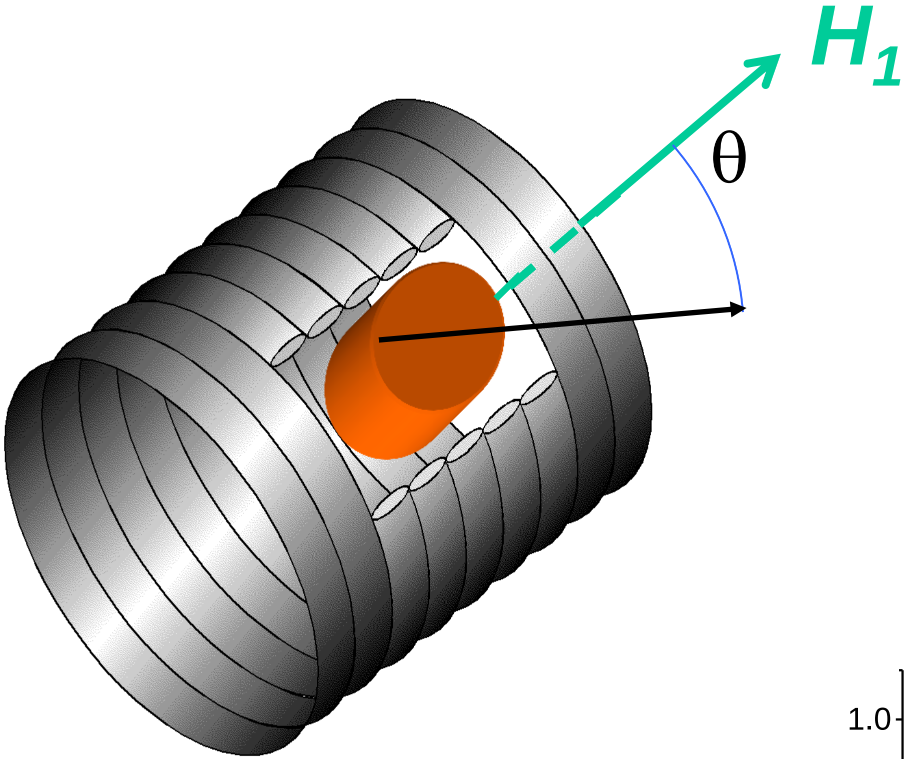


1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
Intensity [a.u.]
θ [degree]

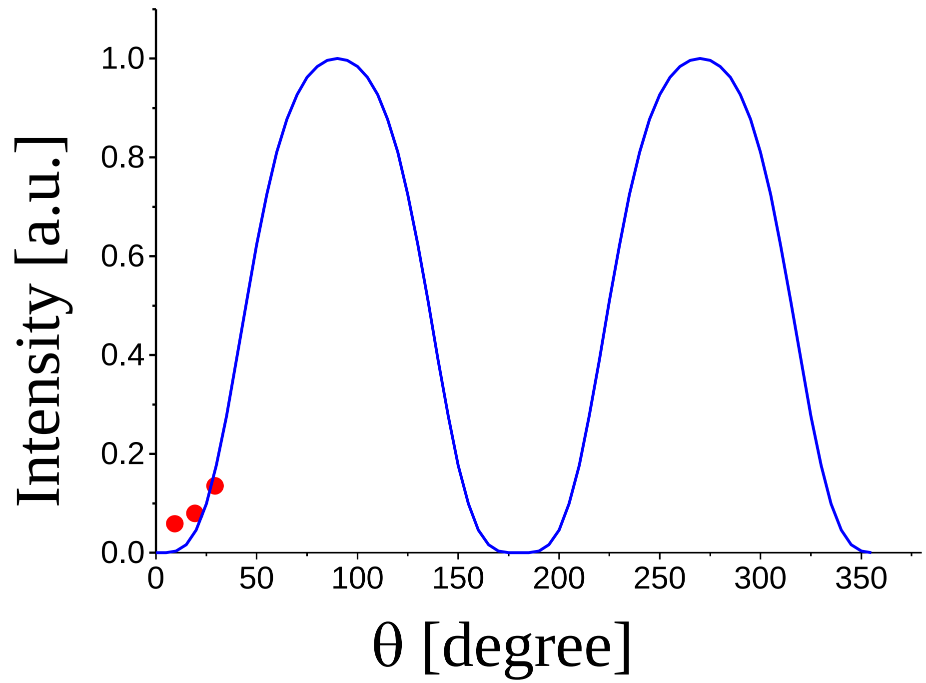

H1
θ

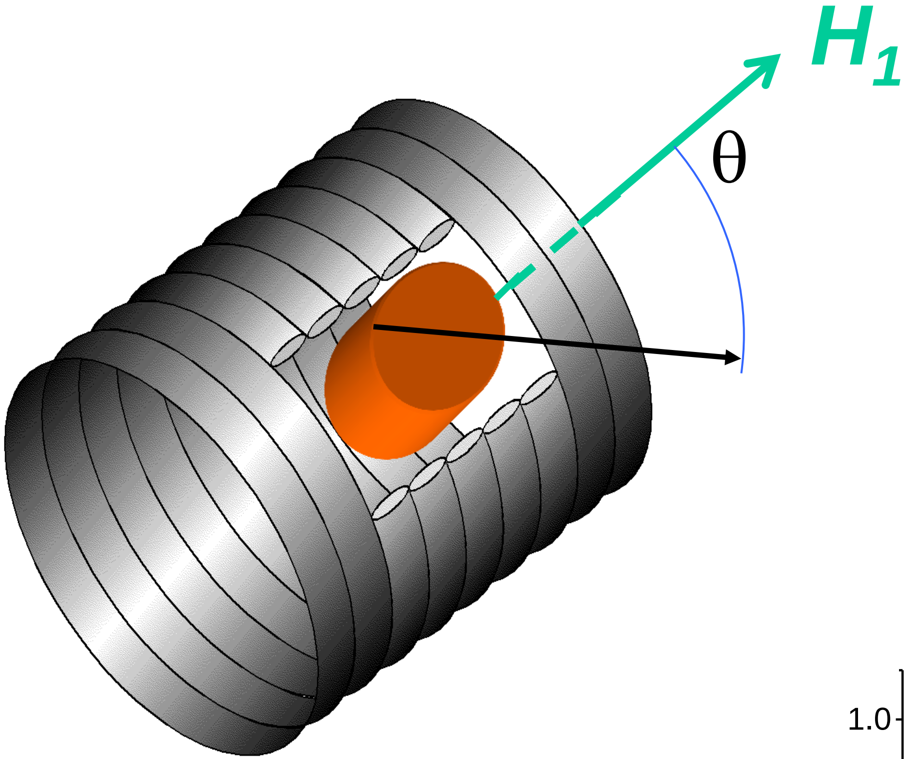
$YBCO_7$


Intensity [a.u.]
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
θ [degree]

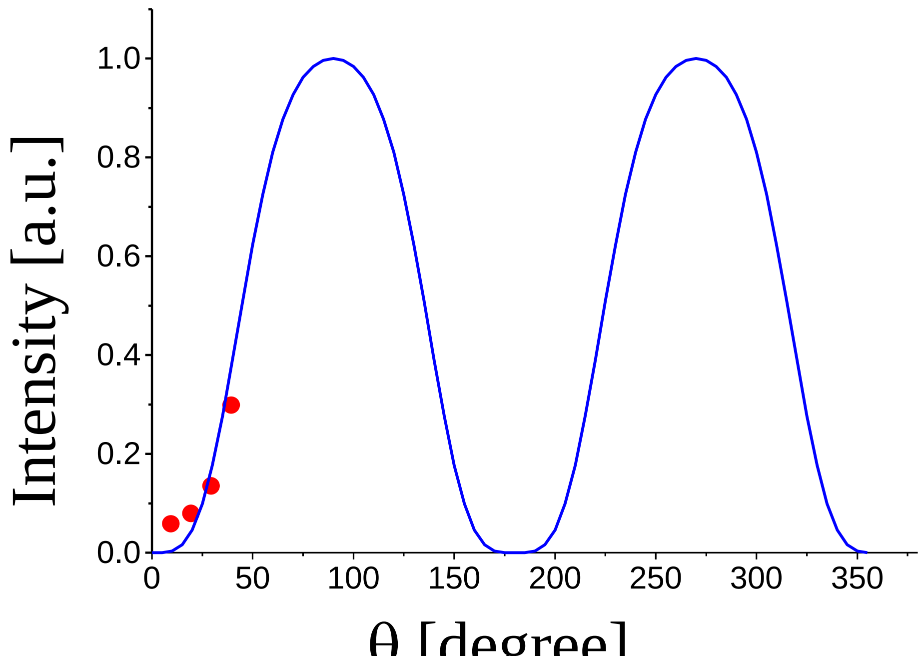

H1
θ

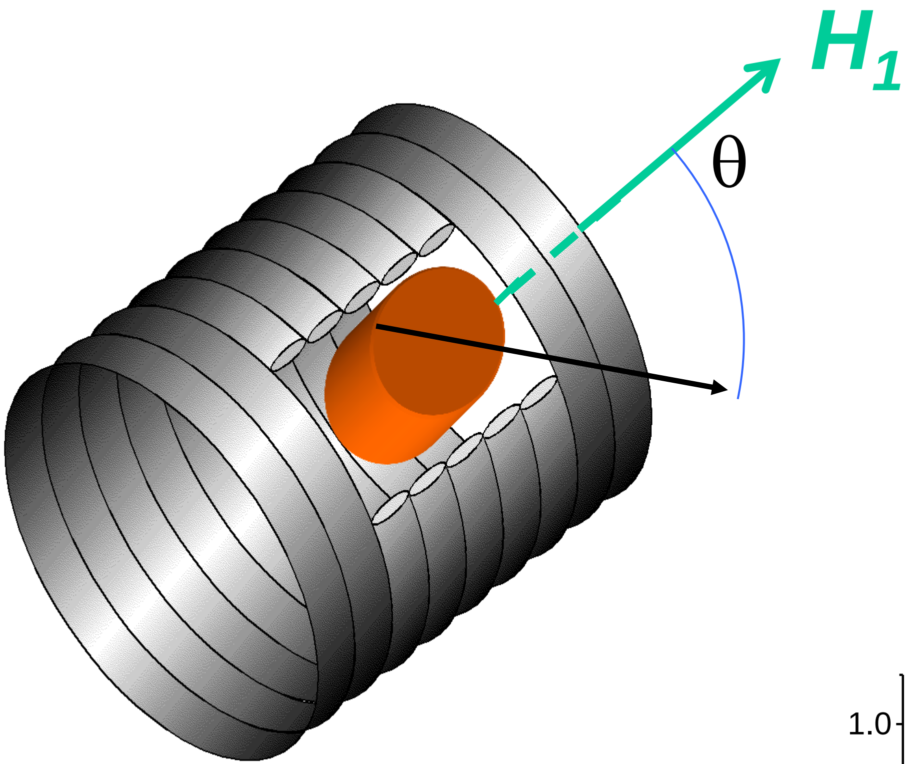
$YBCO_7$

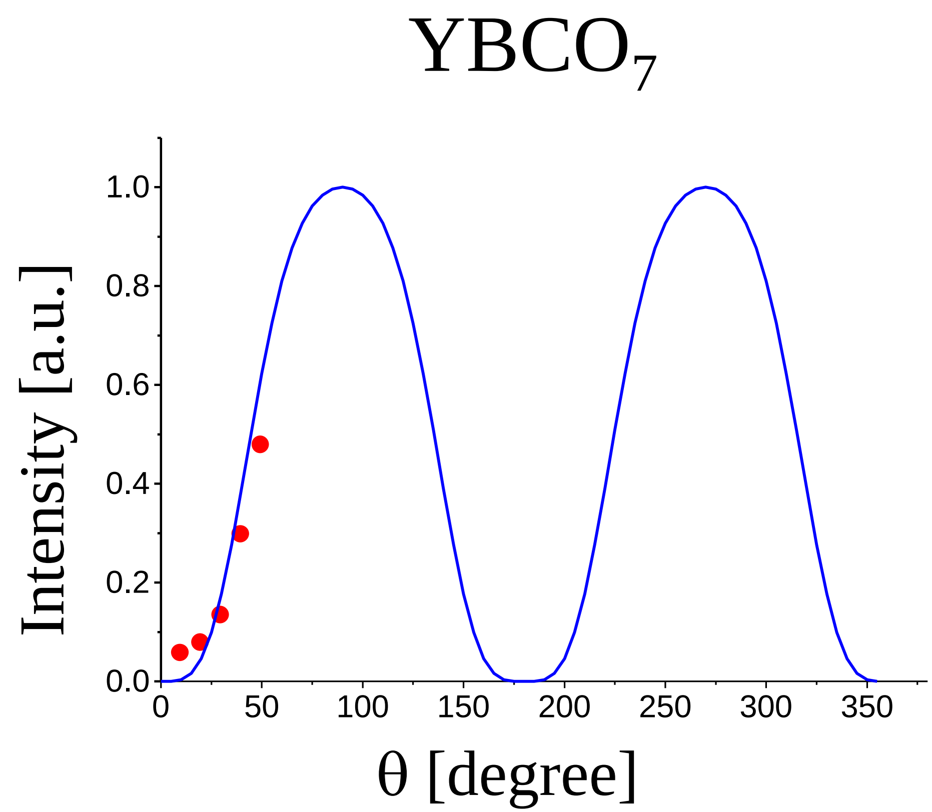

Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

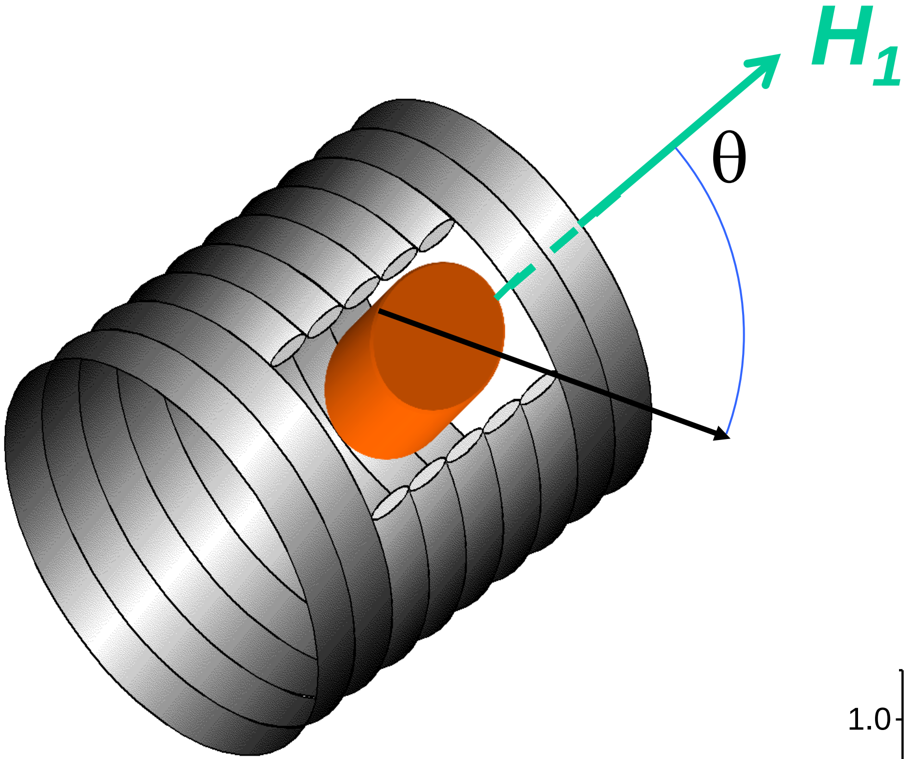

H1
θ

YBCO$_7$

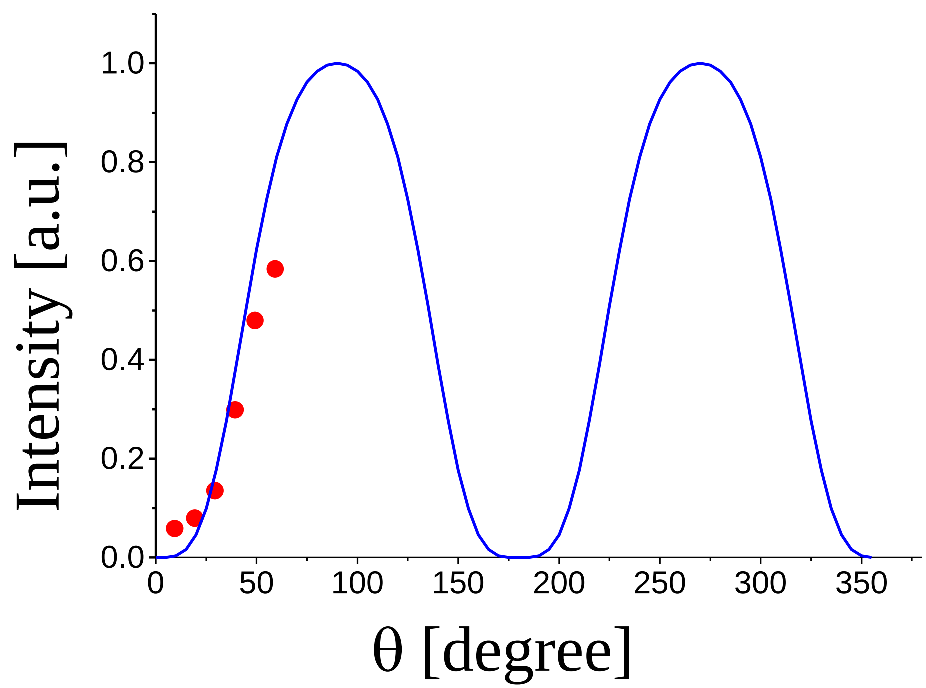

1.0
0.8
0.6
0.4
0.2
0.0
Intensity [a.u.]
0
50
100
150
200
250
300
350
θ [degree]

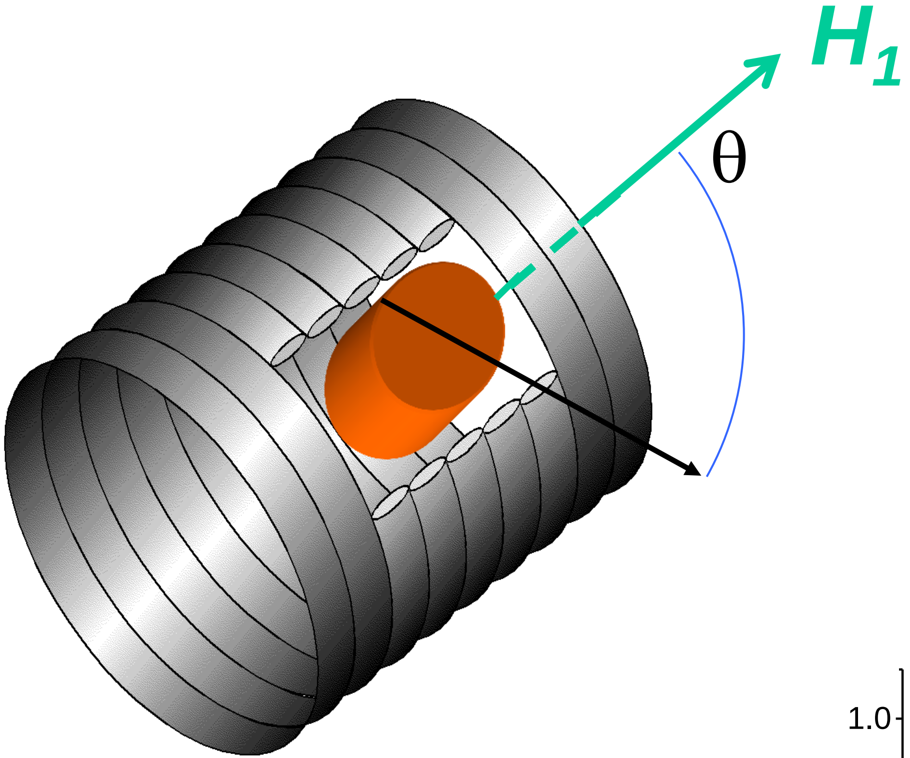

H_1
θ

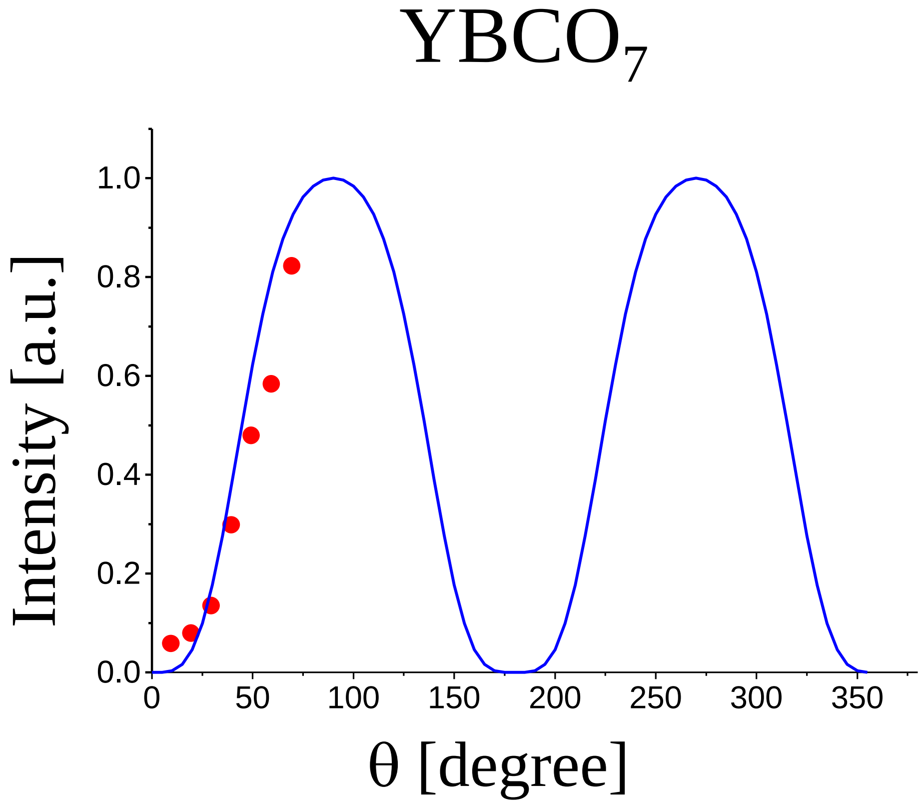

$YBCO_7$
Intensity [a.u.]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350
θ [degree]

