Experimental and numerical study of the low temperature behaviour of $LiYbF_4$

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Outline

Introduction: $LiREF_4$

- RE = Rare Earth ions
  - magnetic : Yb, Ho, Er, Gd, Tb
  - non magnetic : Y

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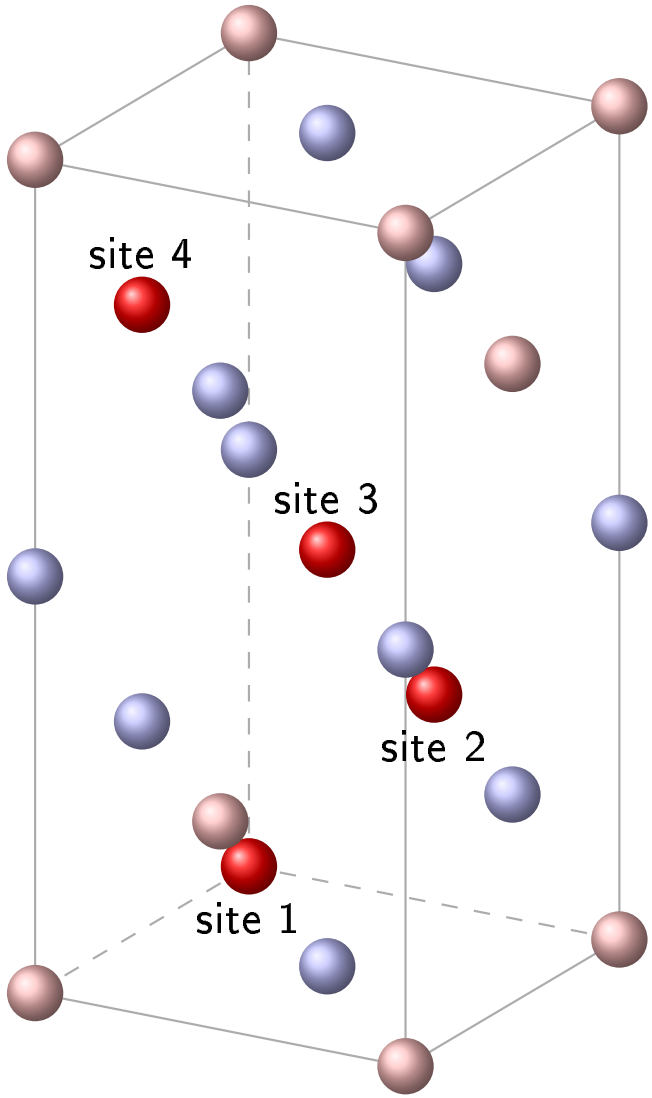
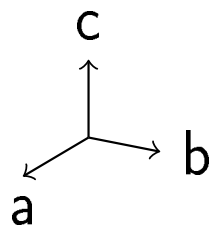
- Dipolar coupled quantum magnets.
- Possible apparition of both ferromagnetic ($LiHoF_4$) and antiferromagnetic ($LiErF_4$, $LiYbF_4$) order.
- Disordered systems with apparition of a spin glass phase:
  - Dilution of the magnetic moments with non magnetic Y ions
  - Mixing of several RE ions with different anisotropies ($LiHo_{1-x}Er_xF_4$ or $LiHo_{1-x}Yb_xF_4$ for instance)

Crystalline structure of $LiREF_4$





Sites coordinates

site 1: $(0, 0, 0)$

site 2: $(0, \frac{1}{2}, \frac{1}{4})$

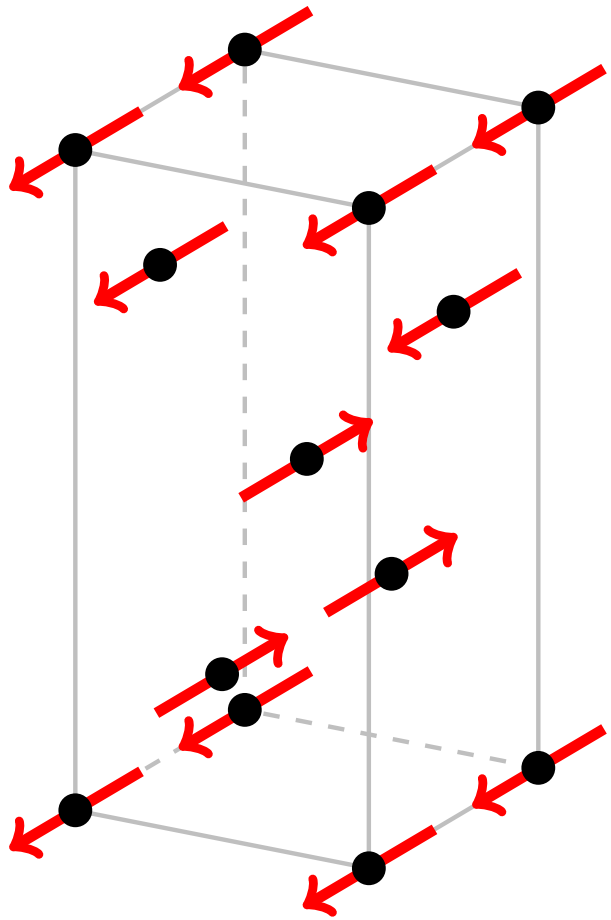
site 3: $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