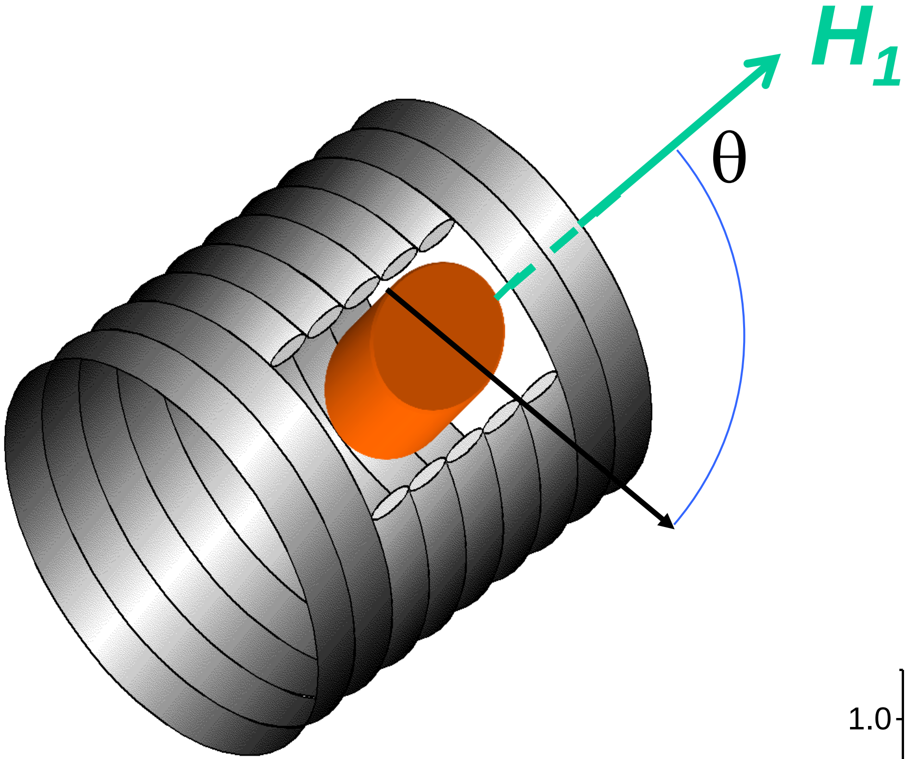

H1
θ

$YBCO_7$

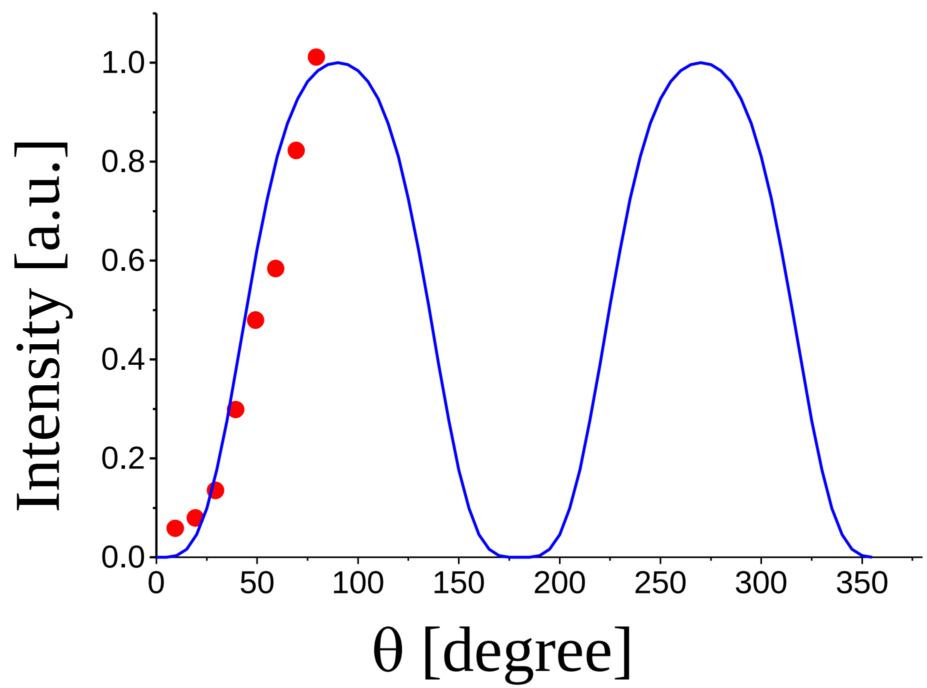

Intensity [a.u.]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350
θ [degree]

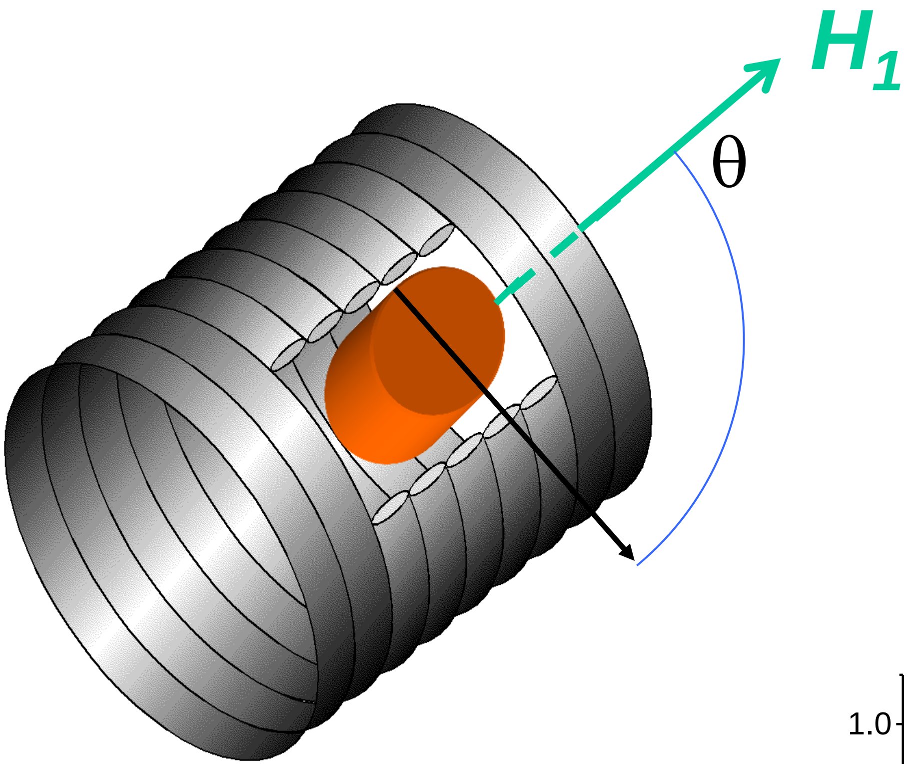

H1
θ

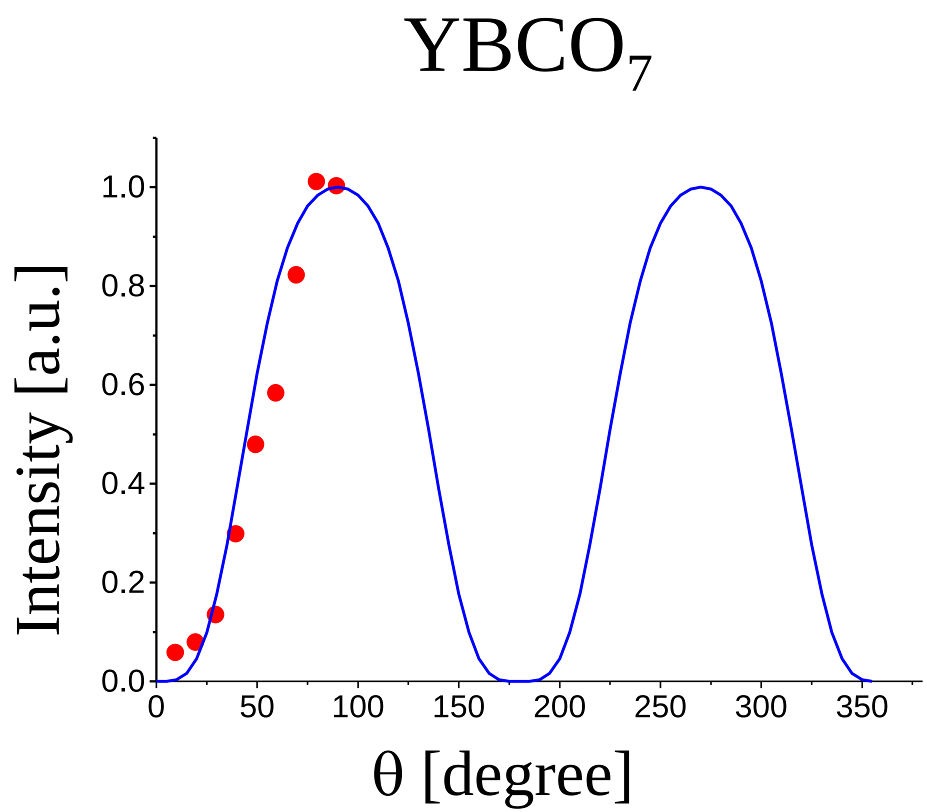

YBCO7
Intensity [a.u.]
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
θ [degree]

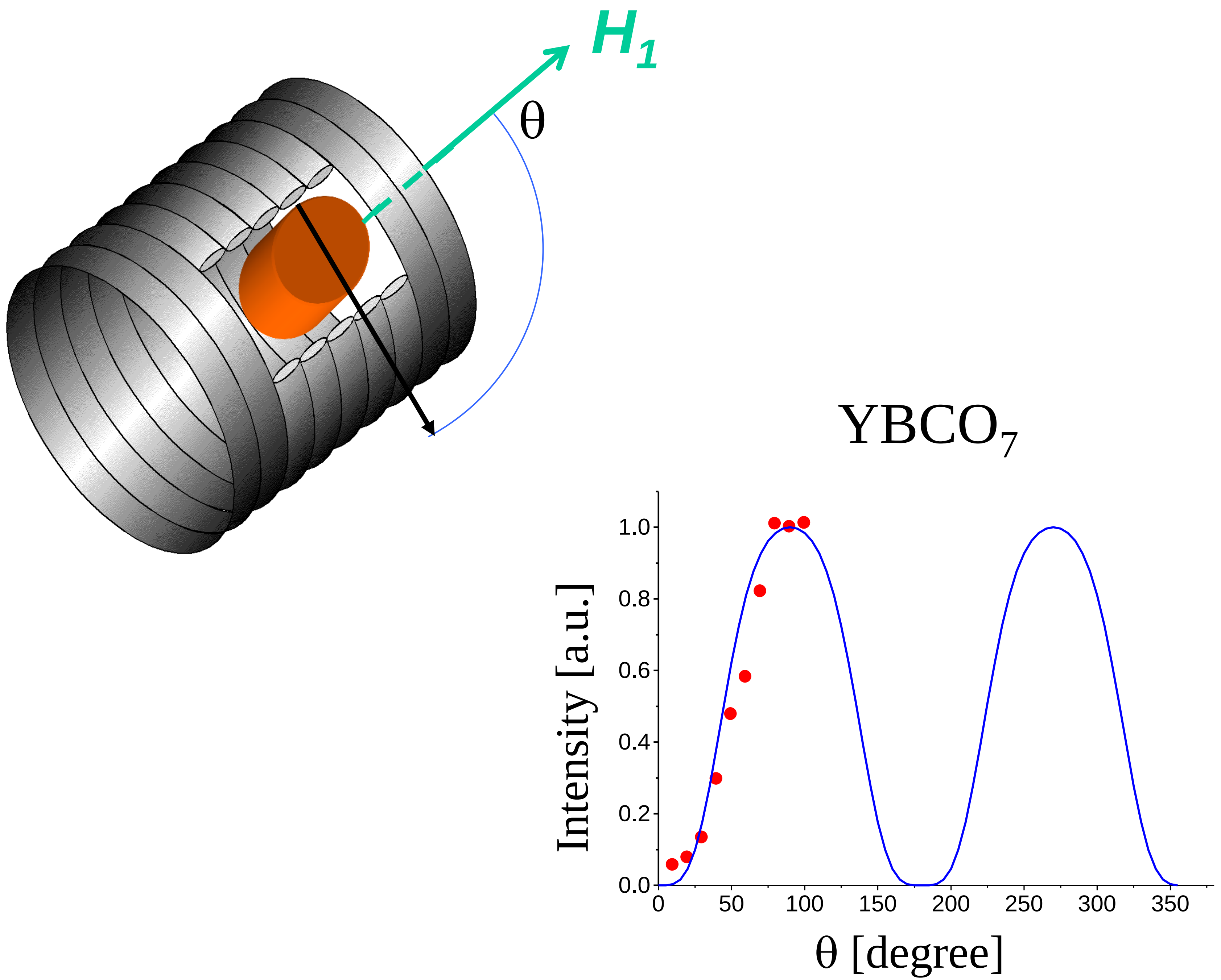

H1
θ

$YBCO_7$

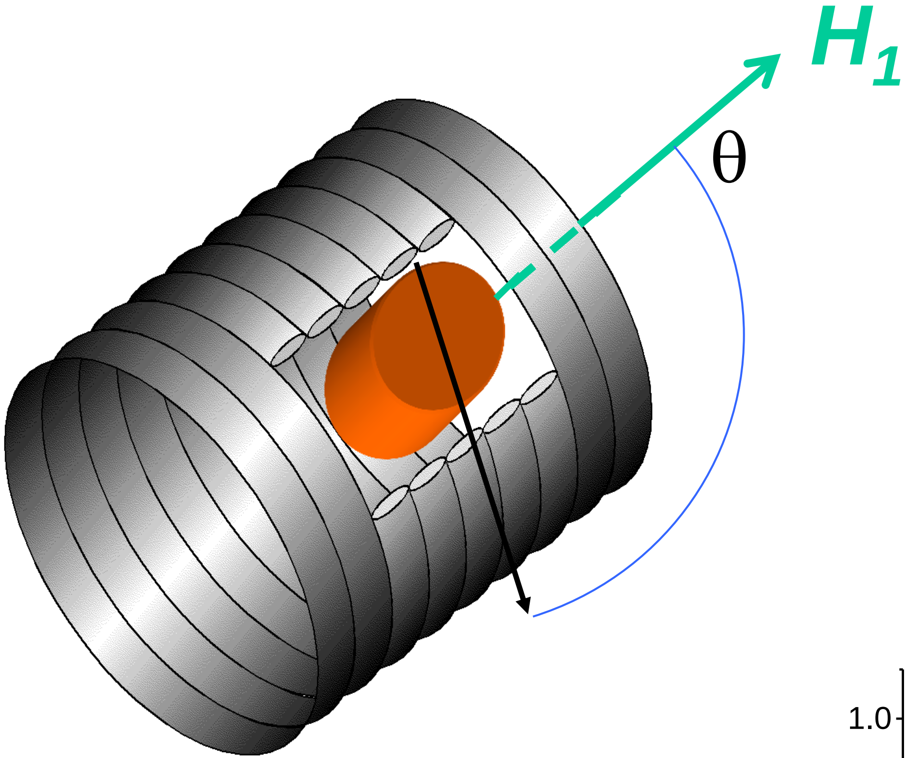

Intensity [a.u.]
θ [degree]
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350

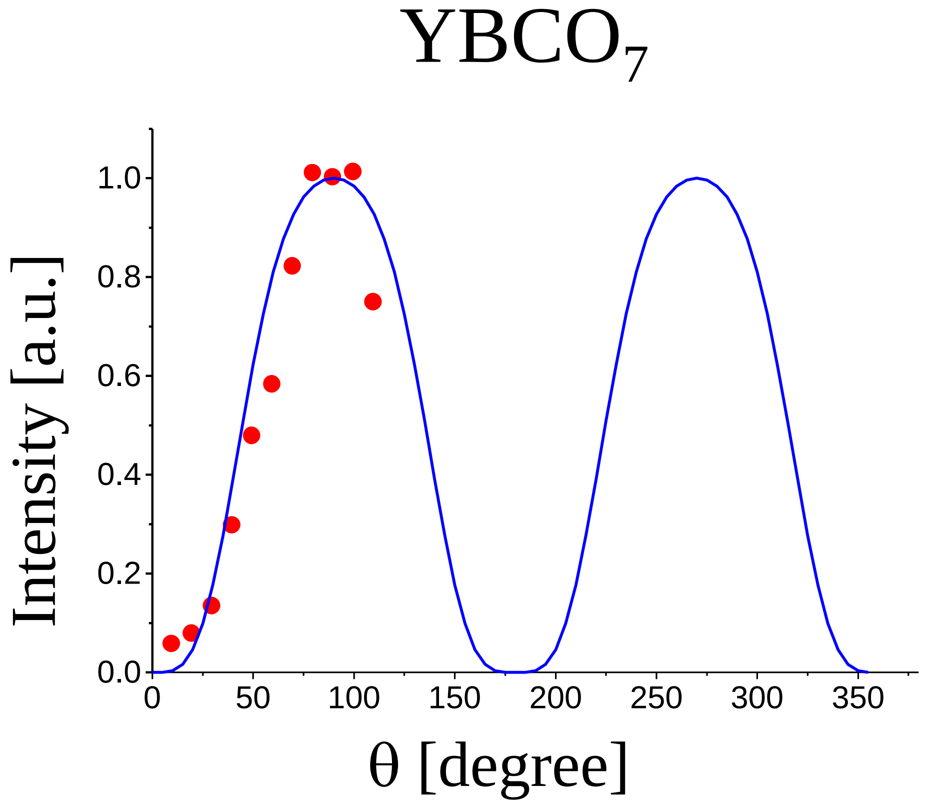

H1
θ

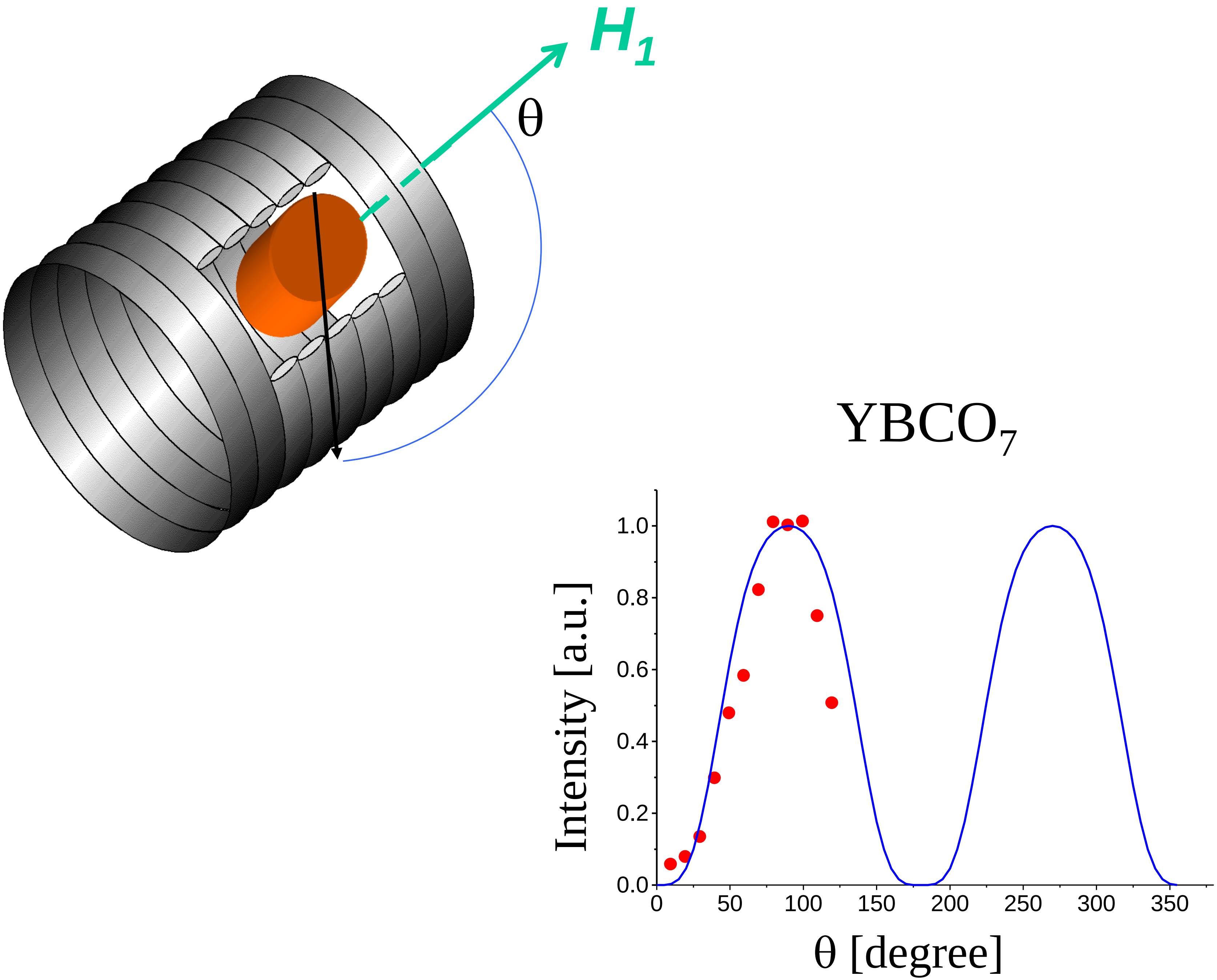

YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350



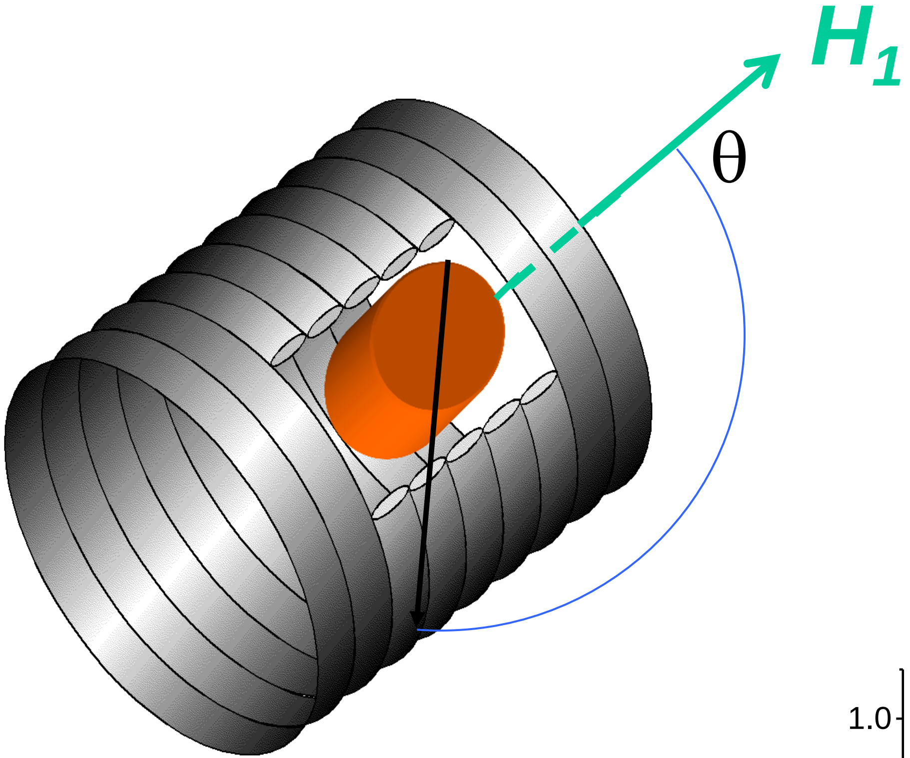
H1
θ
YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350


H1
θ

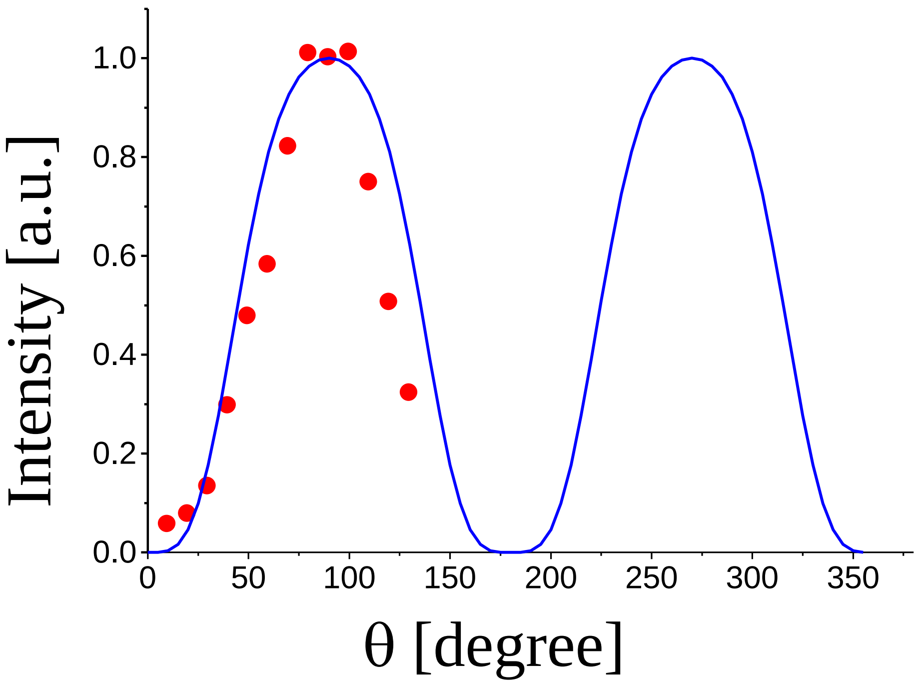

YBCO7
Intensity [a.u.]
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
θ [degree]

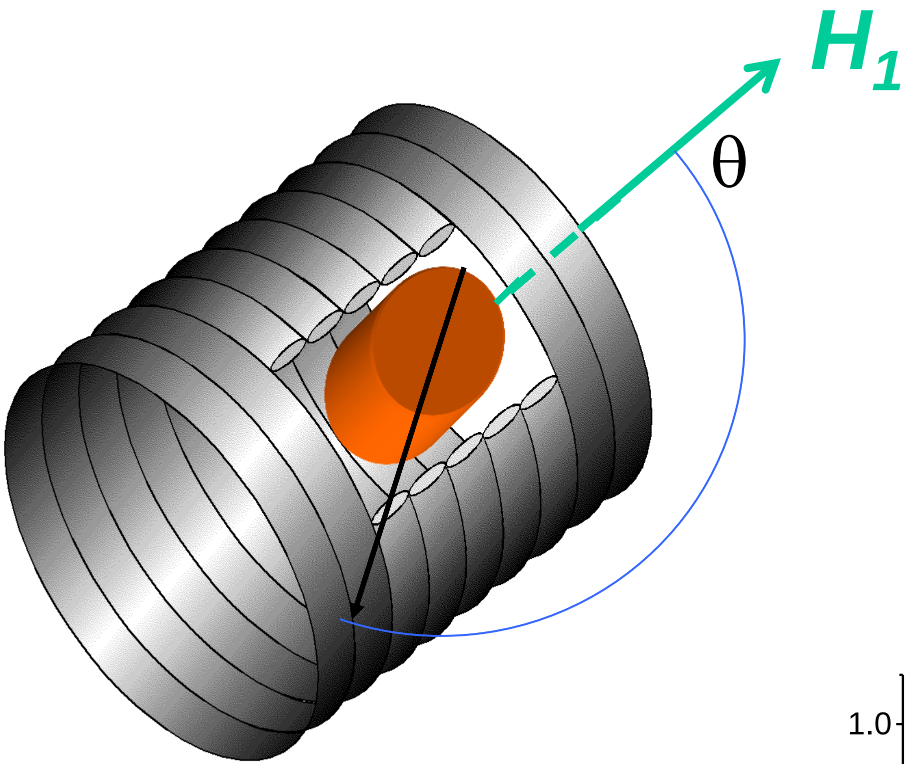


H1
θ
YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

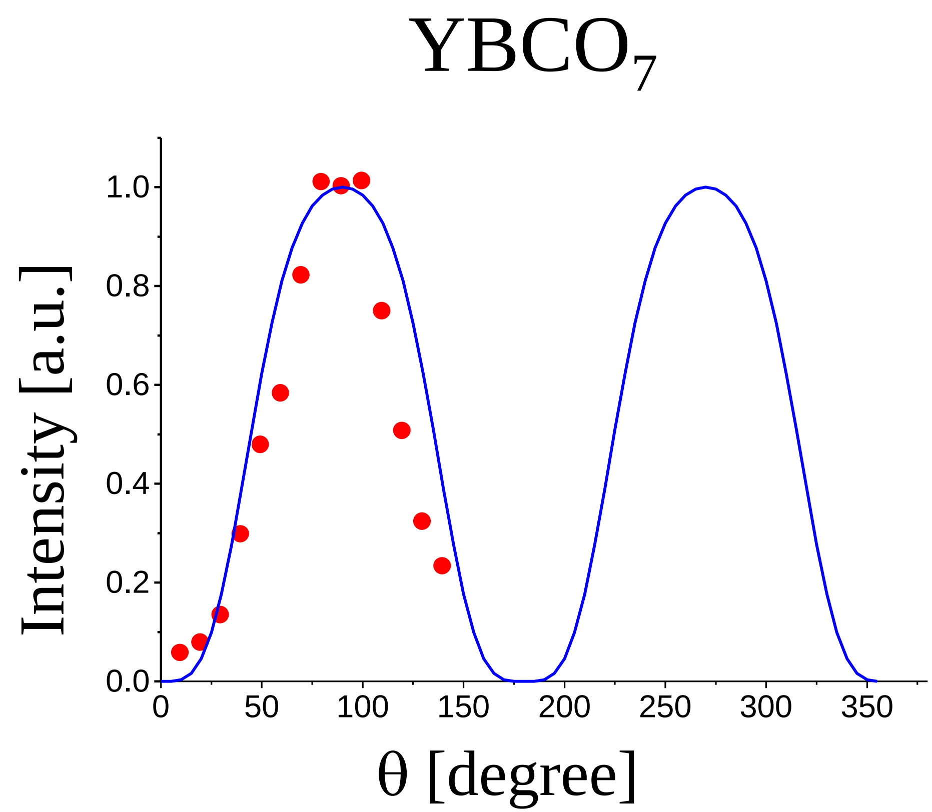

H1
θ

YBCO$_7$

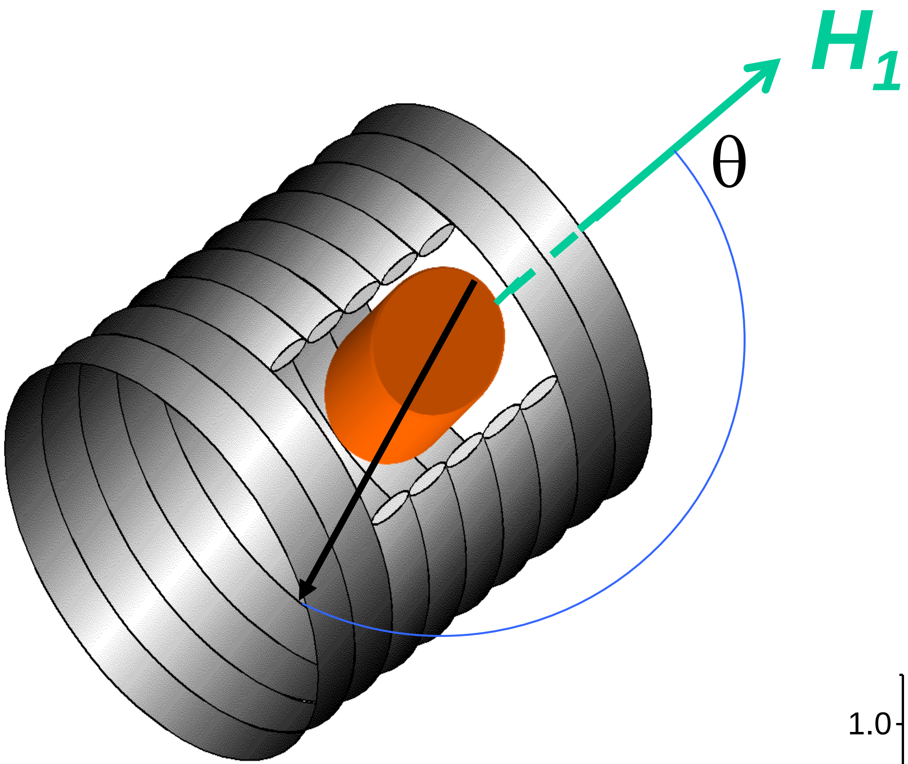

Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350



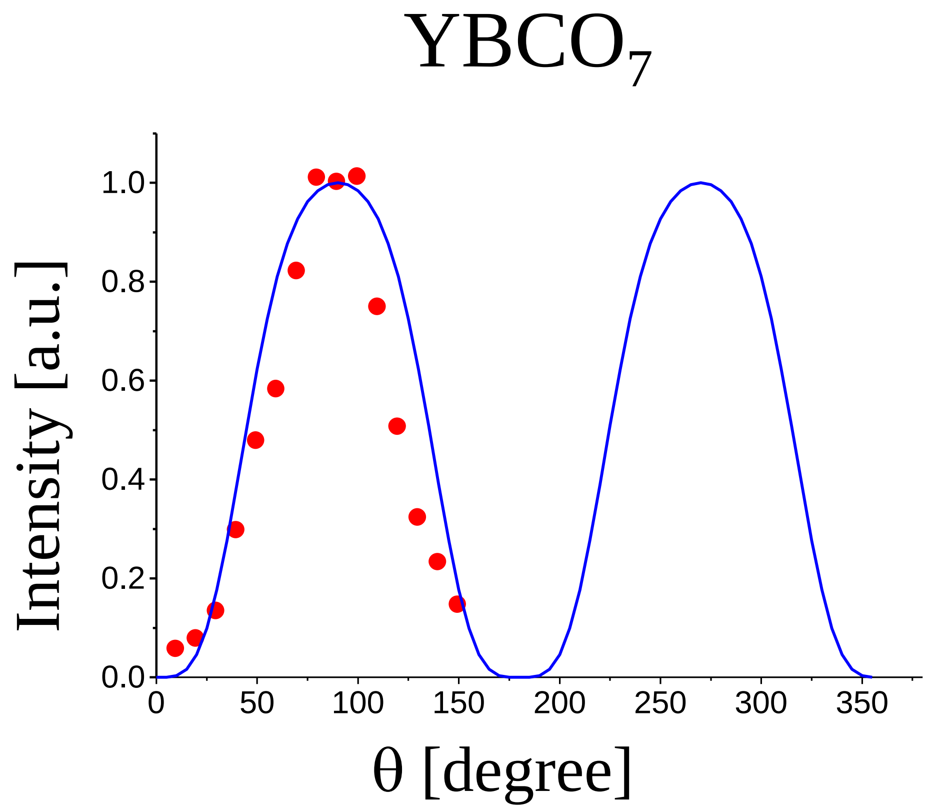
H1
θ



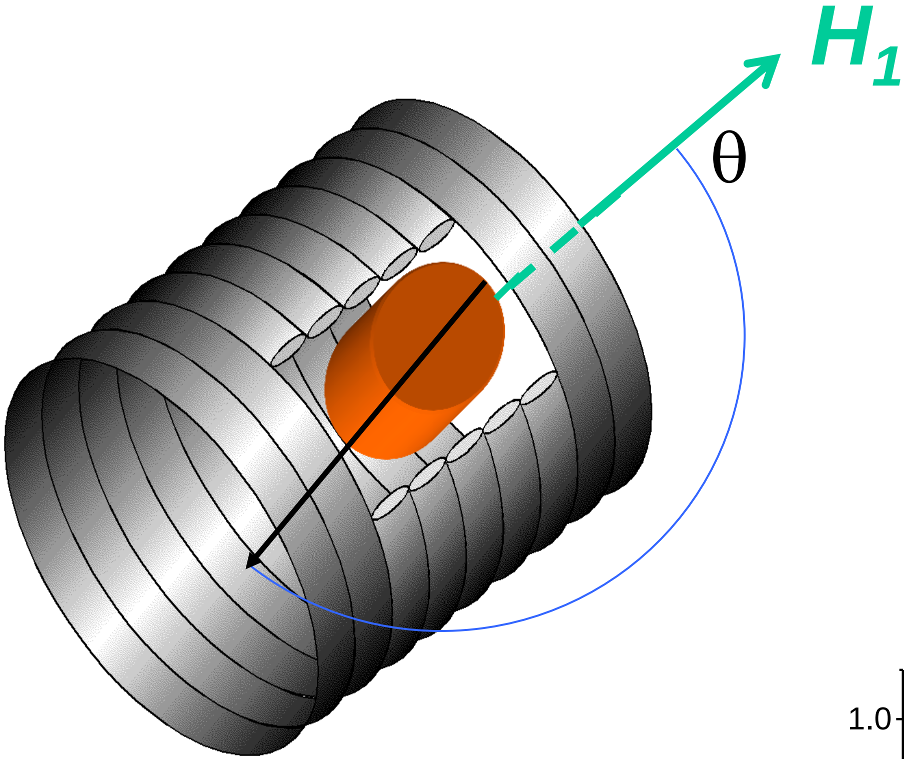
YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350



H1
θ

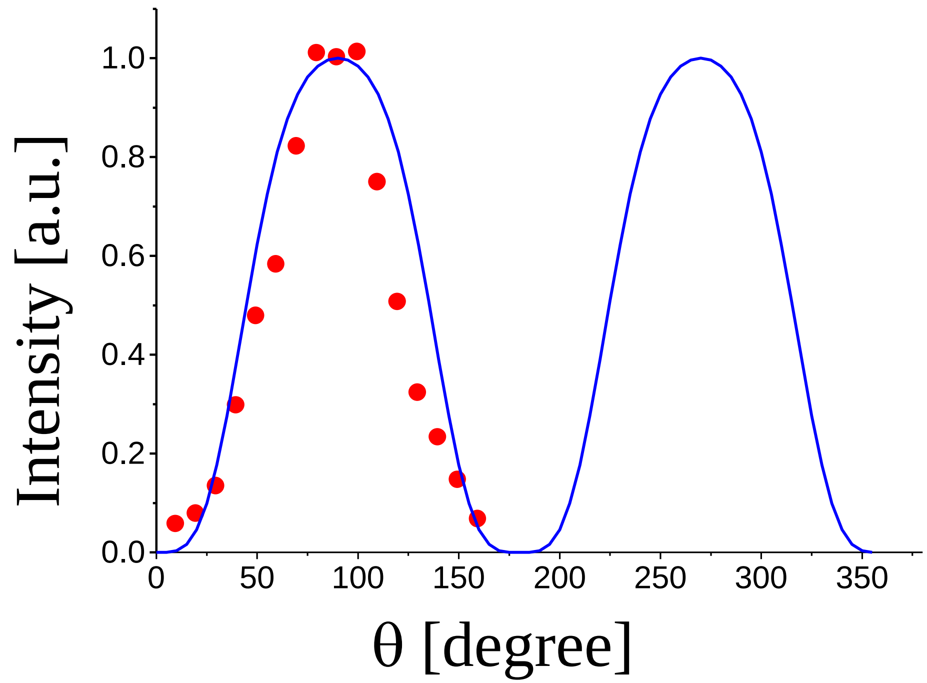


YBCO7
Intensity [a.u.]
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
θ [degree]

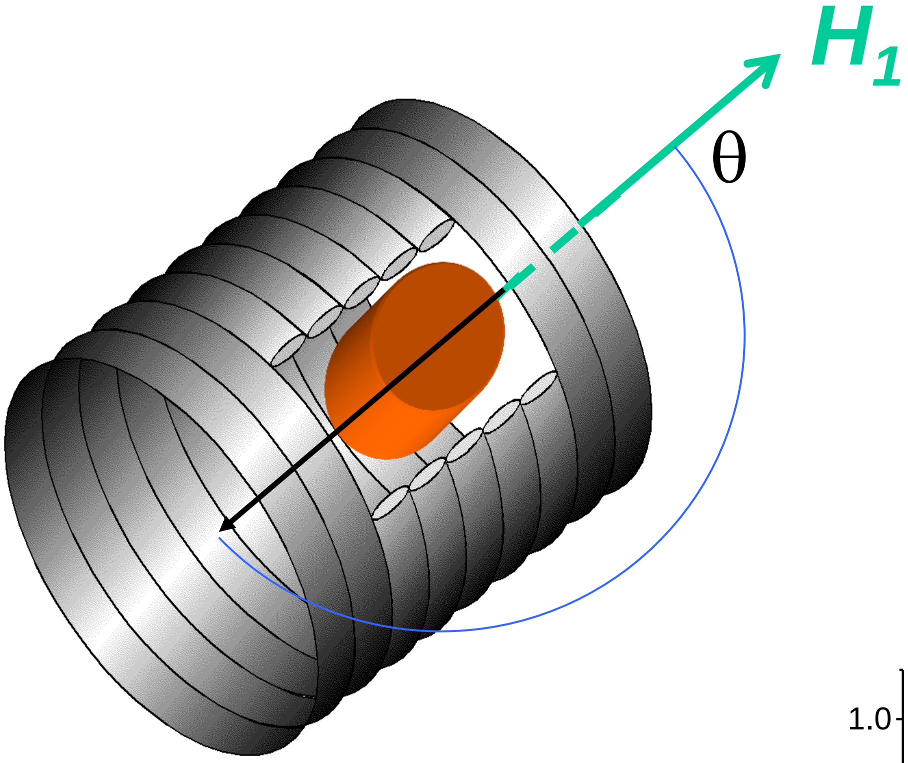


H_1
θ

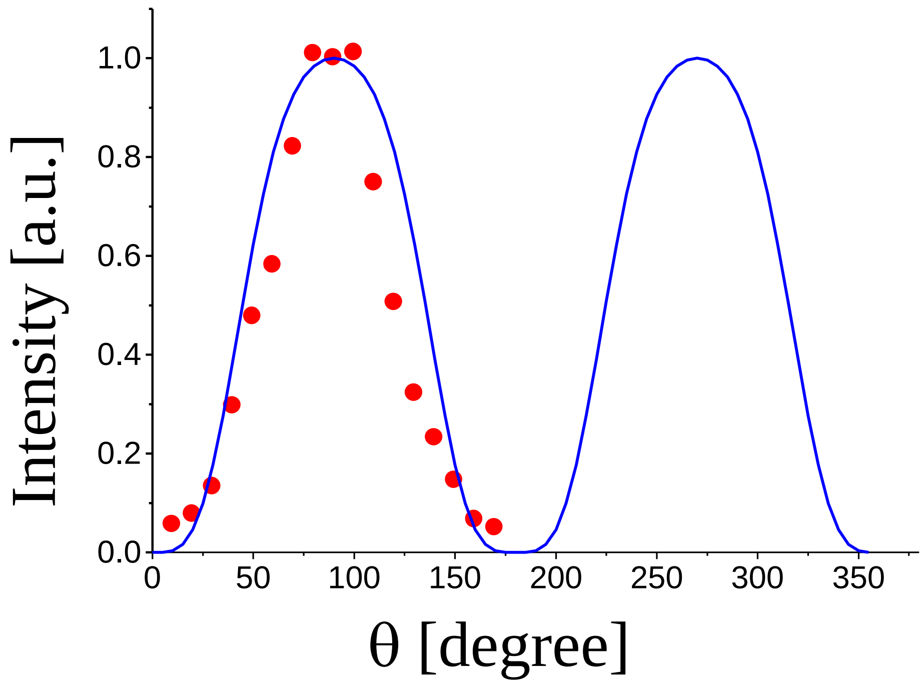
YBCO$_7$

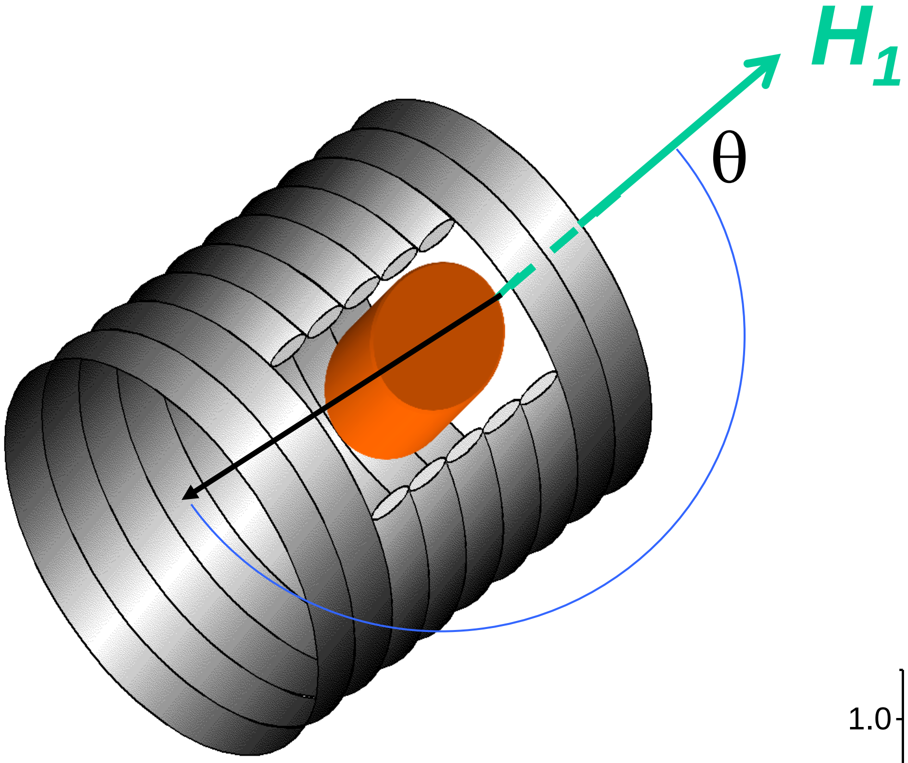


Intensity [a.u.]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350
θ [degree]