site 4 : $(\frac{1}{2}, 0, \frac{3}{4})$

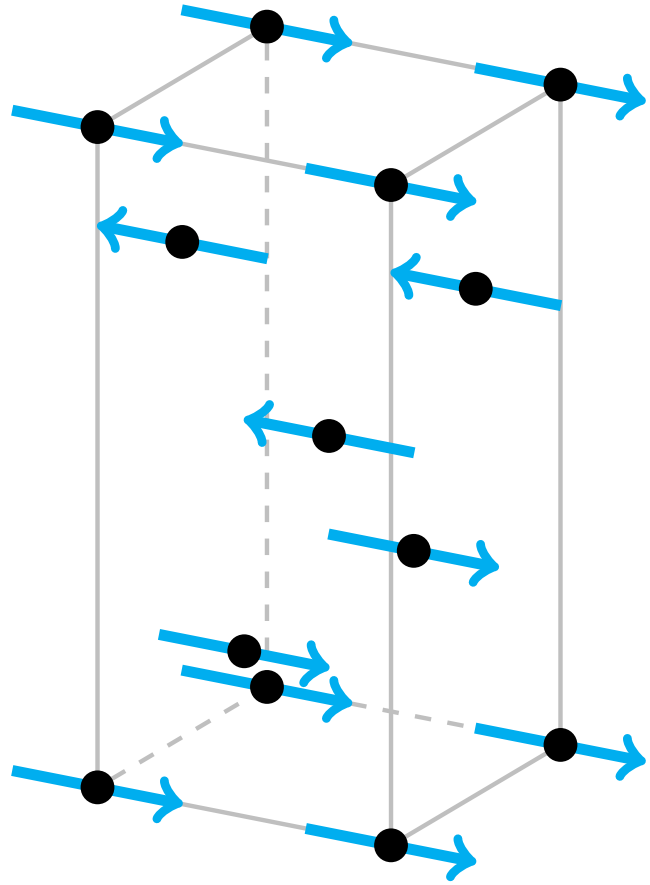
- Rare earth ions on the 4 sites in the unit cell
- Rare earth ions (in the adjacent cells)
- Li ions

The Bi-Layered AntiFerroMagnetic (BLAFM) ordered structure

Moments parallel to the a-axis



Moments parallel to the b-axis



Hamiltonian of the system

$$\mathcal{H} = \mathcal{H}_{single\ ion} + \mathcal{H}_{interactions}$$

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Crystal field

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$$\mathcal{H}_Z = -\mu_B\ g_L\ \vec{J}.\vec{B}$$

Zeeman term

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$$\mathcal{H}_{hyp} = A\ \vec{J} \cdot \vec{I}$$

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$$\mathcal{H}_{dip} = -\frac{1}{2} \sum_{i,j} g_{L_i}\ g_{L_j}\ \mu_B^2\ \vec{J}_i D_{ij} \vec{J}_j$$

Dipolar interactions

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$$\mathcal{H}_{ex} = \sum_{(n.n.)}^{i,j} \mathcal{J}_{ij}\ \vec{J}_i \cdot \vec{J}_j$$

Exchange interactions

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Exchange interactions

Negligible !

$$\mathcal{H}_Z = -\mu_B\ g_L\ \vec{J}.\vec{B}$$

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Dipolar interactions

The crystal field

- Electric field created by the charge distribution around the ion
- Responsible for the magnetic anisotropy

$$\mathcal{H}_{cf} = \sum_i \sum_{lm} B_l^m \hat{O}_l^m(J_i)$$

	$LiYbF_4$	$LiErF_4$	$LiHoF_4$
$10^3 B_2^0$	663 ± 80	60.23	-60.0
$10^3 B_4^0$	12.5 ± 4.5	-0.12	0.350
$10^3 B_4^4(c)$	102 ± 41	-4.33	3.60
$10^5 B_6^0$	-62 ± 73	-0.19	4.0
$10^3 B_6^4(c)$	-16.0 ± 1.7	-0.085	0.070
$10^6 B_6^4(s)$	0	-22.7	9.8

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	$LiYbF_4$	**$LiYbF_4$ (new)**	$LiErF_4$	$LiHoF_4$
$10^3 B_2^0$	663 ± 80	**646.2**	60.23	-60.0
$10^3 B_4^0$	12.5 ± 4.5	**15.3**	-0.12	0.350
$10^3 B_4^4(c)$	102 ± 41	**116.5**	-4.33	3.60
$10^5 B_6^0$	-62 ± 73	**-68.6**	-0.19	4.0
$10^3 B_6^4(c)$	-16.0 ± 1.7	**-15.2**	-0.085	0.070
$10^6 B_6^4(s)$	0	**0**	-22.7	9.8

Mean field approximation

- Fluctuations are neglected and effective mean fields are introduced :

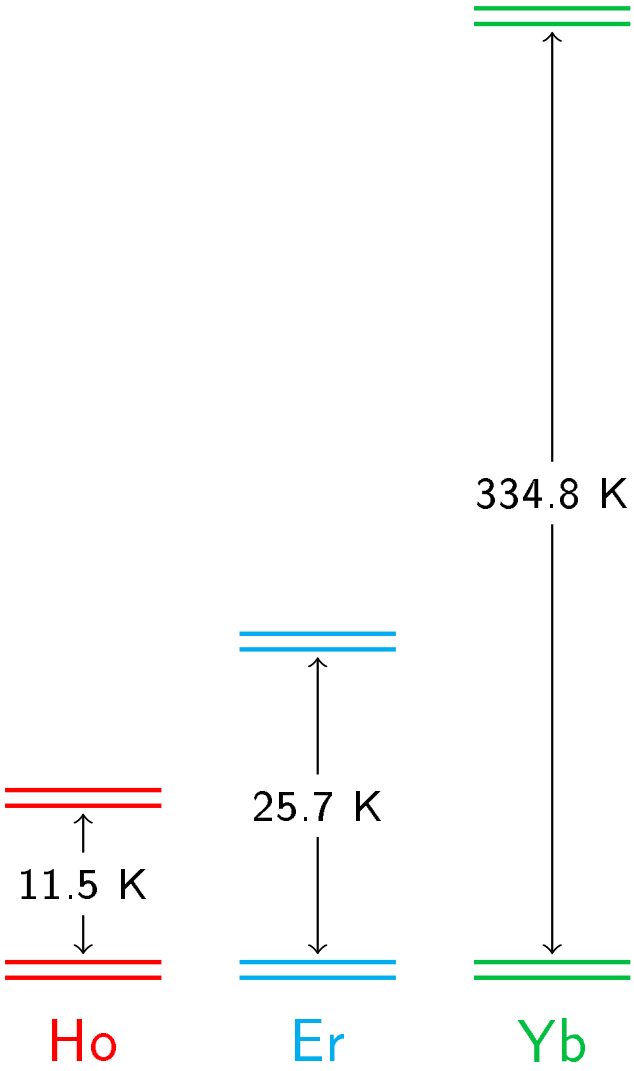
$$\vec{h}^i_{\text{eff}} = \sum_{j=1}^{4} \tilde{D}_{ij} \langle \mu_B \; g_{L_j} \; \vec{J}_j \rangle$$

- Hamiltonians decoupled for each site :

$$\mathcal{H}^{\text{MF}}_{dip} = \sum_{i=1}^{4} g_{L_i} \; \mu_B \; \vec{J}_i \cdot \vec{h}^i_{\text{eff}}$$

- Algorithm :
  - Computation of $\tilde{D}_{ij}$
  - Initialization of the moments $\langle J_i \rangle$
  - Computation of h^i_{eff} for the current configuration
  - Diagonalization of $\mathcal{H}^{\text{MF}}_i$ and update of $\langle J_i \rangle$
  - Evaluation of $\Delta = \sum_i |\langle J_i \rangle^{new} - \langle J_i \rangle^{old}|$

Monte Carlo calculation: the quantum effective model



Effective model for $\mathcal{H}_0 = \mathcal{H}_{cf} + \mathcal{H}_Z$

- Diagonalization of $\mathcal{H}_0$
- Projection of J and $\mathcal{H}_0$ on the subspace of the doublet
- Diagonalization of $\tilde{J}_z$
- Obtention of a basis $\{|+\rangle, |-\rangle\}$

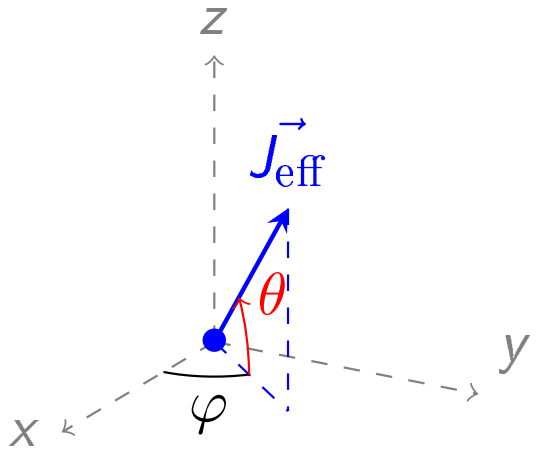
State:

$$|\alpha, \beta\rangle = \cos(\alpha)\,|+\rangle + e^{i\beta}\sin(\alpha)\,|-\rangle$$

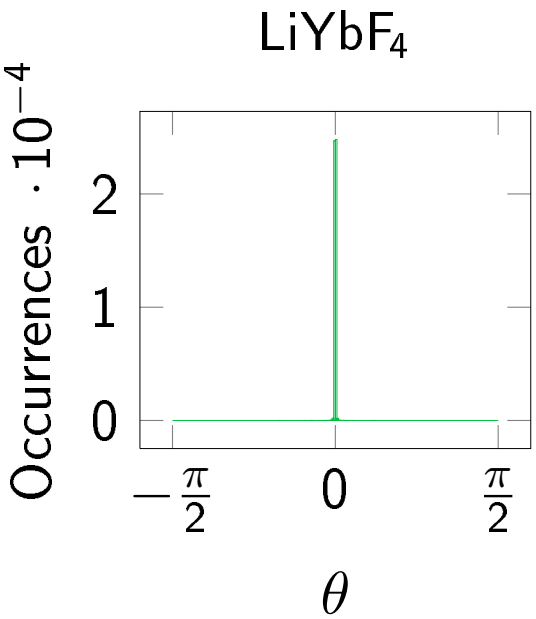
where $\alpha \in [0, \frac{\pi}{2}]$ and $\beta \in [0, 2\pi]$.

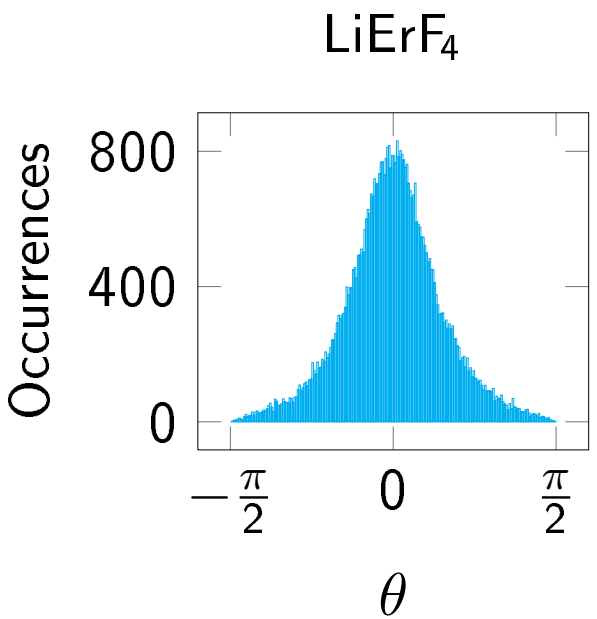
The classical effective model

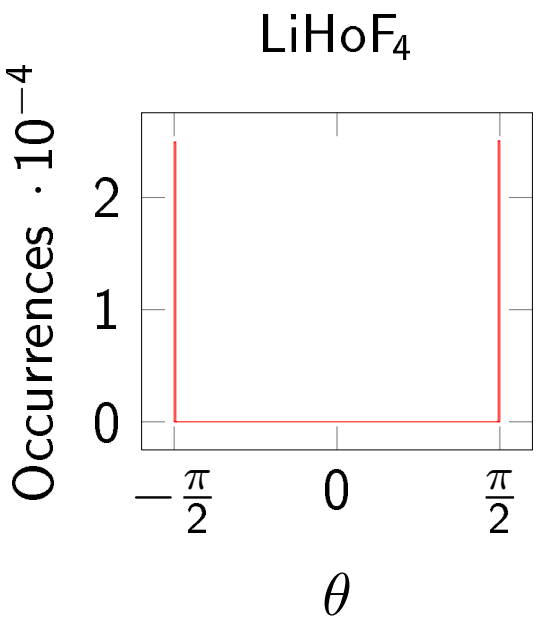
- 2 parameters: α and β
- Classical moment: $\vec{J_{eff}} = \langle \alpha, \beta | \vec{J} | \alpha, \beta \rangle$