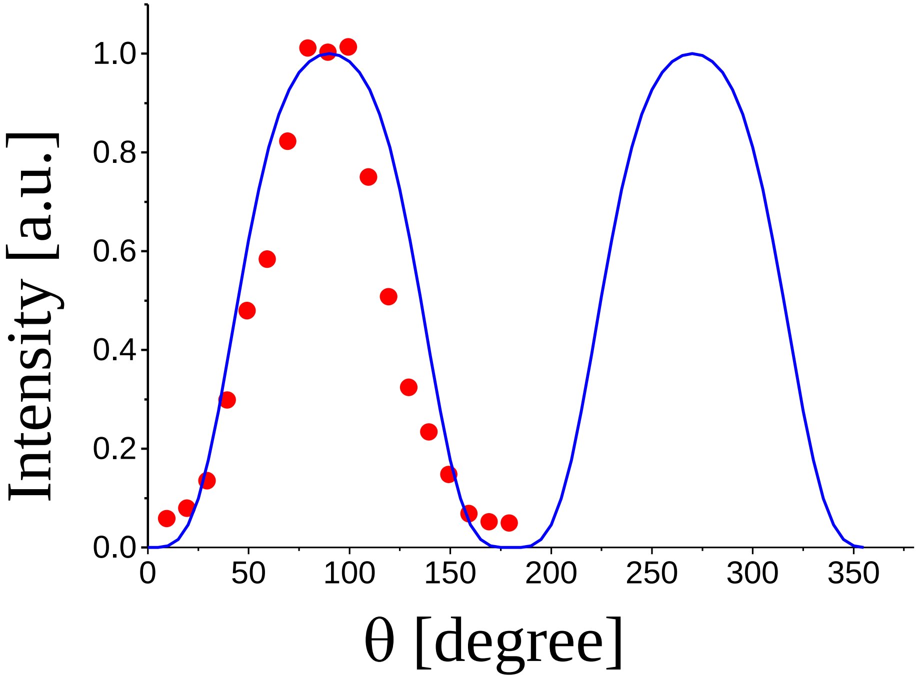

H1
θ

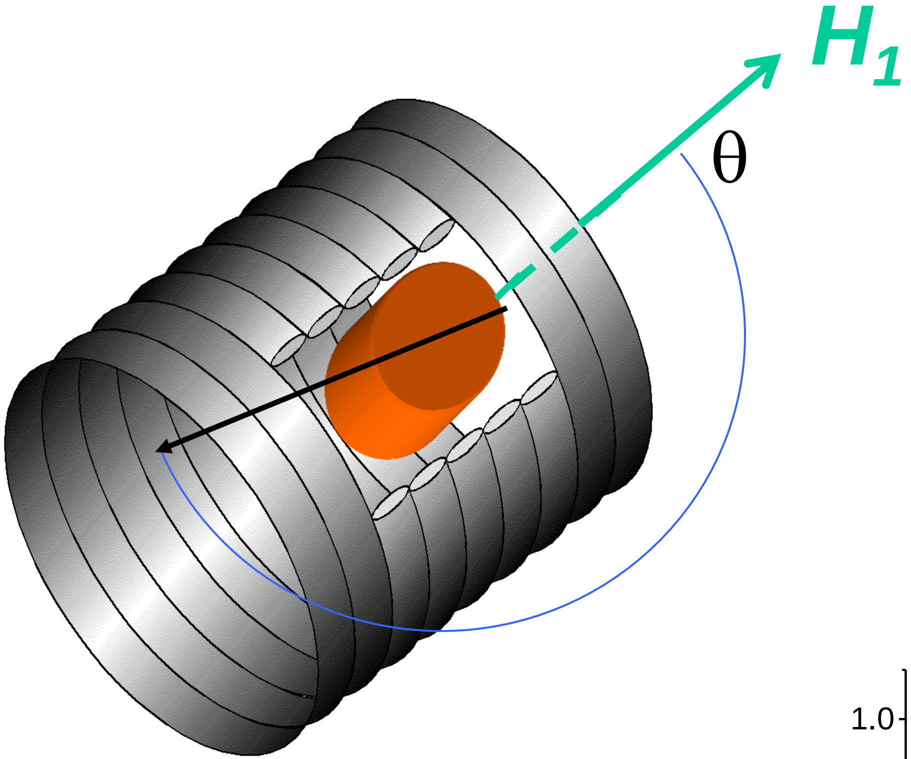
YBCO$_7$


Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

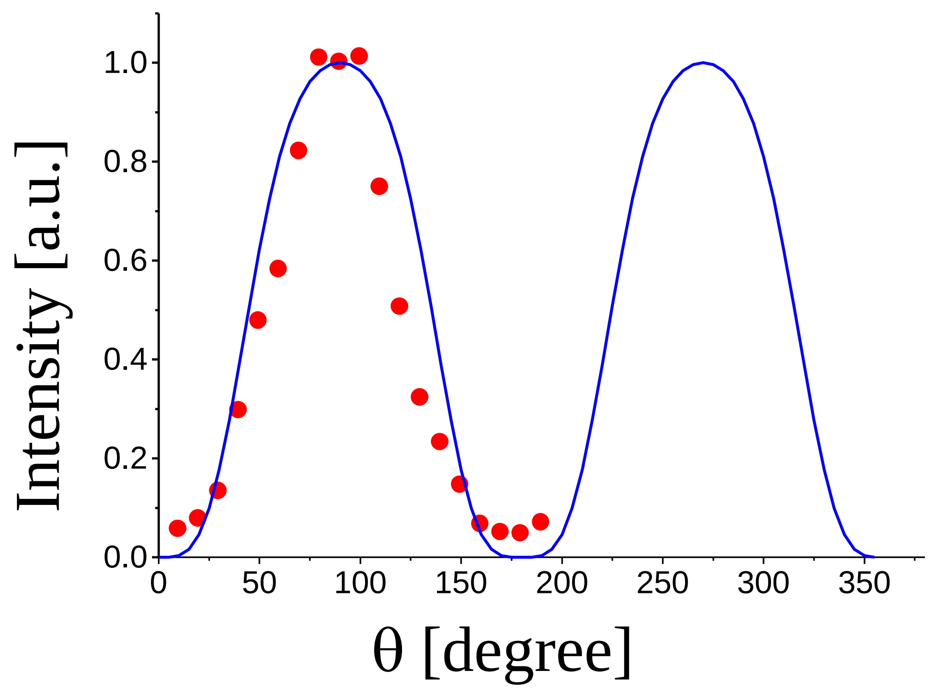

H1
θ

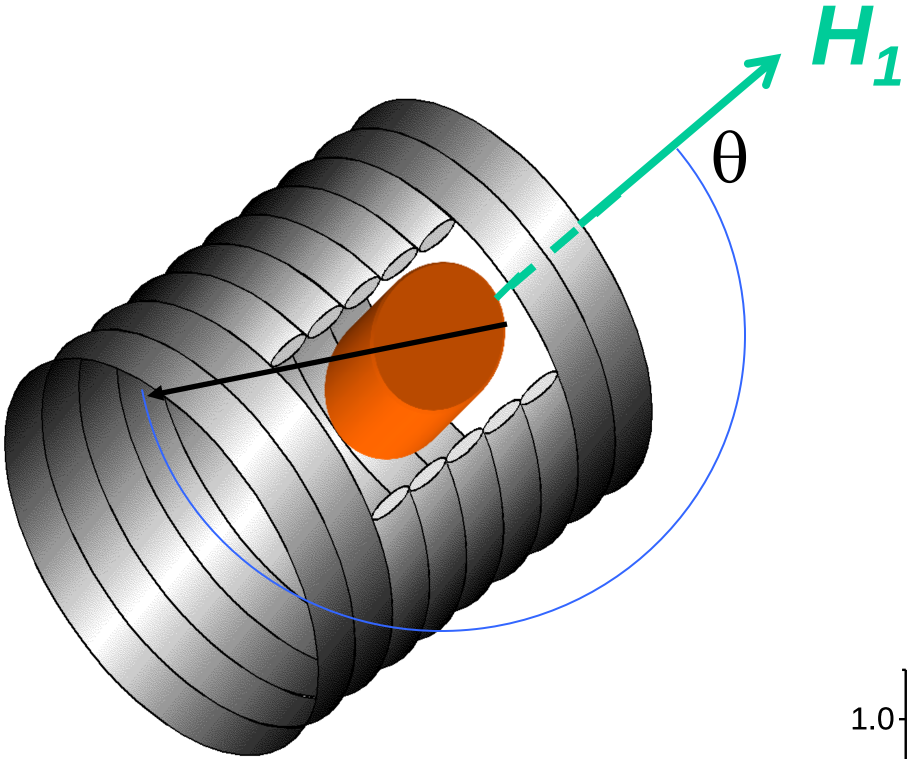
YBCO$_7$

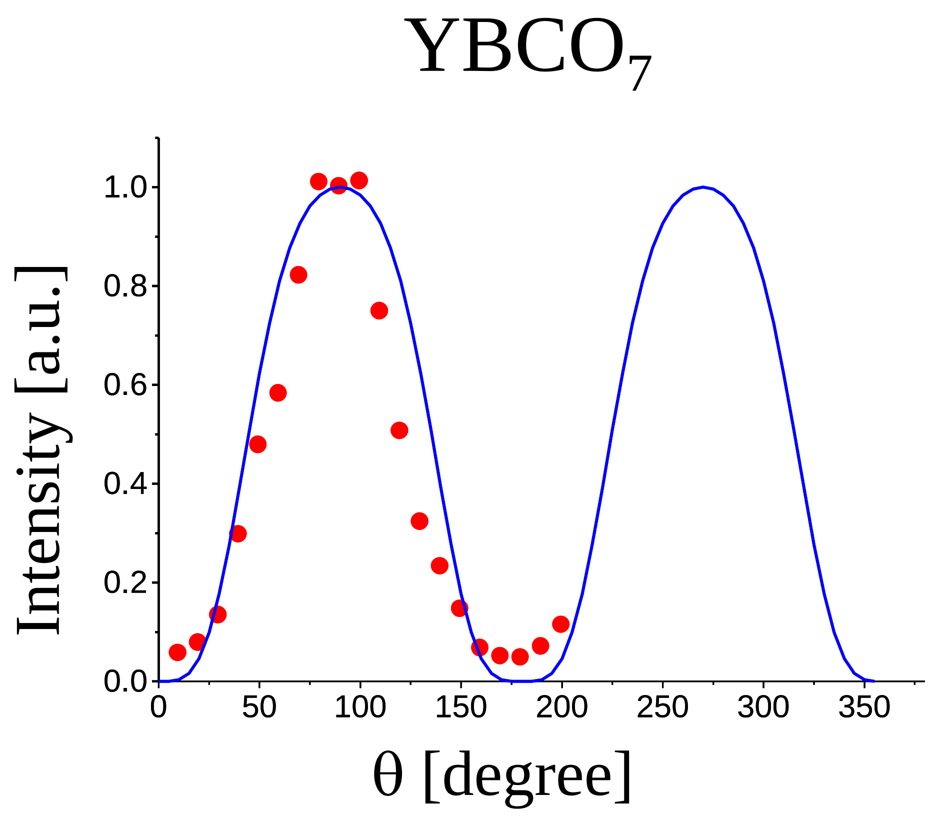

Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

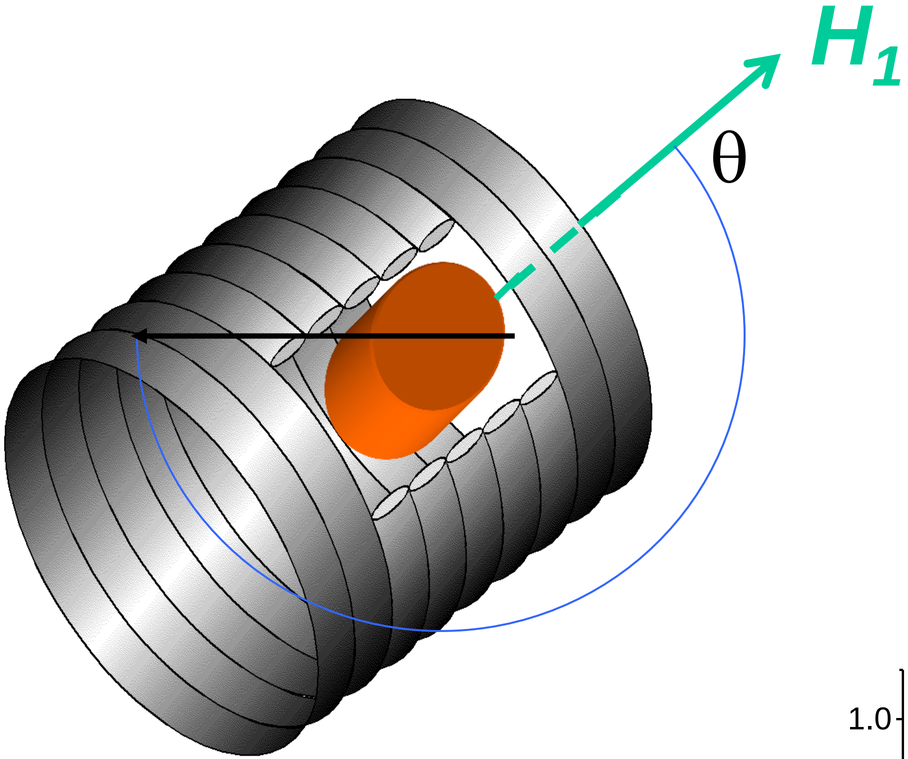

H_1
θ

$YBCO_7$


Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

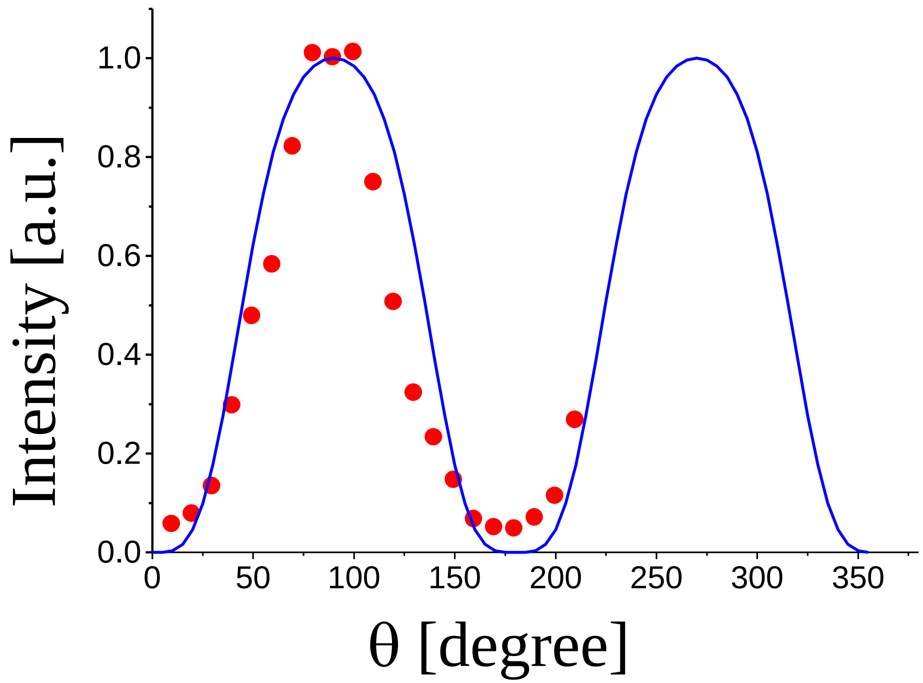

H1
θ


YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

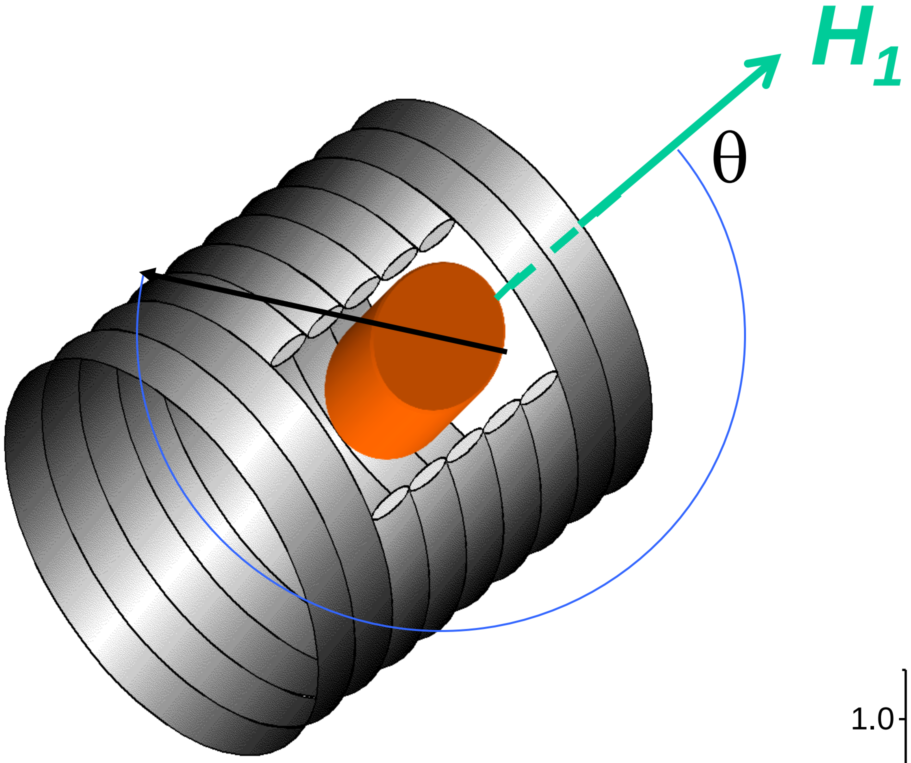


H1
θ

$YBCO_7$

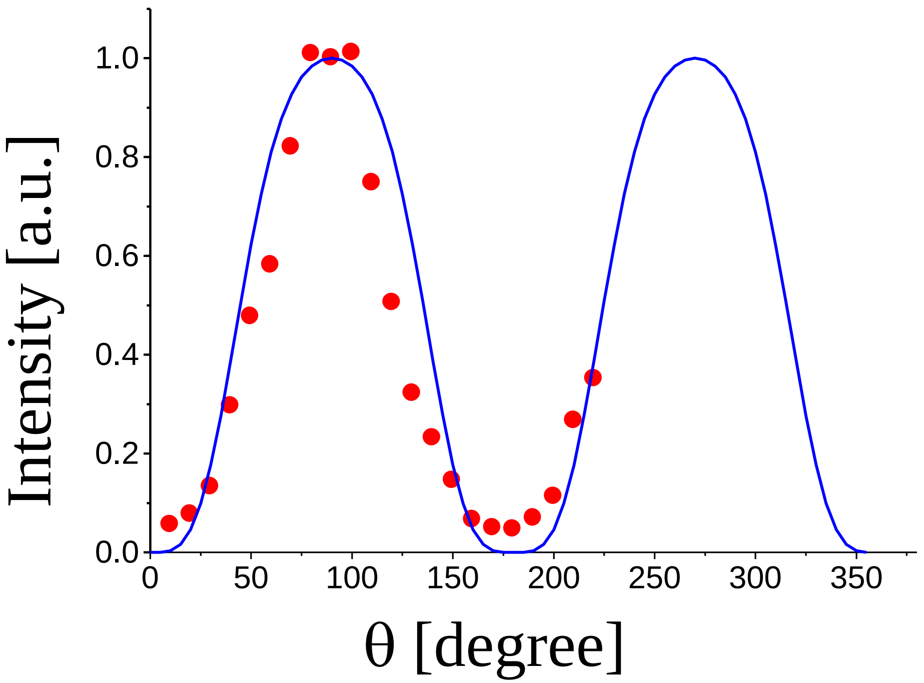


Intensity [a.u.]
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
θ [degree]