Distribution of θ







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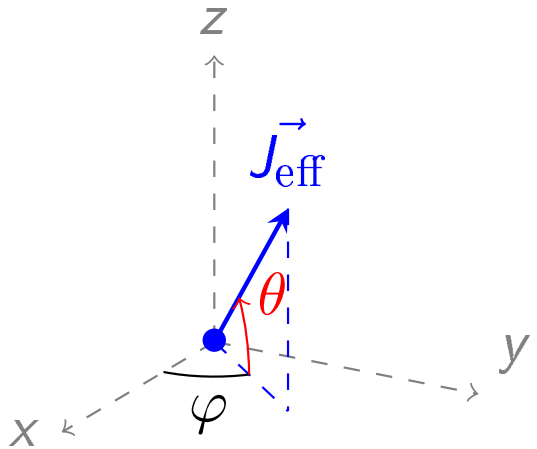

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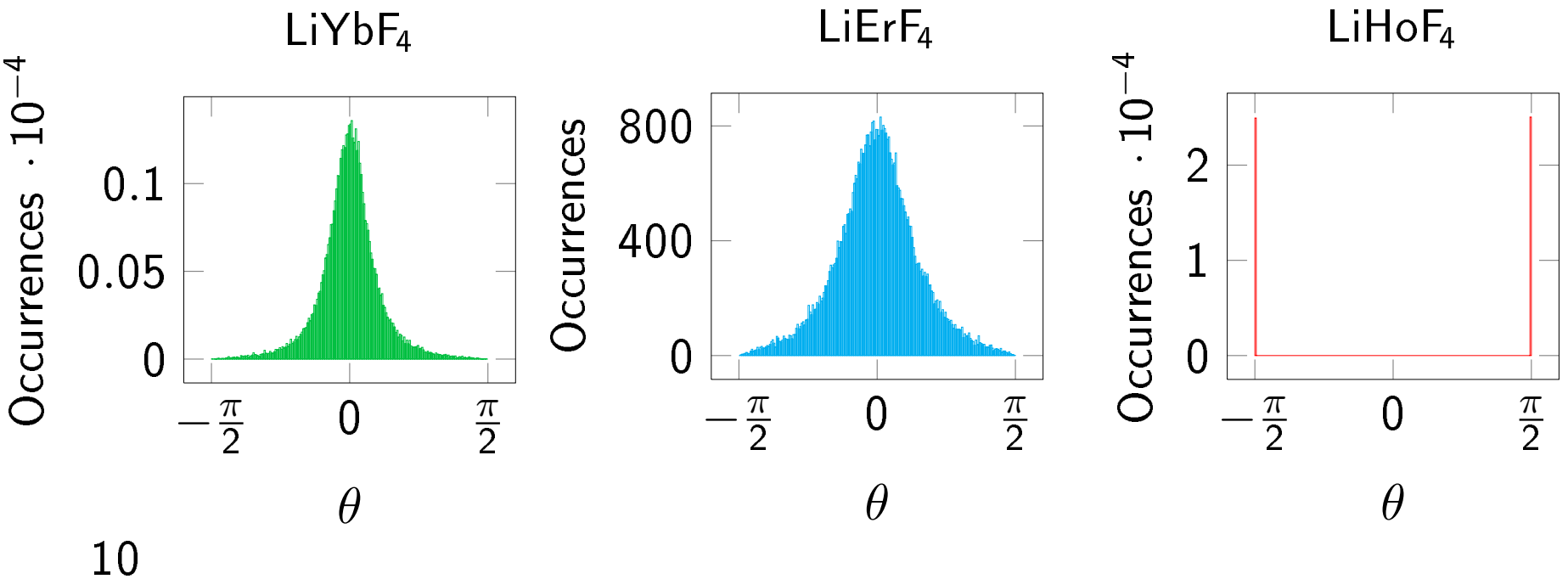
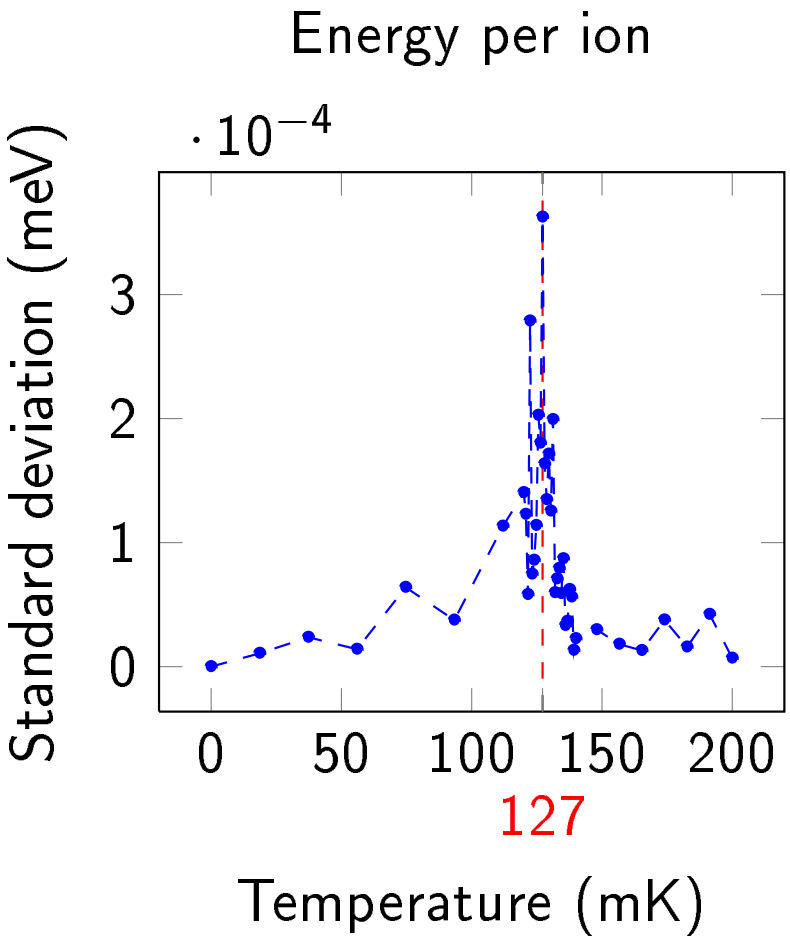


Critical exponents

$$C \propto |T - T_N|^{-\alpha}$$
$$J_{xy}^{alt} \propto |T - T_N|^{\beta}$$
$$\chi \propto |T - T_N|^{-\gamma}$$

Exponent		α	β	γ
Mean-field		0	0.5	1
3D	Ising	-0.11	0.32	1.24
	XY	0.01	0.35	1.32
	Heisenberg	0.12	0.36	1.39
2D	Ising	0	0.125	1.75
	XY/h4		0.1-0.25	
	$LiErF_4$ (at T_N)	0.28 ± 0.04	0.15 ± 0.02	0.82 ± 0.04
	$LiErF_4$ (at H_c)		0.31 ± 0.02	1.44 ± 0.2

Monte Carlo simulation of $LiErF_4$



- $T_N = 127$ mK Exp: 373 mK

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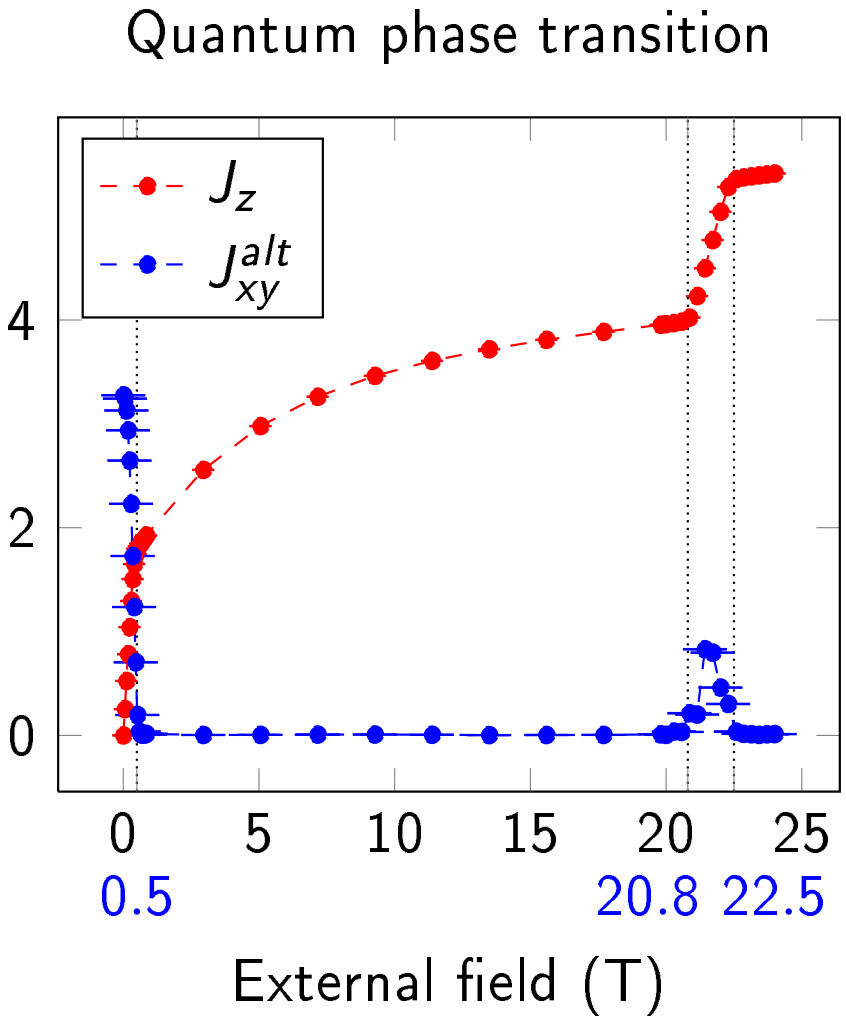
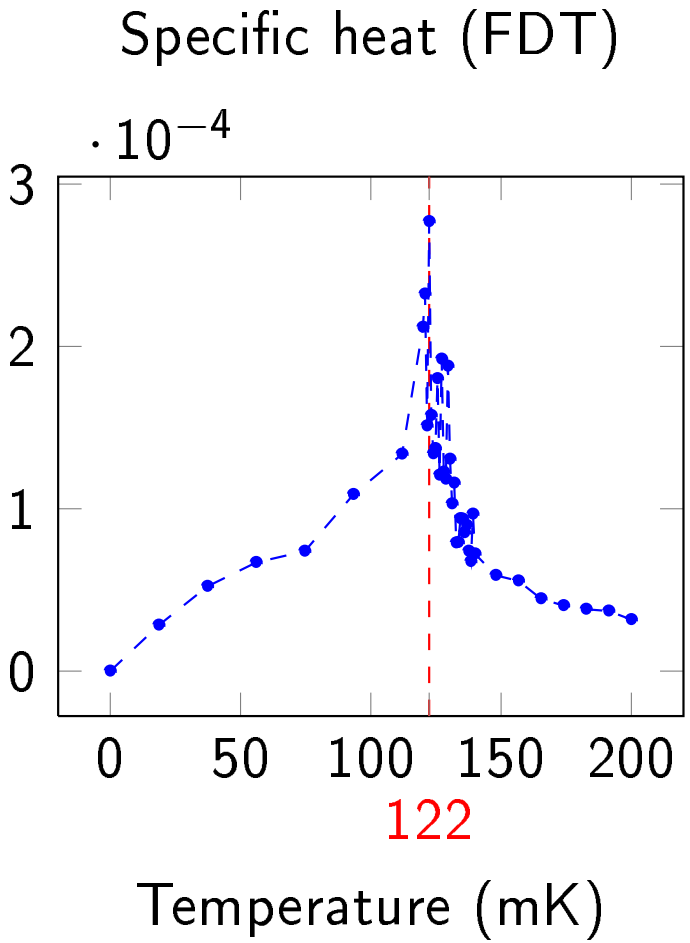


- $T_N = 127$ mK Exp: 373 mK
- $H_C = 0.5$ T Exp: 0.4 T

Monte Carlo simulation of $LiErF_4$



- T_N $= 127$ mK Exp: 373 mK
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- α_{FDT} $= 0.33$ Exp: 0.28