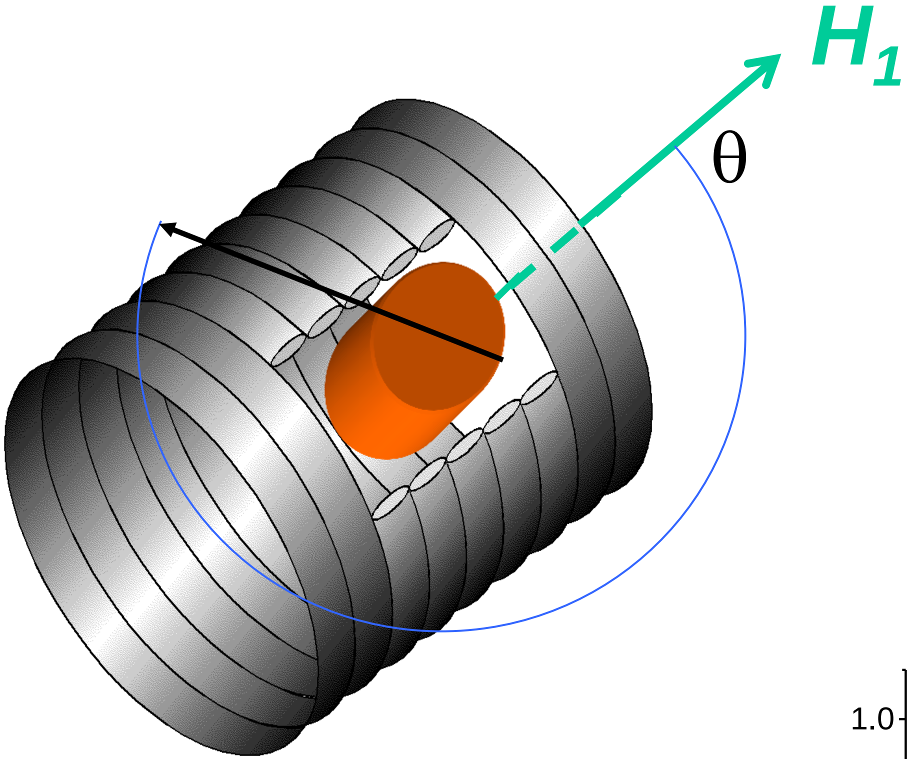


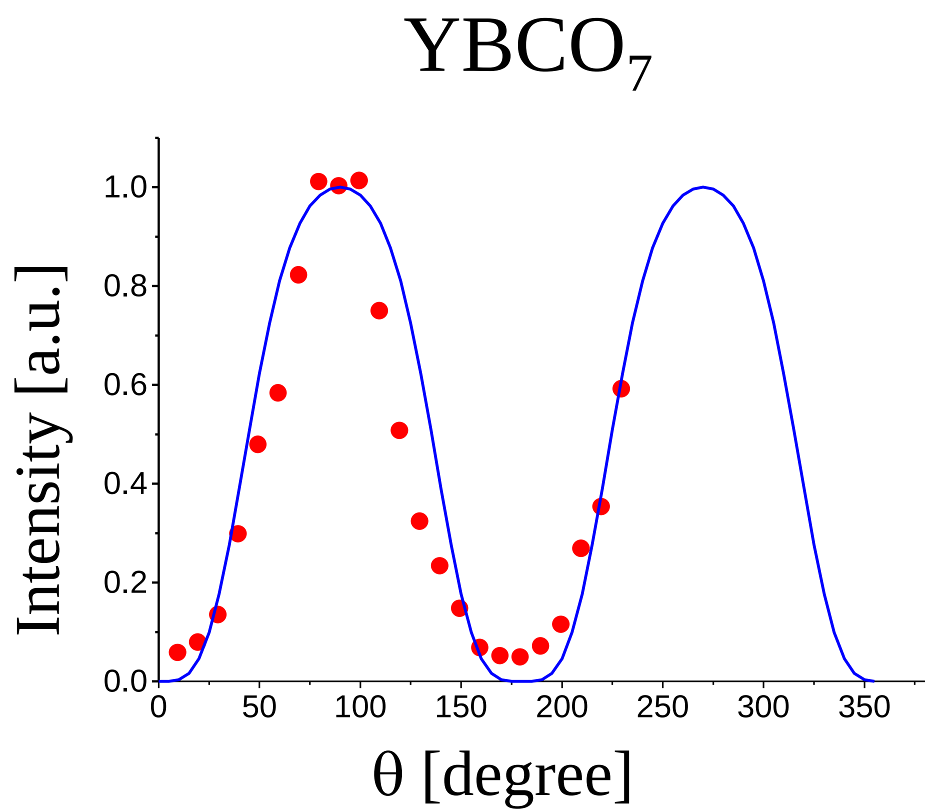
H1
θ

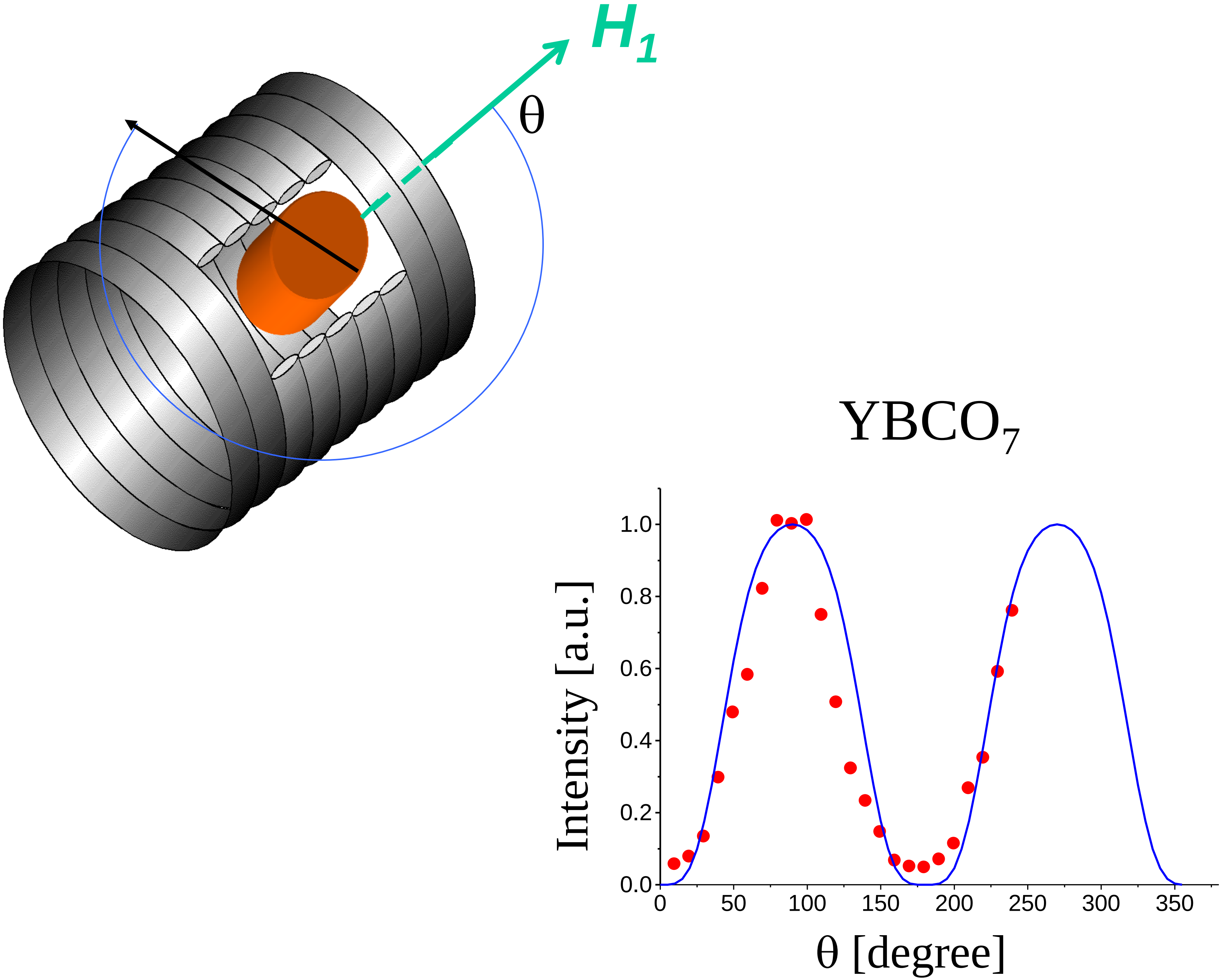
YBCO$_7$



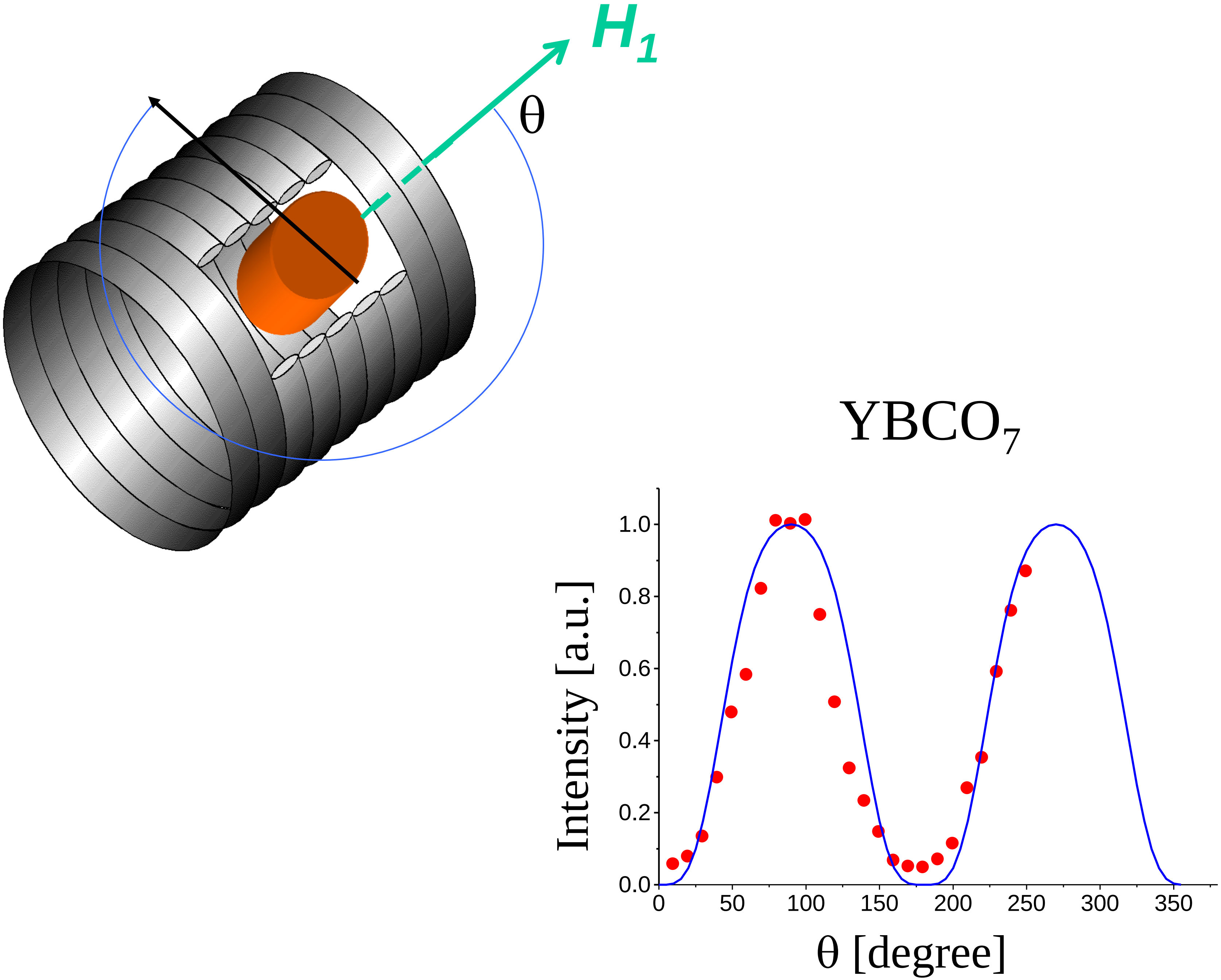
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350


H1
θ

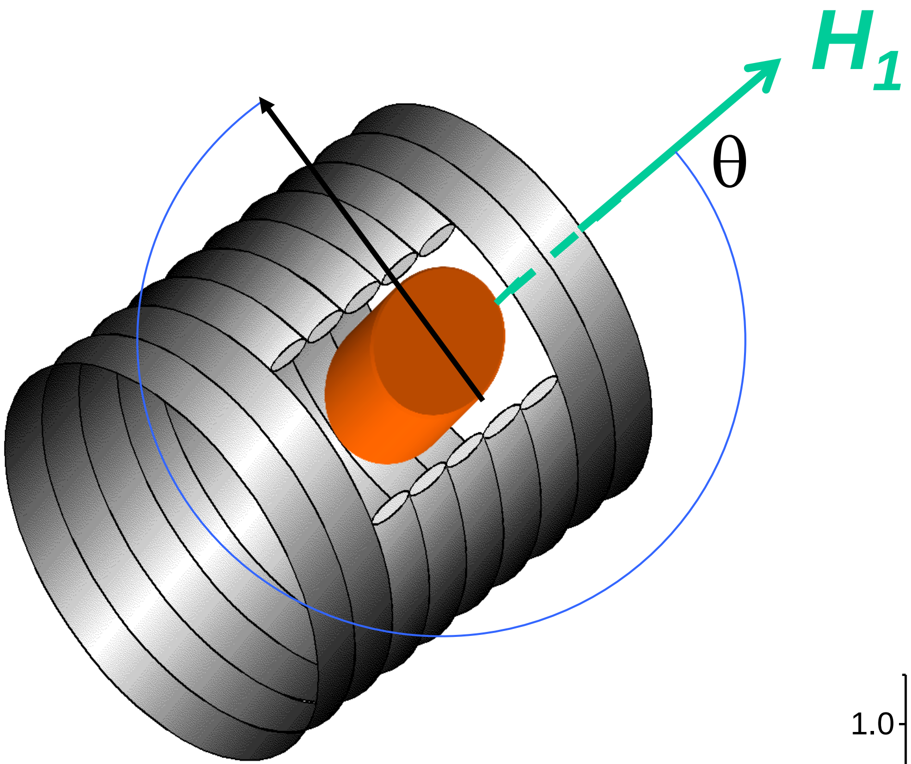

YBCO7
Intensity [a.u.]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350
θ [degree]

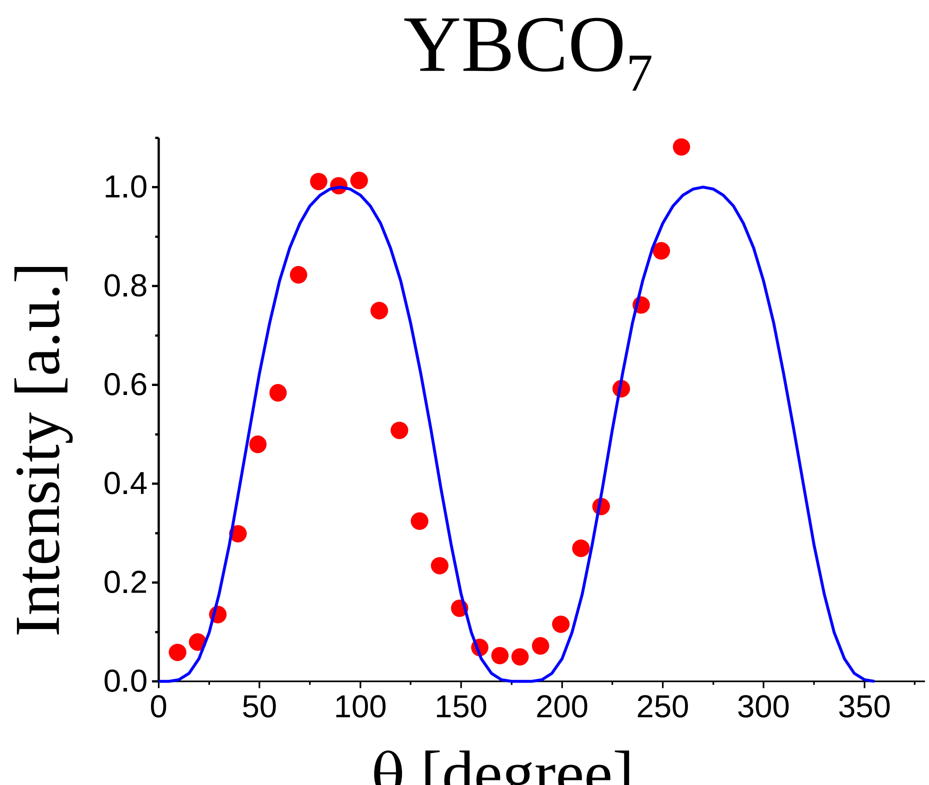


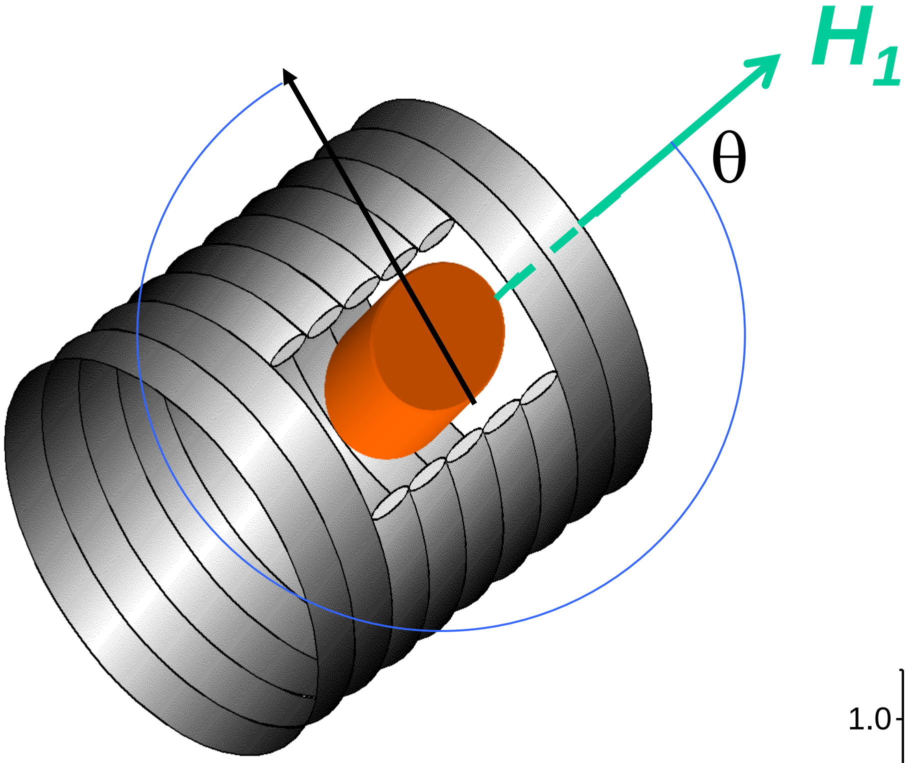
H1
θ
YBCO7
Intensity [a.u.]
θ [degree]
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350

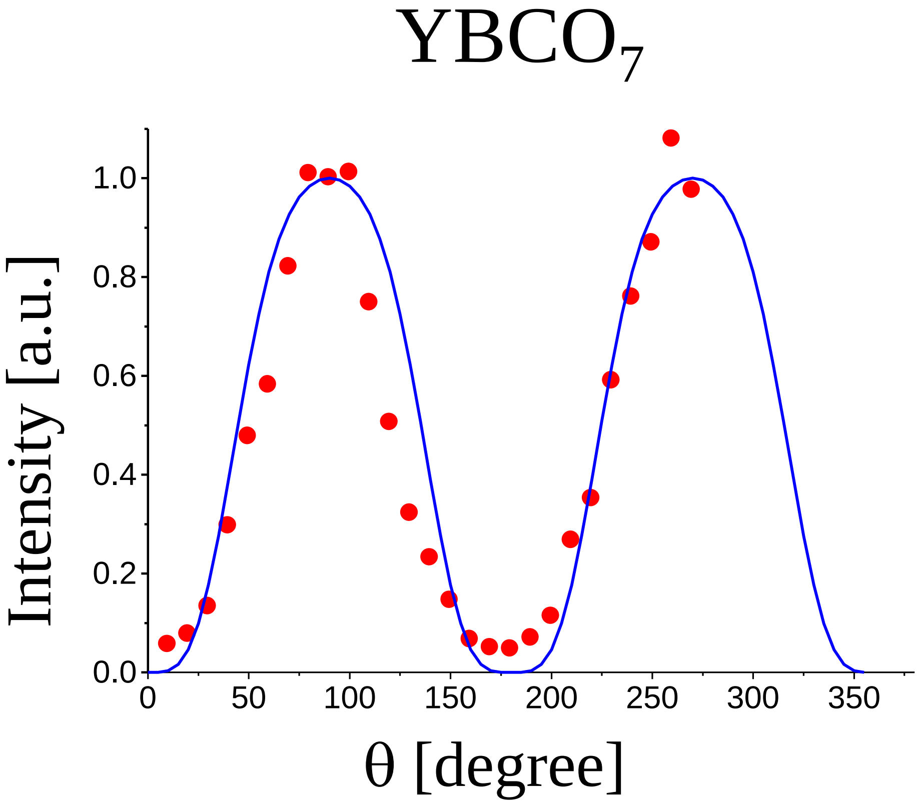


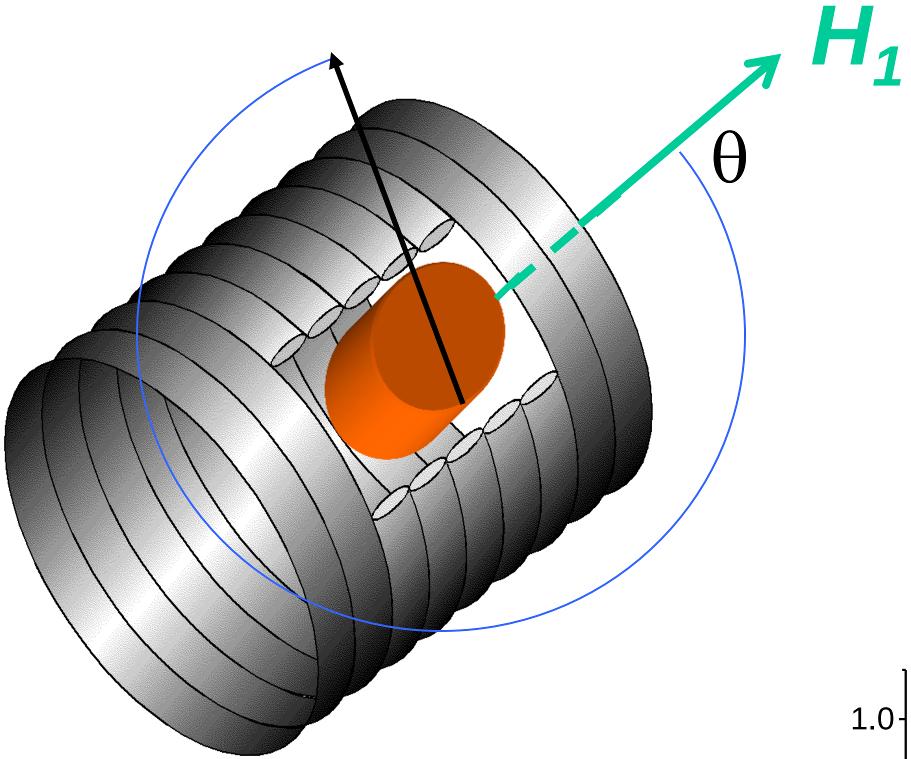
H1
θ
YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350