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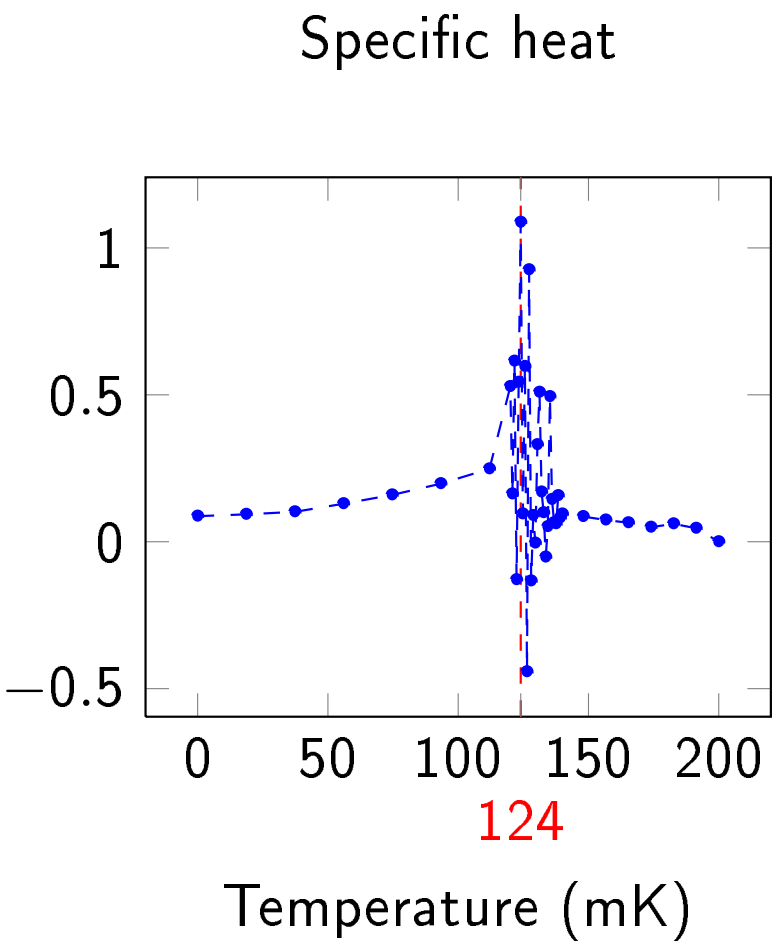

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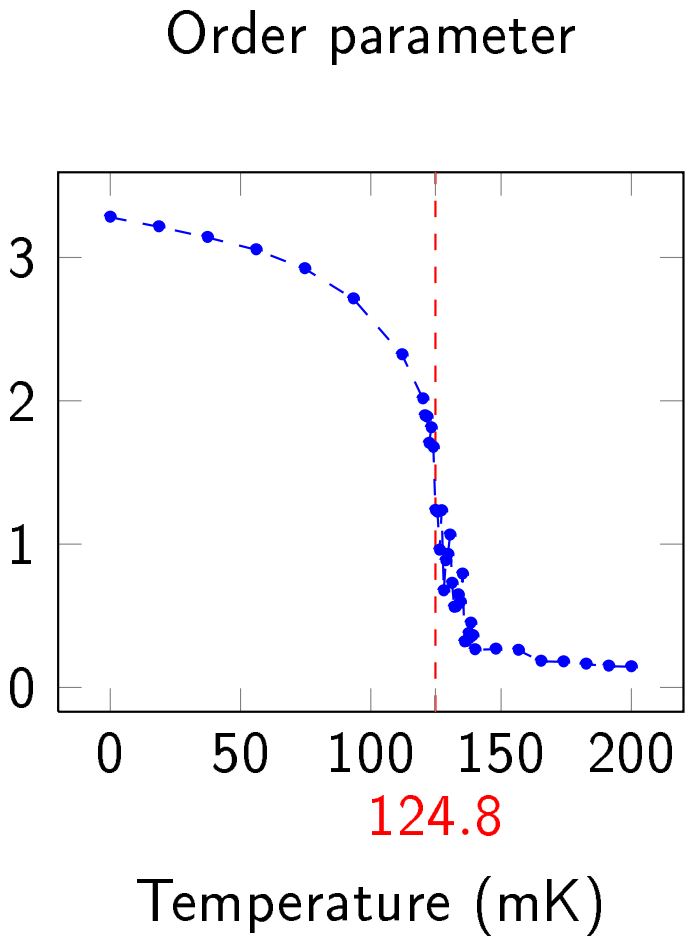

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- β $= 0.15$ Exp: 0.15

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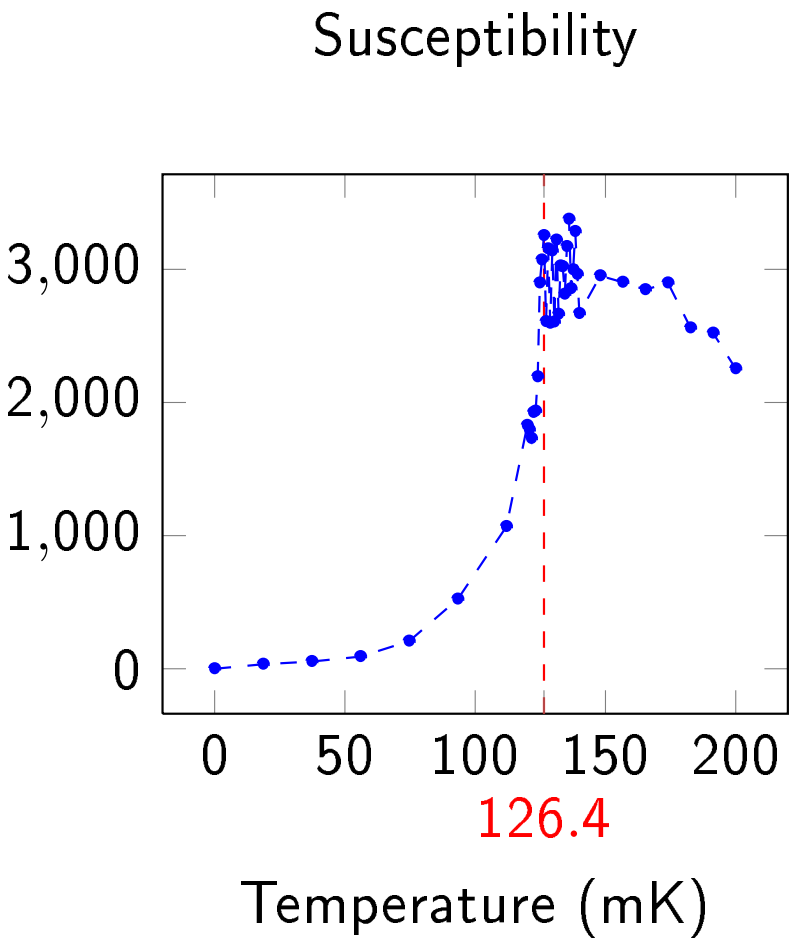

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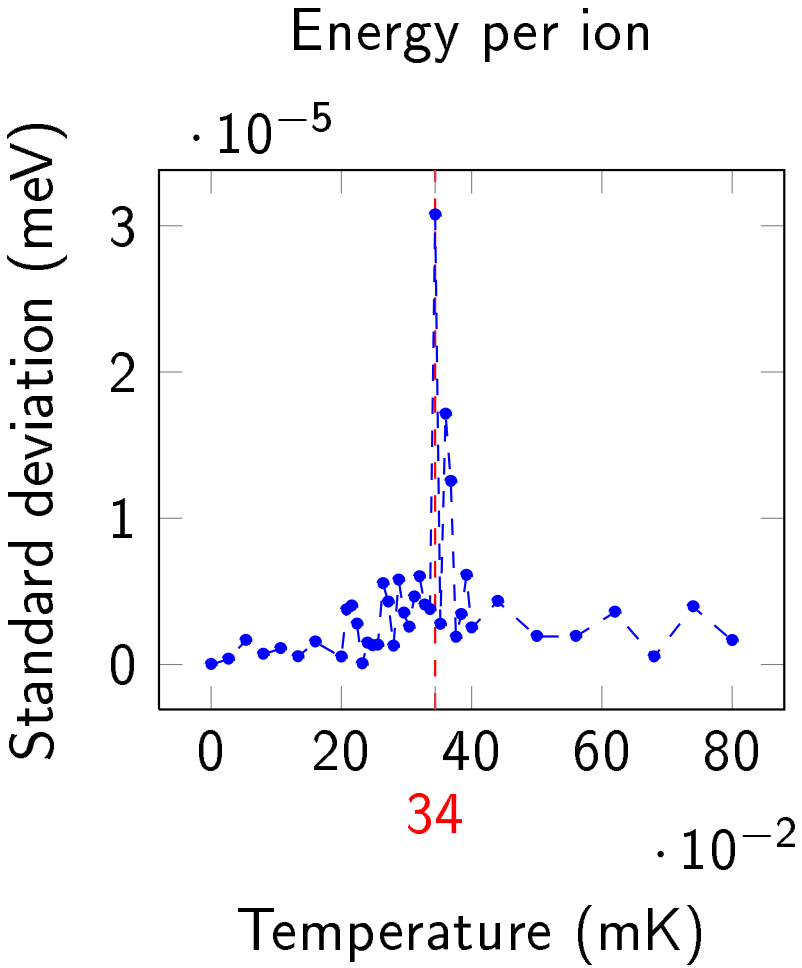
- α = 0.27 Exp: 0.28
- β = 0.15 Exp: 0.15
- γ = 0.91 Exp: 0.82

Monte Carlo simulation of $LiYbF_4$

Wrong CF parameters !



- T_N = 34.4 mK Exp: 128.6 mK

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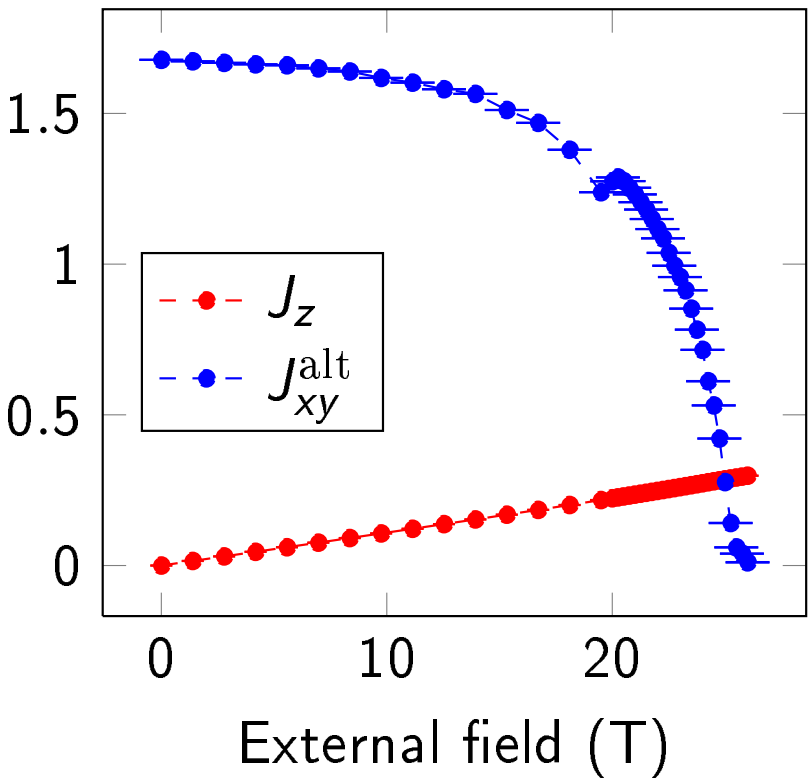
Quantum phase transition