H1
θ

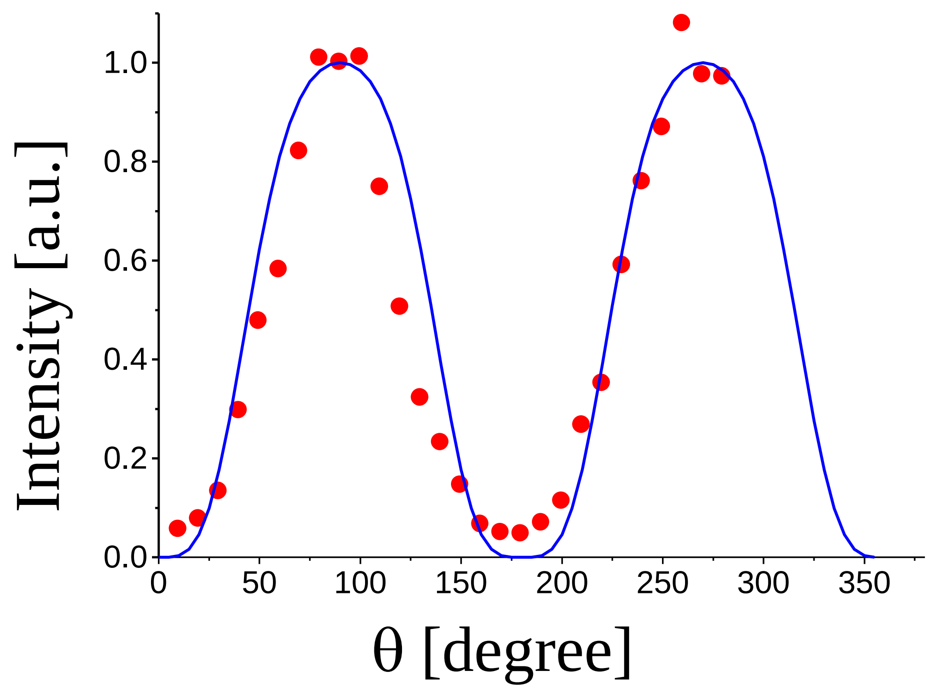

YBCO7
Intensity [a.u.]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350
θ [degree]

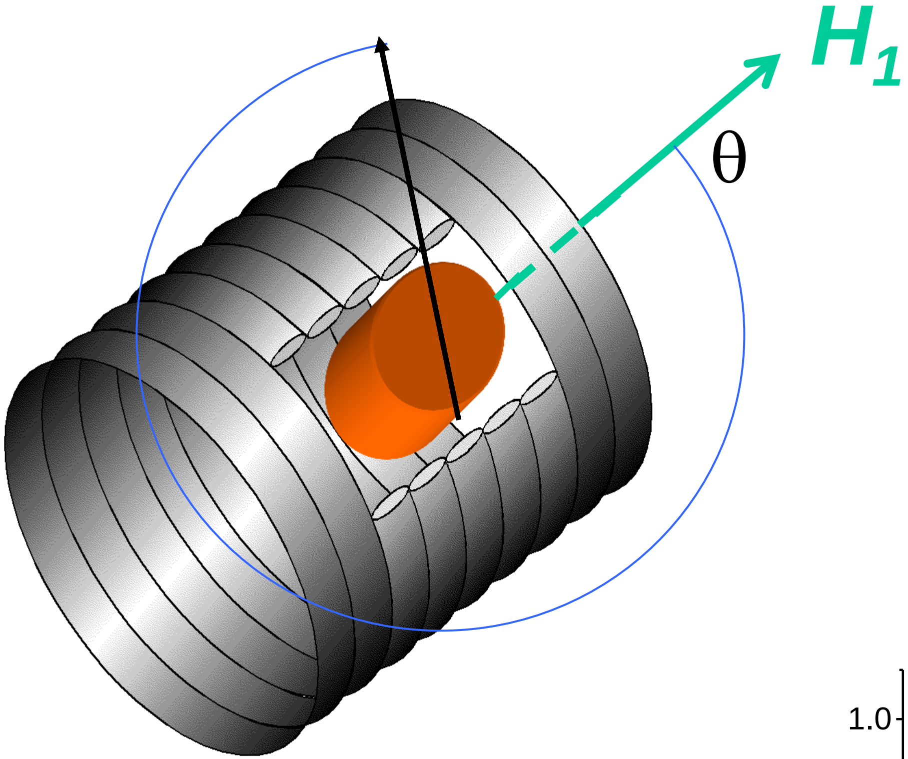

H1
θ

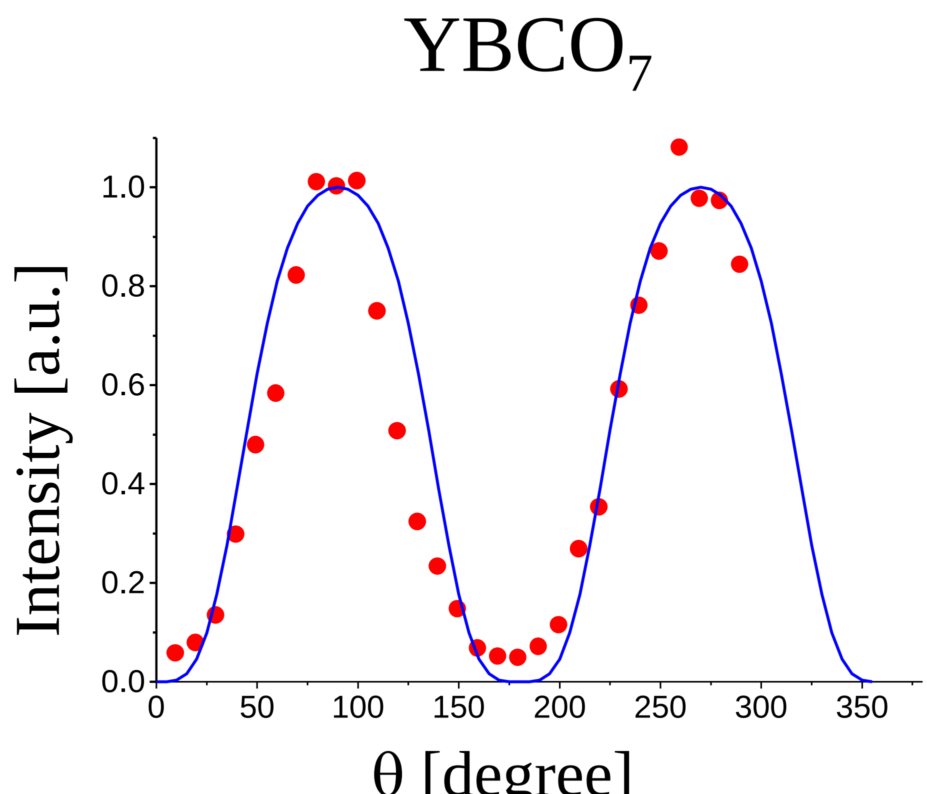

YBCO7
Intensity [a.u.]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350
θ [degree]

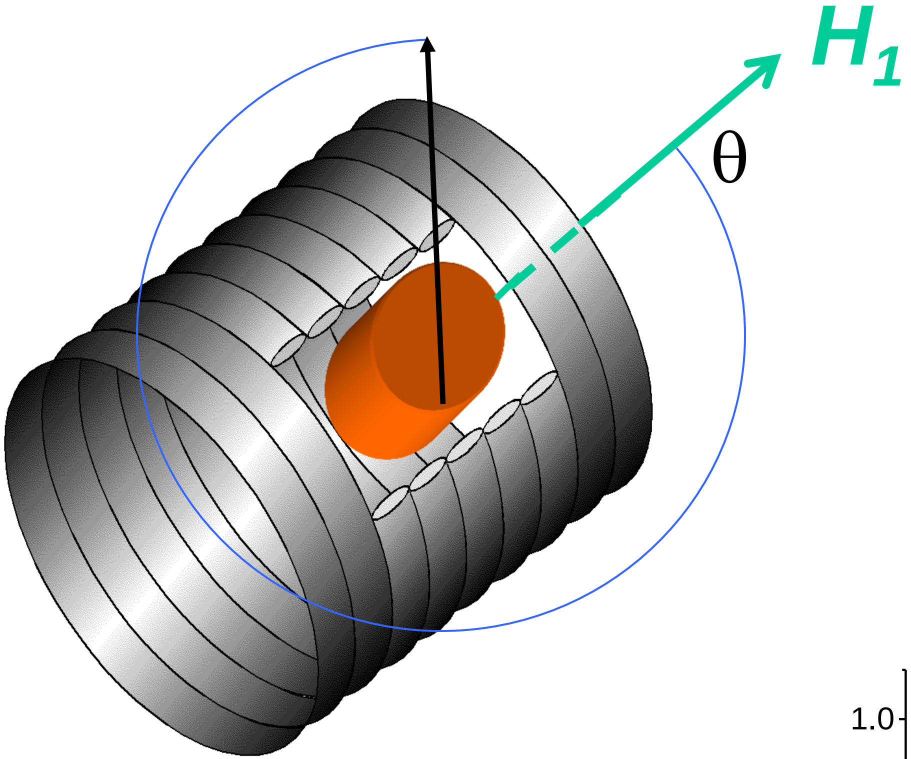

H1
θ

$YBCO_7$

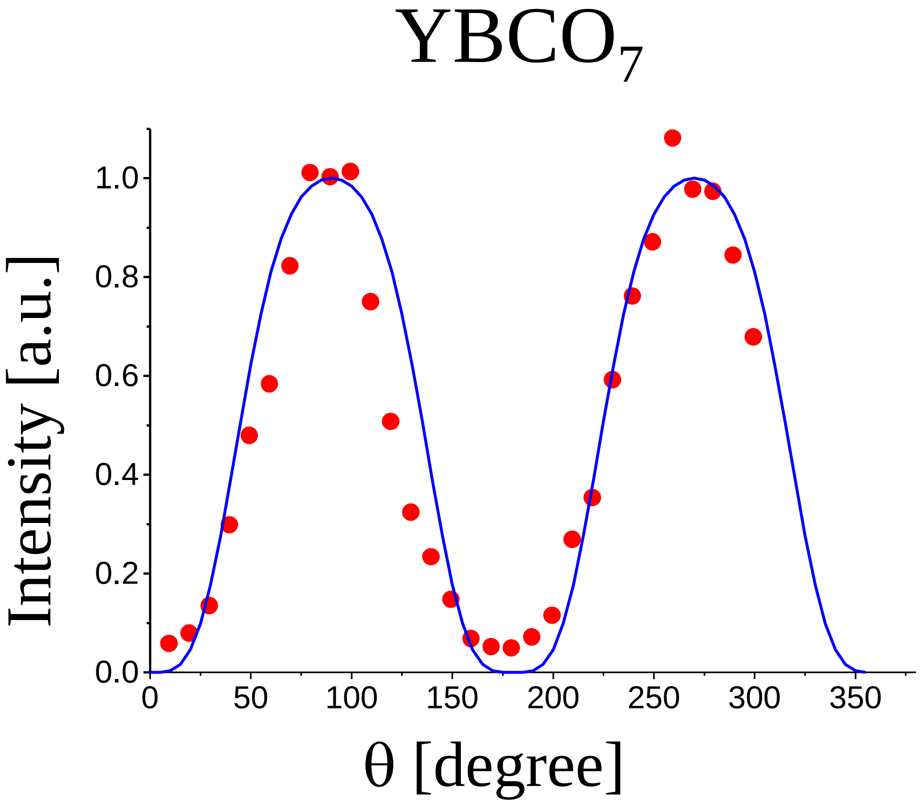

Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350


H1
θ

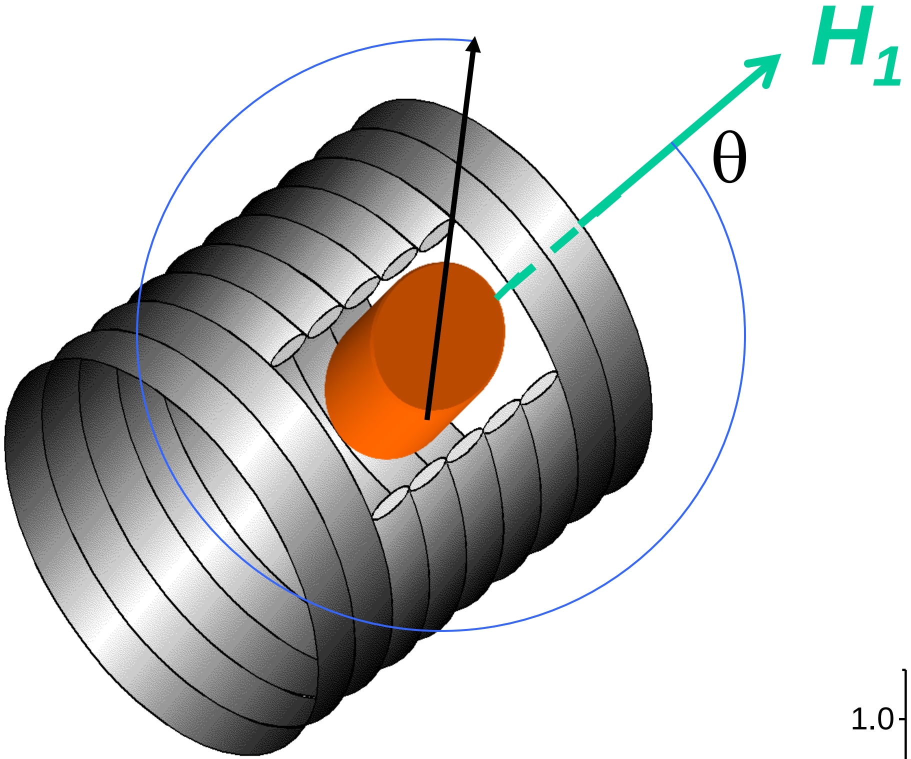

YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350



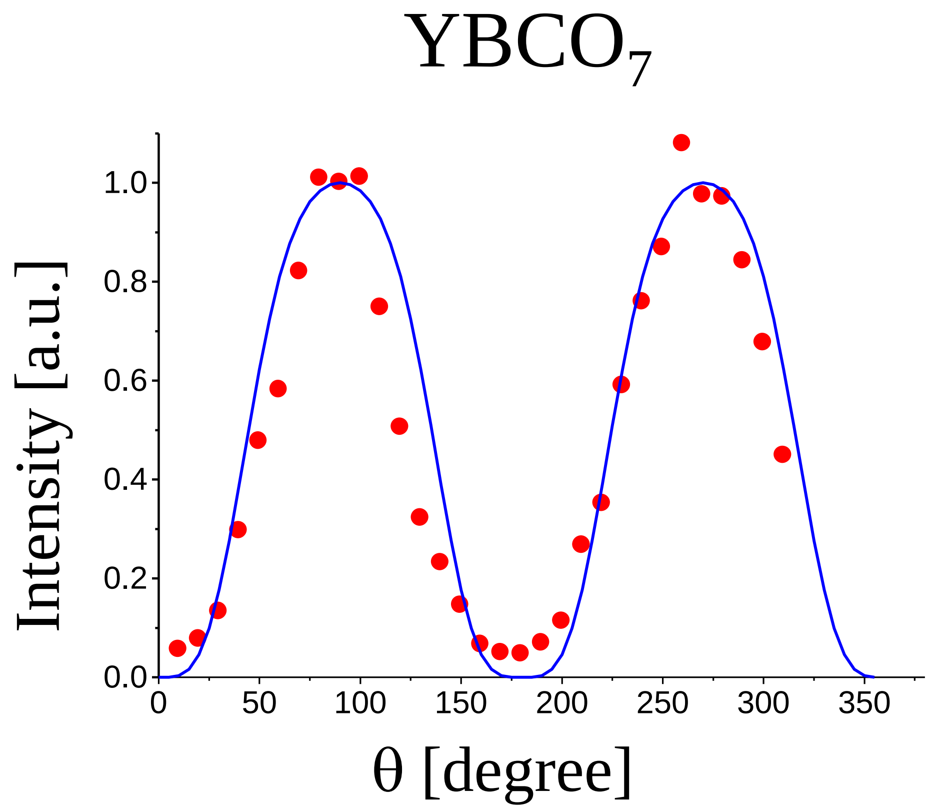
H1
θ



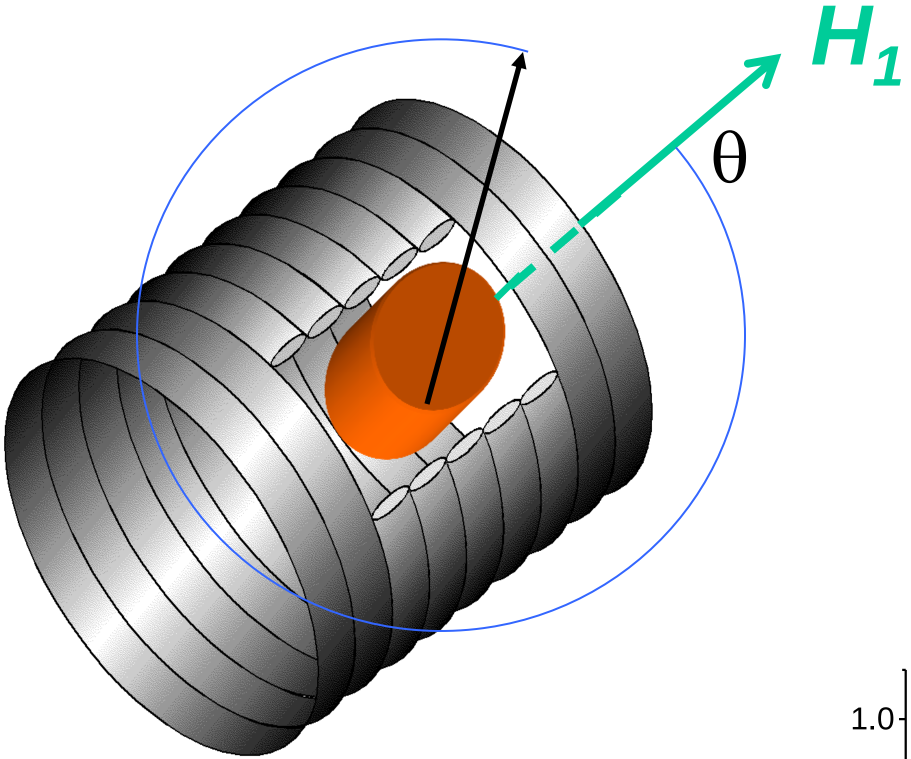
YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

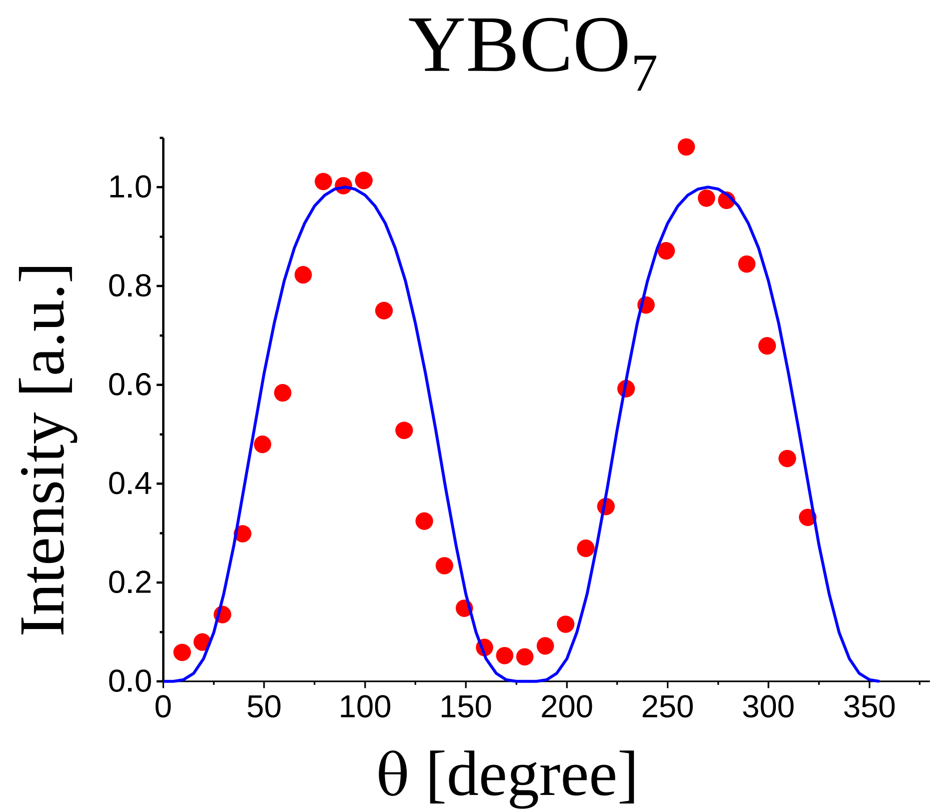


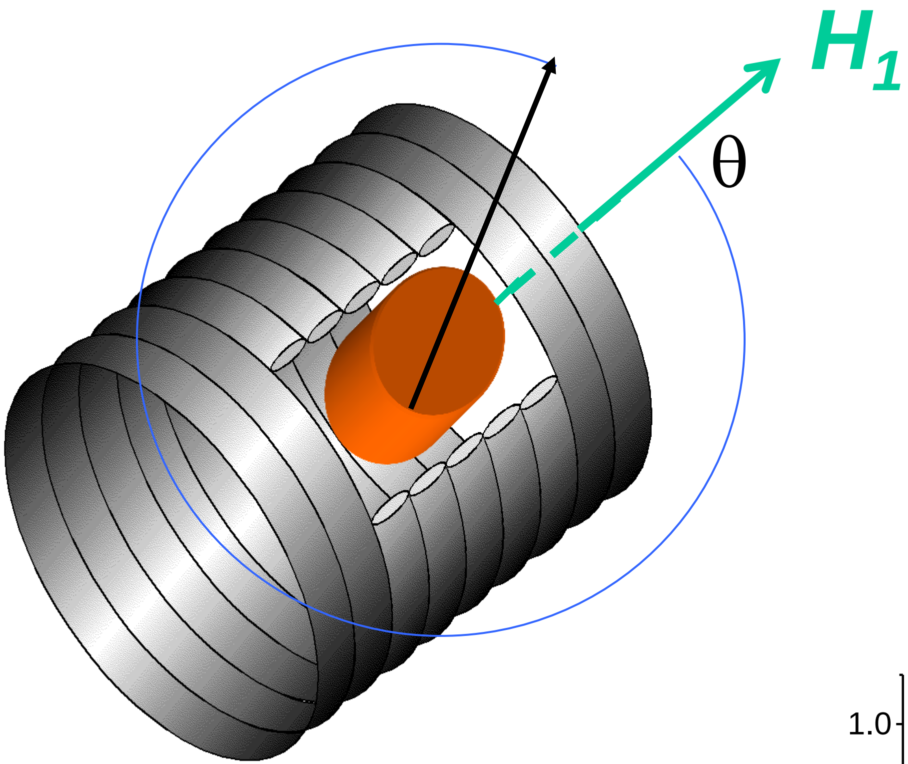
H1
θ



YBCO7
Intensity [a.u.]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350
θ [degree]

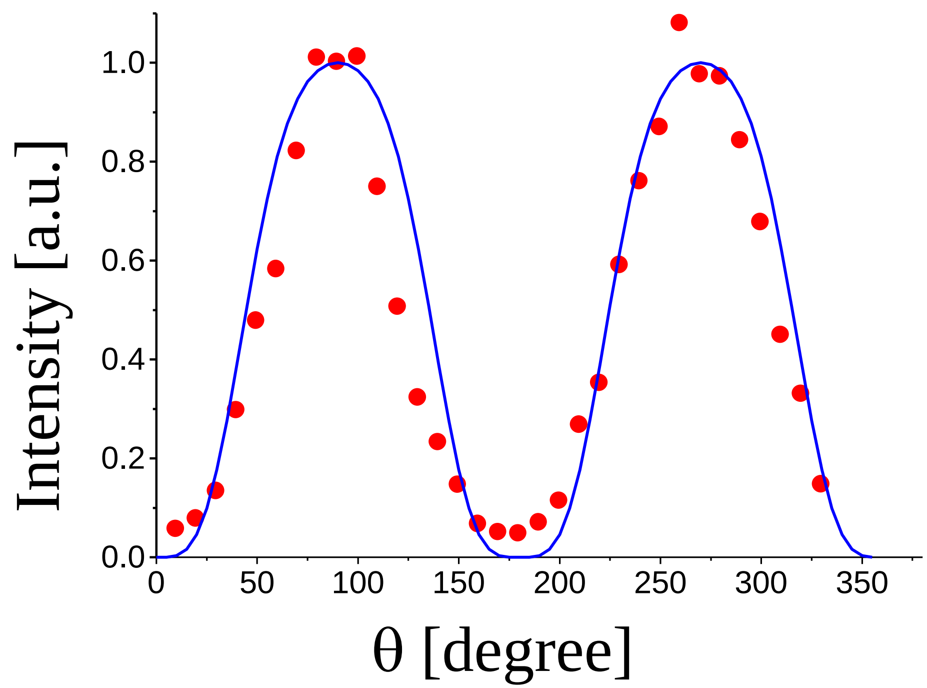

H1
θ


YBCO7
Intensity [a.u.]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350
θ [degree]

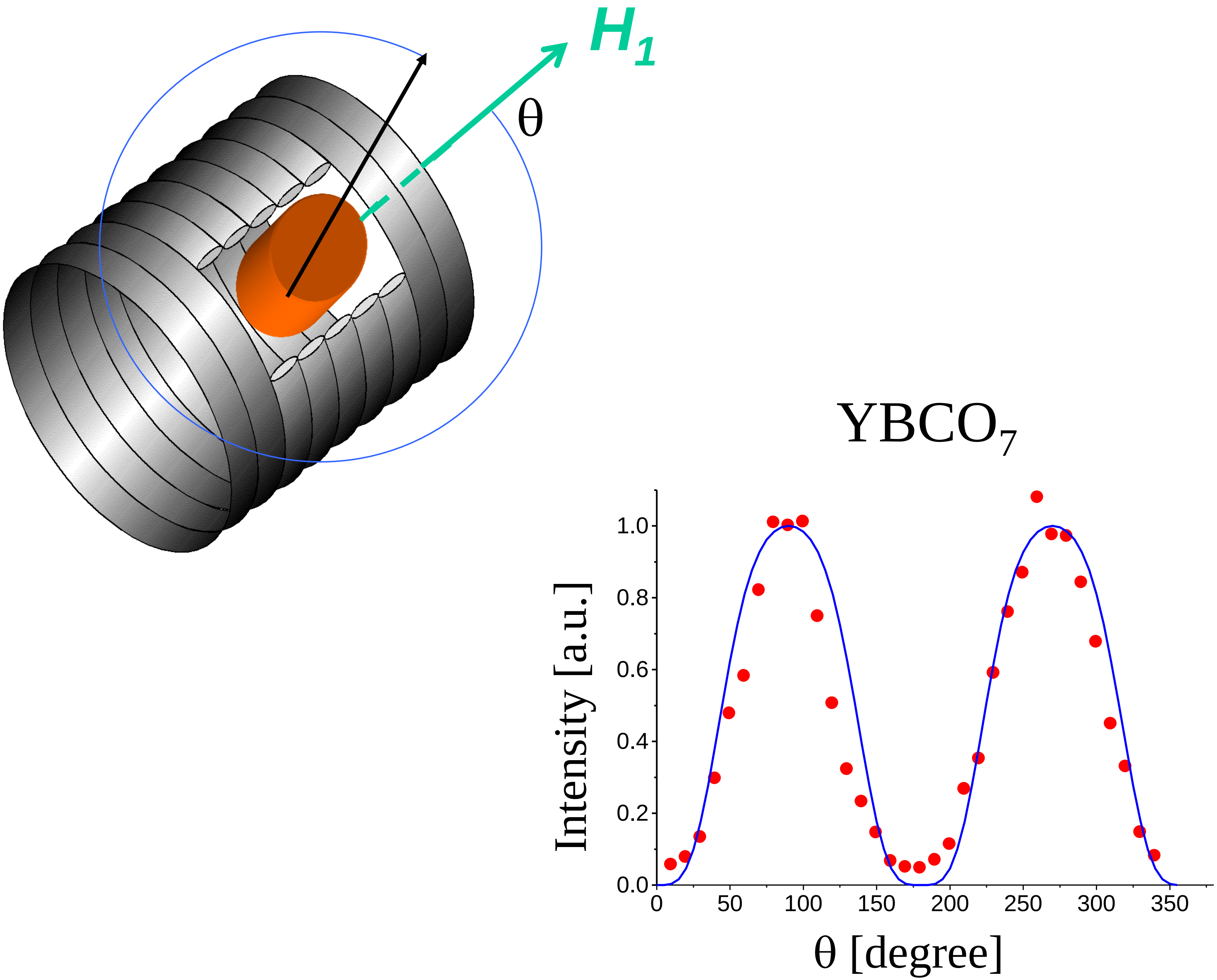


H_1
θ

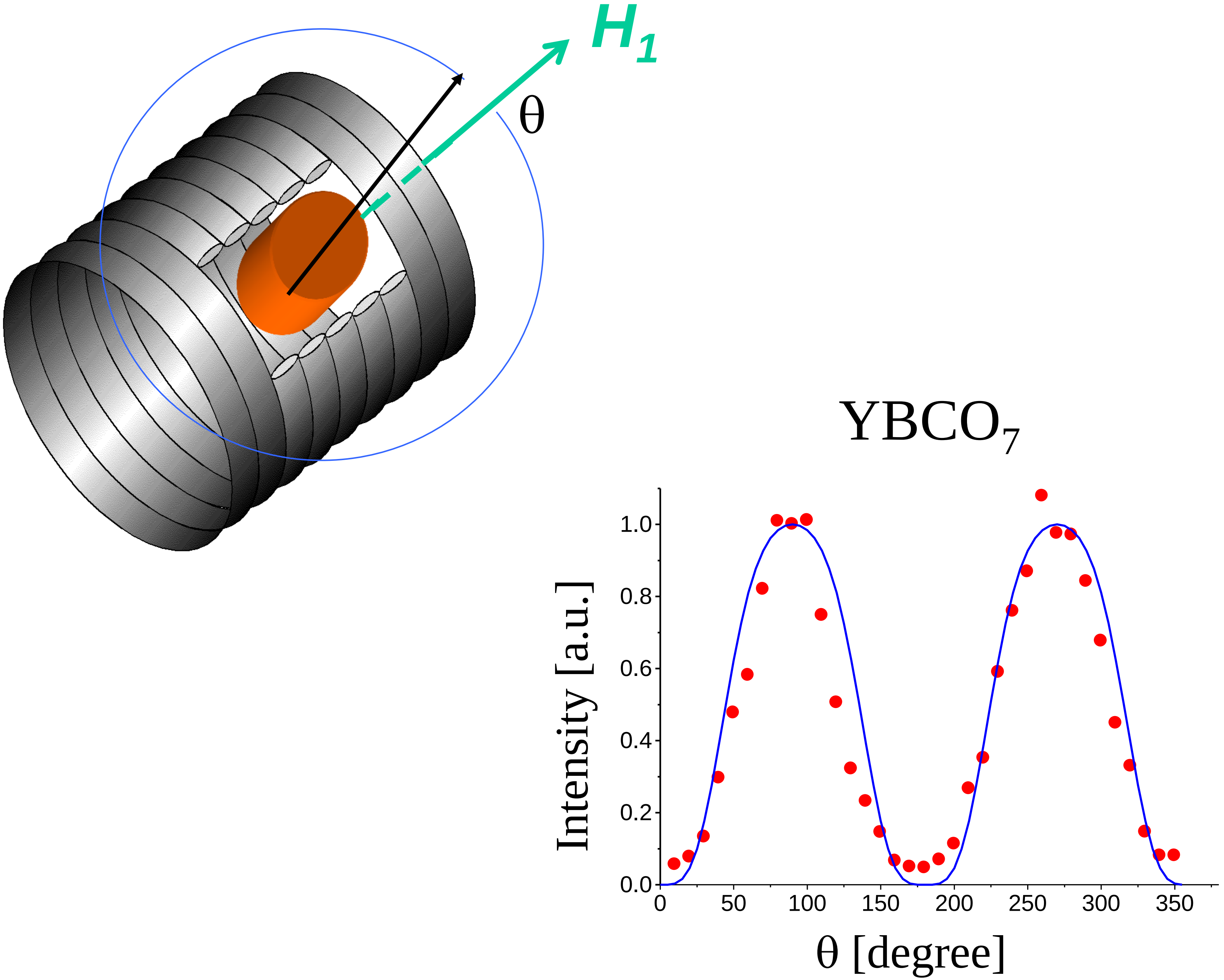
$YBCO_7$



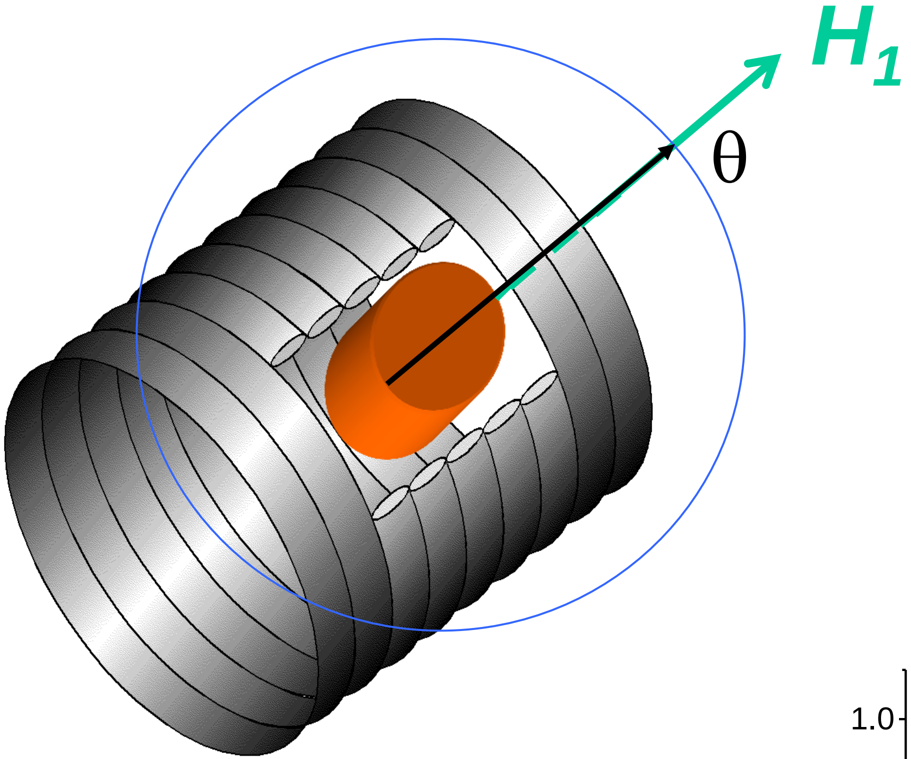
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

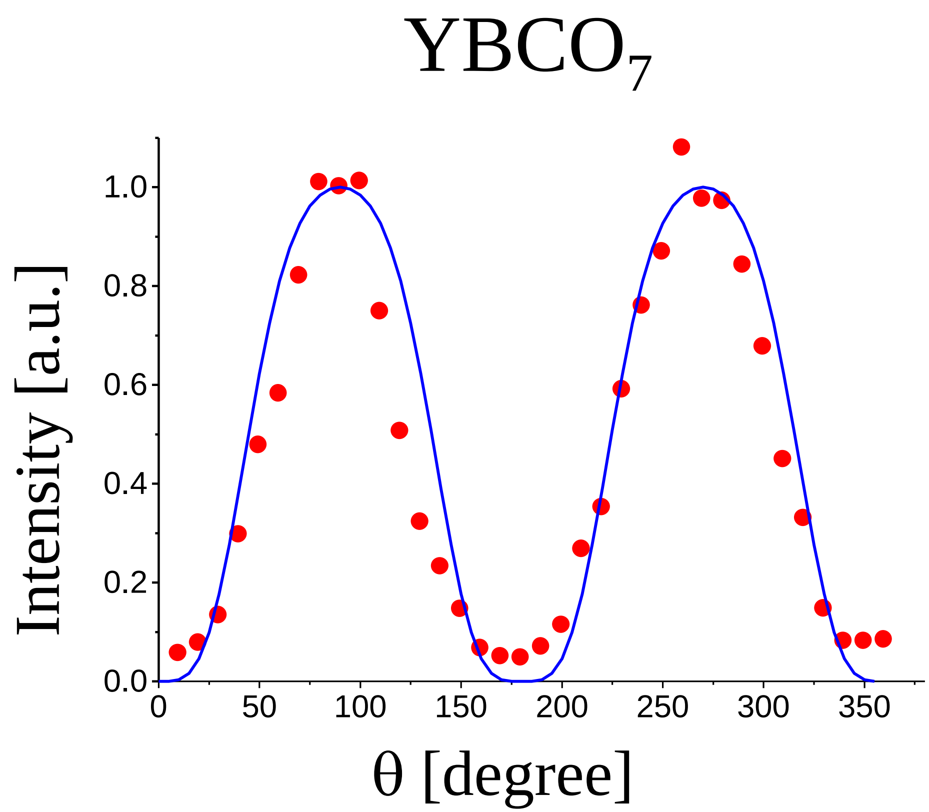


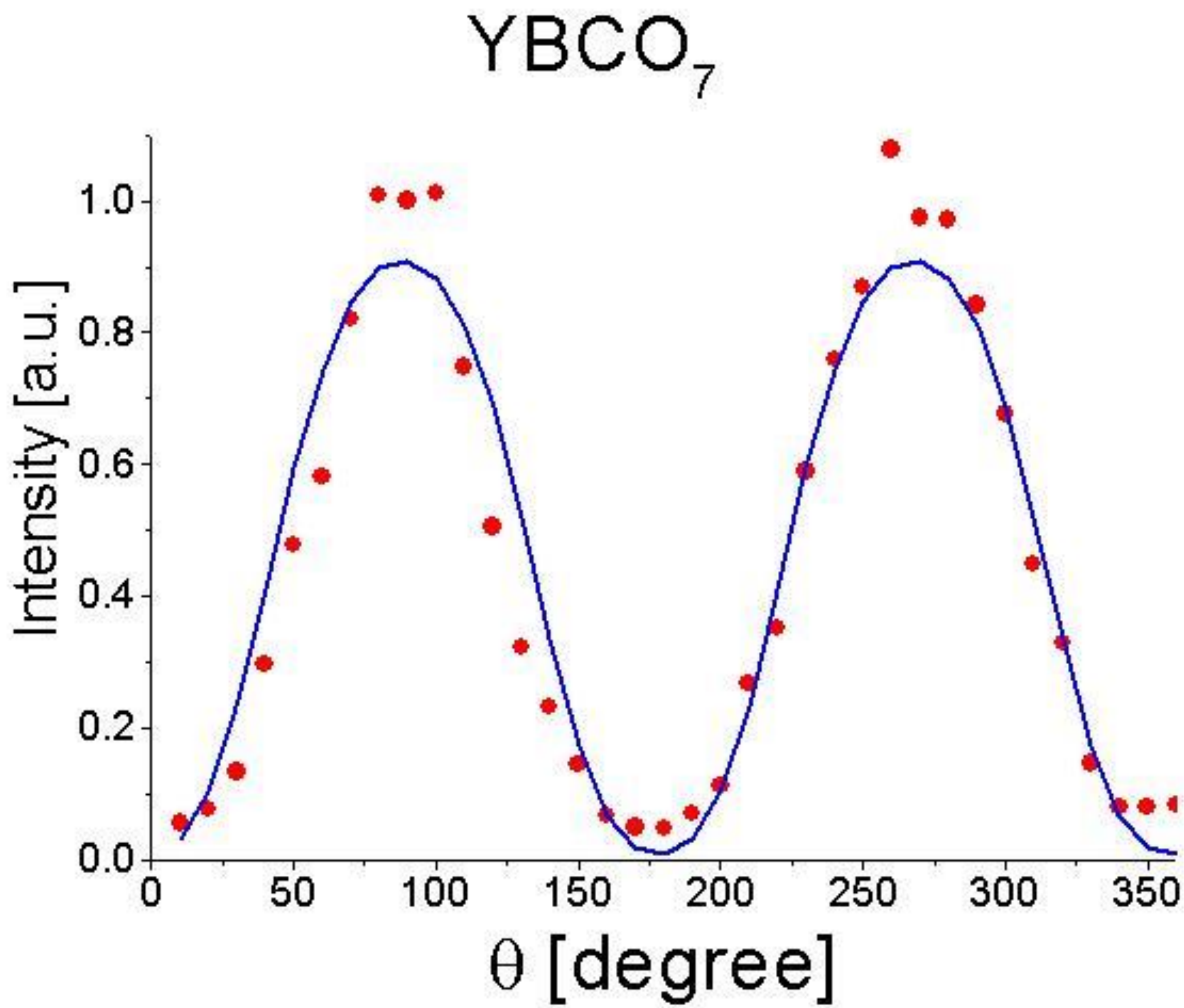
H1
θ
YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350



H1
θ
YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350


H1
θ


YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

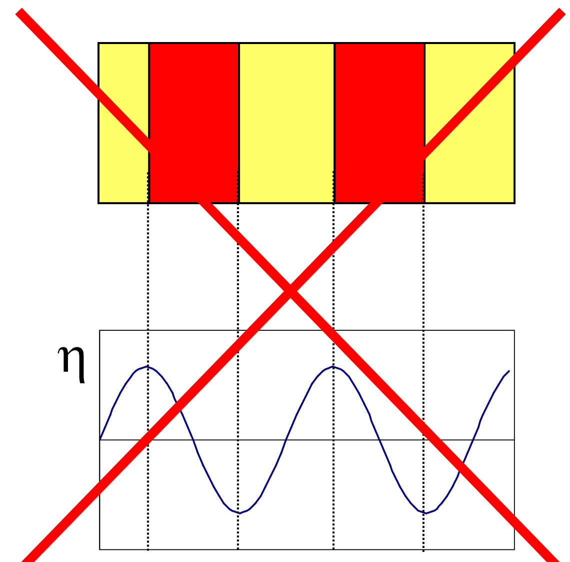

YBCO7
Intensity [a.u.]
θ [degree]
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
350

Intermediate Conclusions:

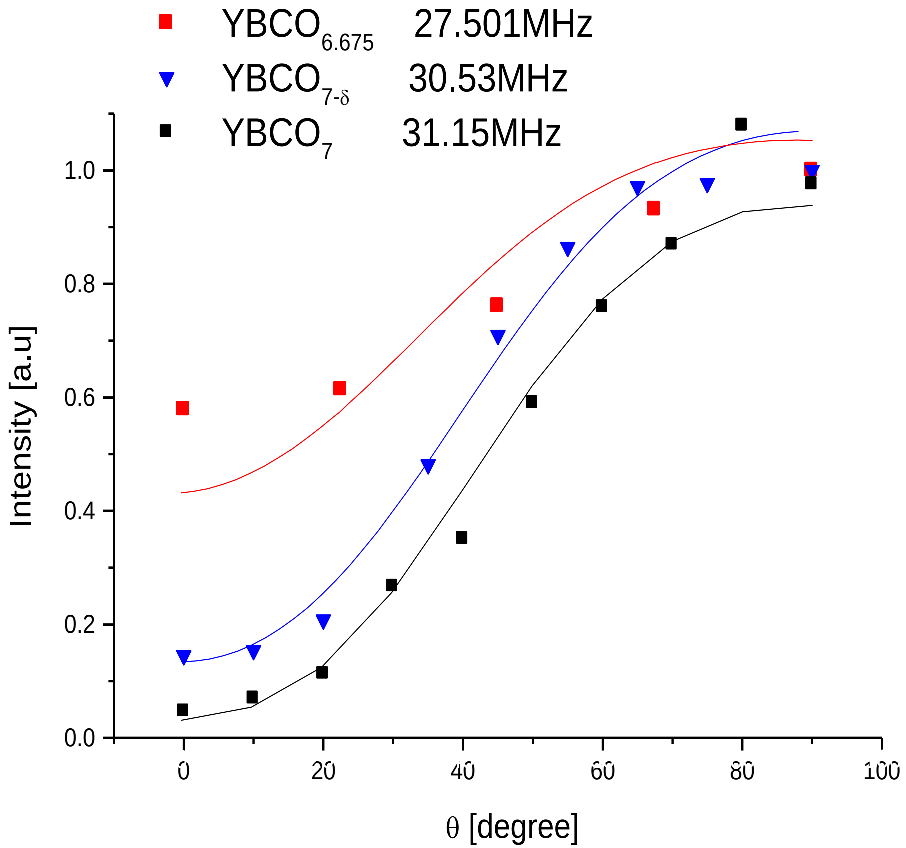
- ADNQR can be applied successfully to measure η.
- For $YBCO_7$ we obtained $\eta=0 \pm 0.1$. This agrees with the known result.
- Since we measure $|\eta|$ we can further conclude that there is no spatial fluctuation in the charge distribution.

$\langle \eta \rangle = 0$

$\langle |\eta| \rangle \neq 0$



Results of ADNQR for different samples



$\eta=1 \pm 0.1$ $YBCO_{6.675}$

$\eta=0.6 \pm 0.1$ $YBCO_{7-\delta}$

$\eta=0 \pm 0.1$ $YBCO_7$

Higher doping ⇒ Higher homogeneity

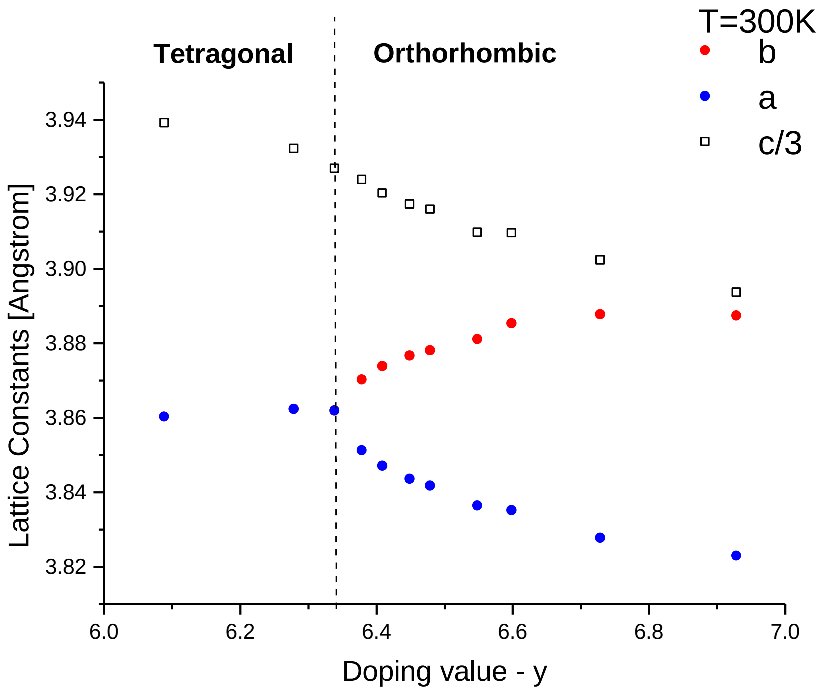
Motivation - Stripes

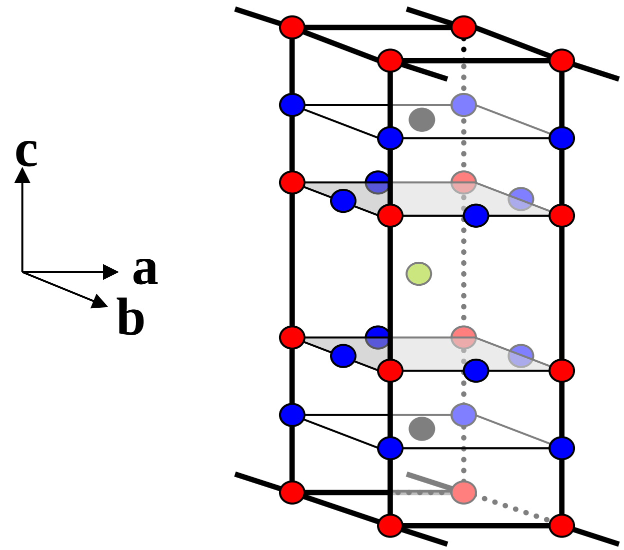
- The stripes theory claims that one dimensional charge structures in the planes play a crucial role in the mechanism of superconductivity.

- Higher doping $\Rightarrow$ more stripes $\Rightarrow$ inhomogeneity
  higher T_c

- There are experimental evidences for stripes.

Is it a structural or a charge effect?





J. D. Jorgensen *et al*, PRB , **41**, 1863 (1990)

a=b ⇒ η=0 Theory **a ≠ b ⇒ η ≠ 0** ⇒ $\eta_{6.675} < \eta_7$

Experiment $\eta_{6.675} > \eta_7$

The effect is due to charges and not to lattice structure

Summary:

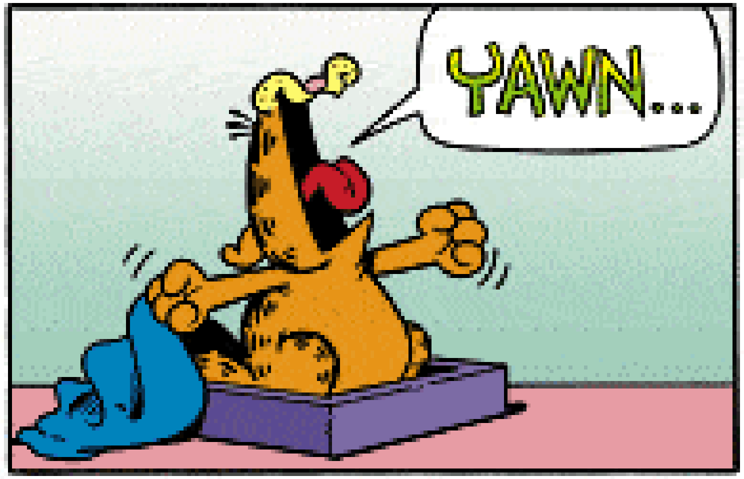
•ADNQR can be applied successfully to measure η.

• For $YBCO_7$ we obtained η=0 (high homogeneity).

• We found the first evidence for charge inhomogeneity in the bulk of highly doped YBCO ($YBCO_{6.675}$).

•We can safely say that $YBCO_{6.675}$ is less homogenous than $YBCO_7$.

There is an anticorrelation between T_c and homogeneity



Acknowledgements

Prof. Amit Keren

Prof. Emil Polturak

Galina Bazalitsky

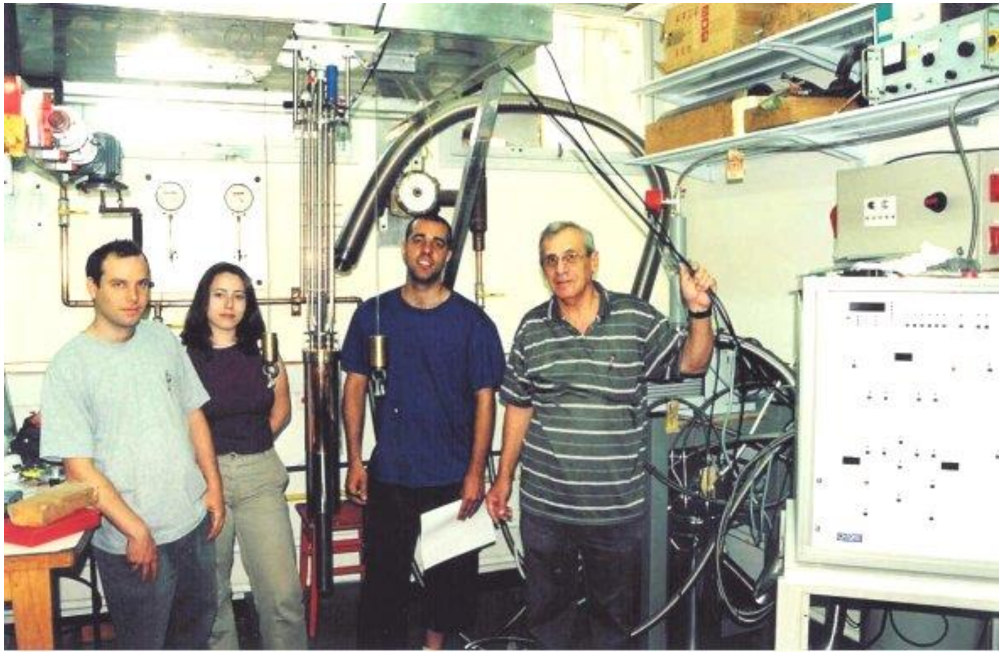
Mordehai Ayalon

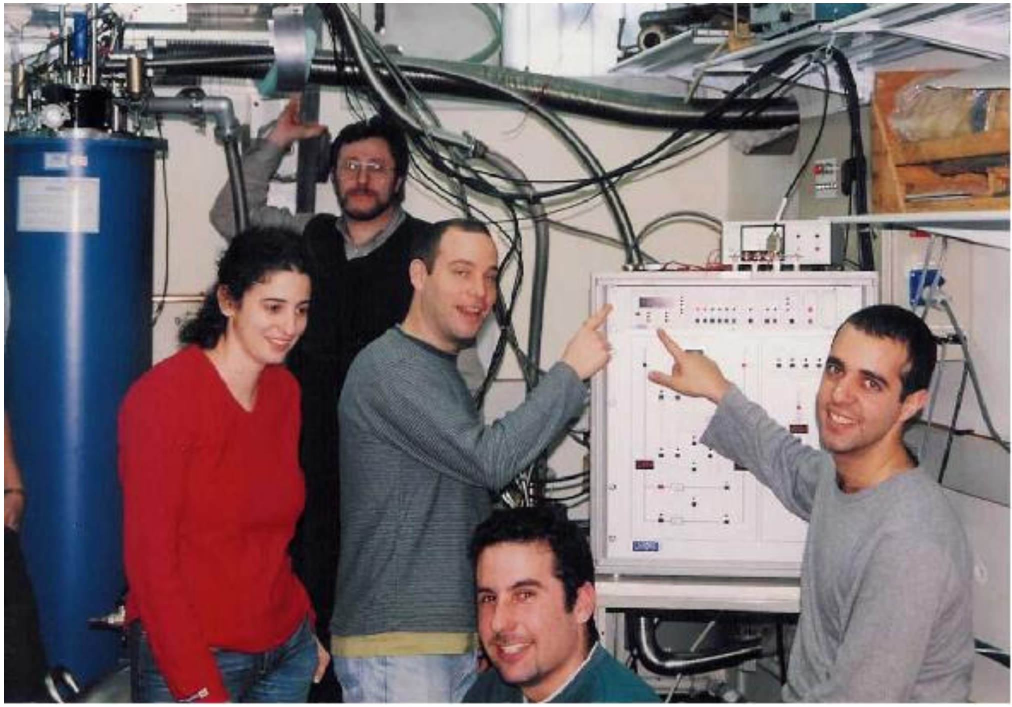
Shmuel Hoida

Leonid Iomin

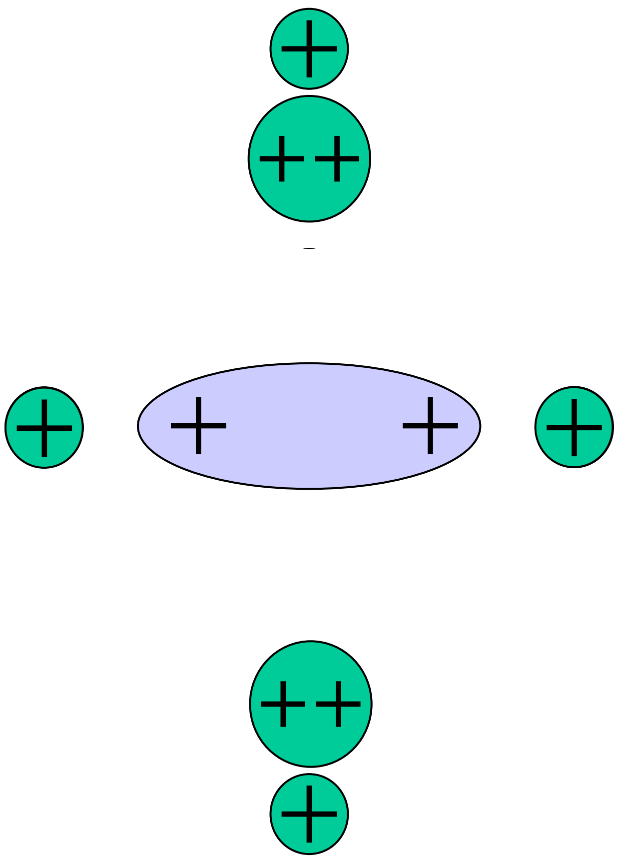
Rinat Assa, Ariel Maniv, Oshri Peleg, Eva Segal, Oren Shafir, Meni Shay, Lior Shkedy

Amit Kanigel





Electric quadrupole interaction



$$V(\mathbf{r}) \Longrightarrow V_{ij} = \frac{\partial^2 V}{\partial r_i \partial r_j}$$

$$V_{xx} + V_{yy} + V_{zz} = 0$$

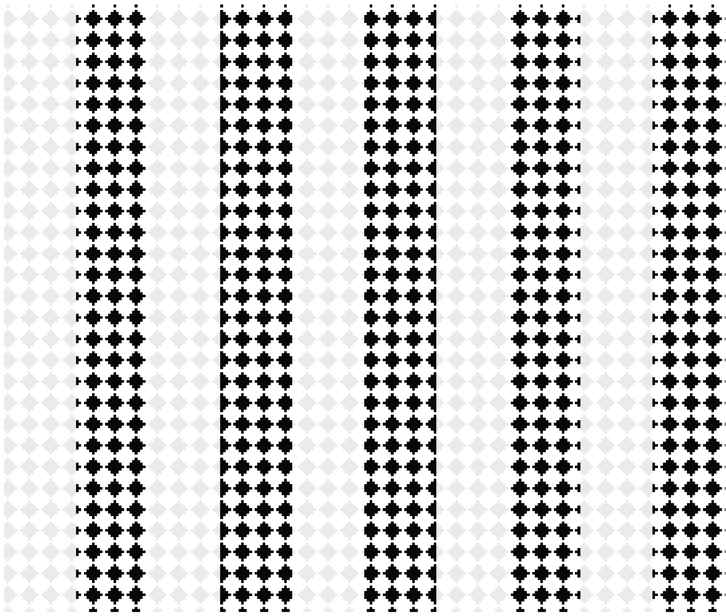
$$\nu_q \propto \frac{V_{zz}}{e} \qquad \eta = \frac{V_{xx} - V_{yy}}{V_{zz}} \Rightarrow \quad 0 \le |\eta| \le 1$$

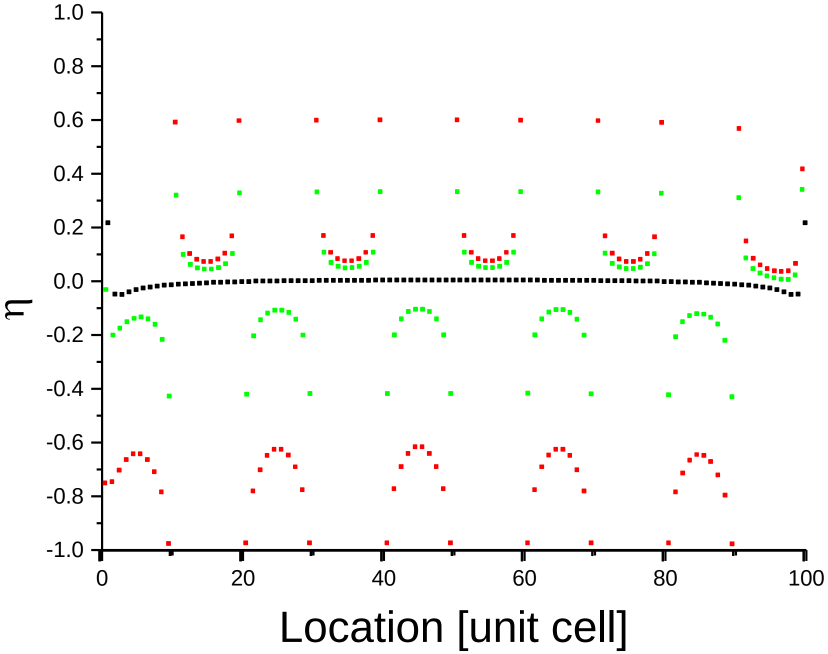
$$V_{ij} = \nu_q \begin{bmatrix} -\frac{1-\eta}{2} & 0 & 0 \\ 0 & -\frac{1+\eta}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\Downarrow$$

Nucleus $I_x^2 \quad I_y^2 \quad I_z^2$ $\Longrightarrow$

$$\hat{H}_q = \frac{\hbar \nu_q}{6}\left[3\hat{I}_z^2 - \hat{I}^2 + \eta(\hat{I}_x^2 - \hat{I}_y^2)\right]$$

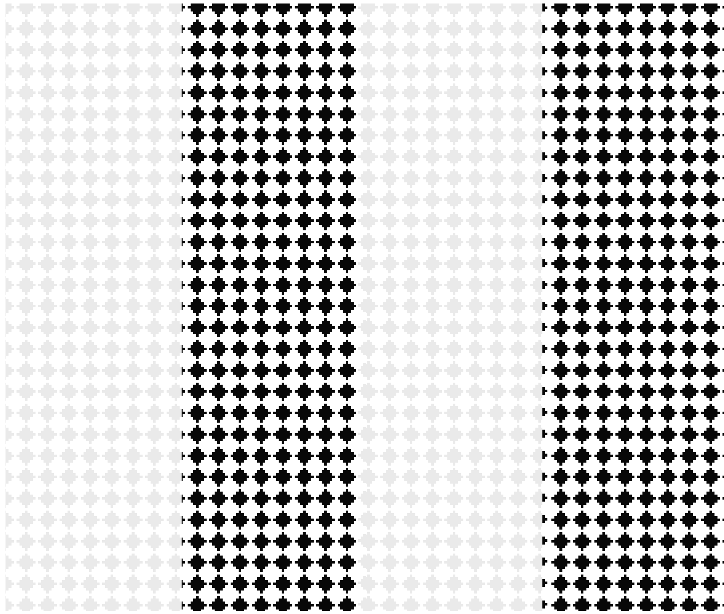


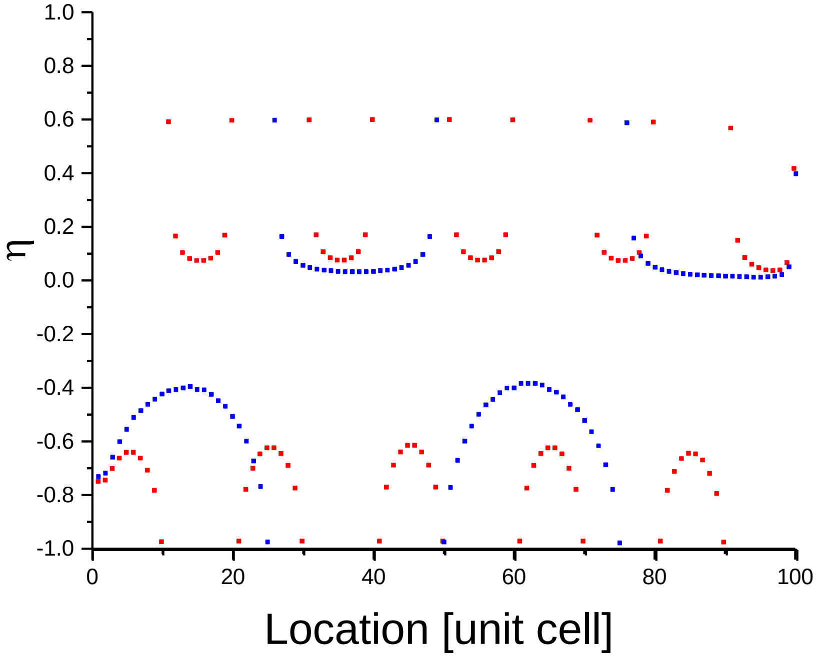


$< |\eta| > = 0.01$

$< |\eta| > = 0.15$

$< |\eta| > = 0.47$




1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
η
0
20
40
60
80
100
Location [unit cell]

< |η| >=0.32

< |η| >=0.47