- $T_N = 34.4$ mK Exp: 128.6 mK
- $H_C = 25$ T Exp: 0.48 T

Monte Carlo simulation of $LiYbF_4$

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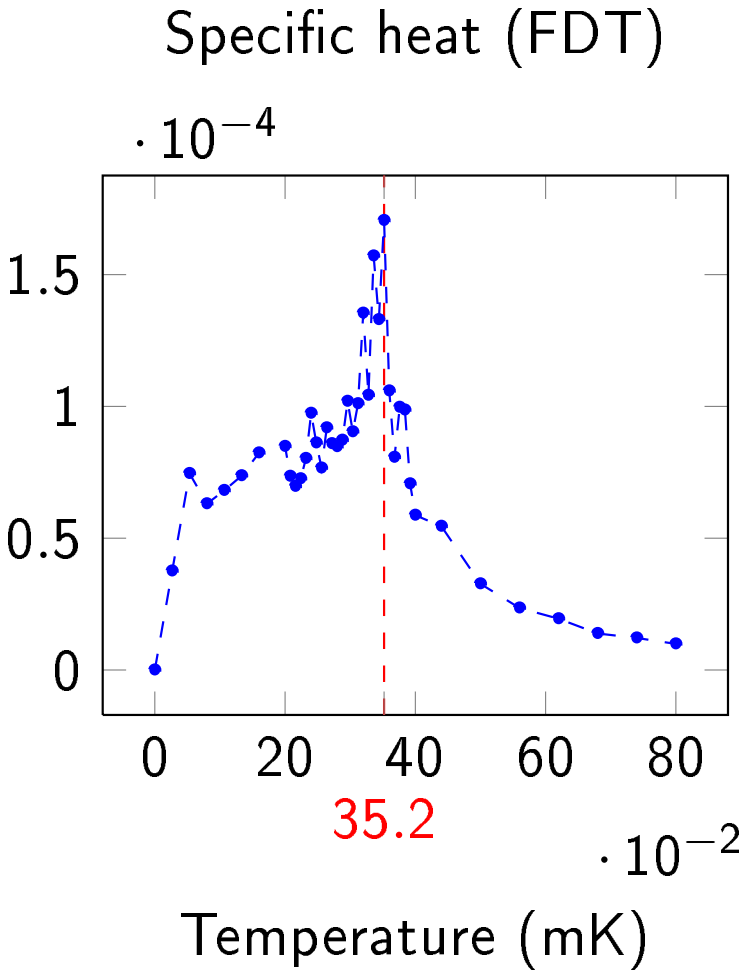

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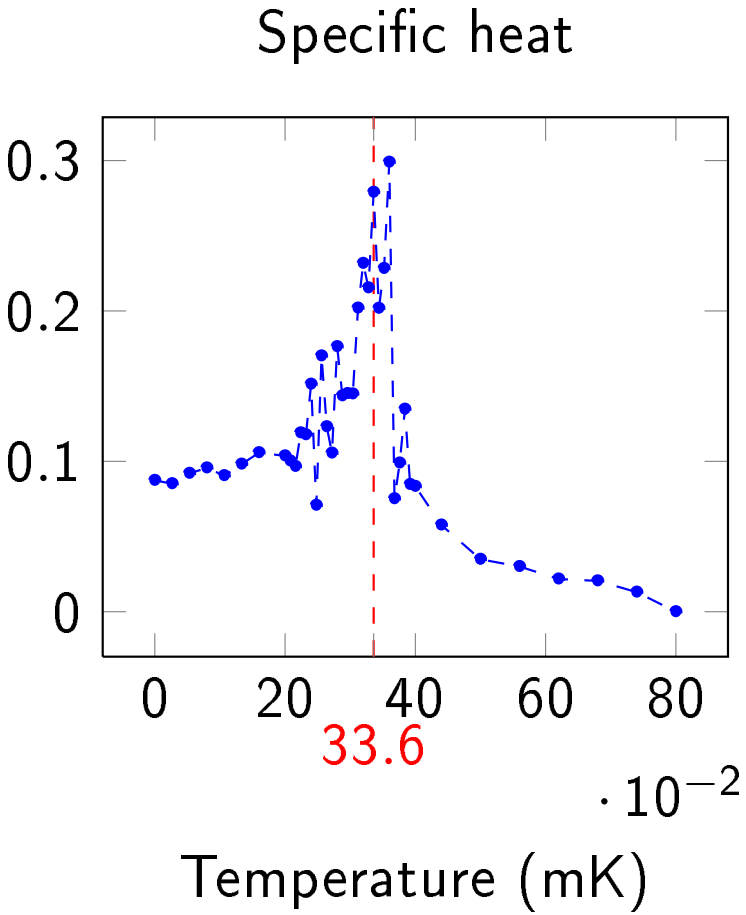

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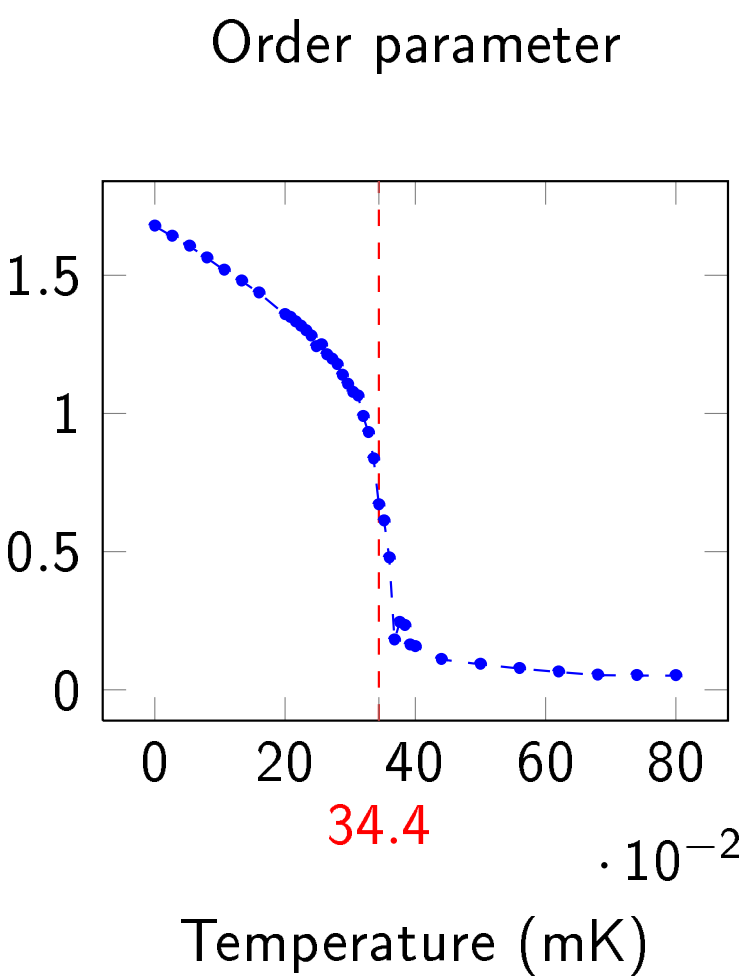

- T_N = 34.4 mK Exp: 128.6 mK
- H_C = 25 T Exp: 0.48 T
- α_{FDT} = 0.25
- α = 0.28
- β = 0.18

Monte Carlo simulation of $LiYbF_4$

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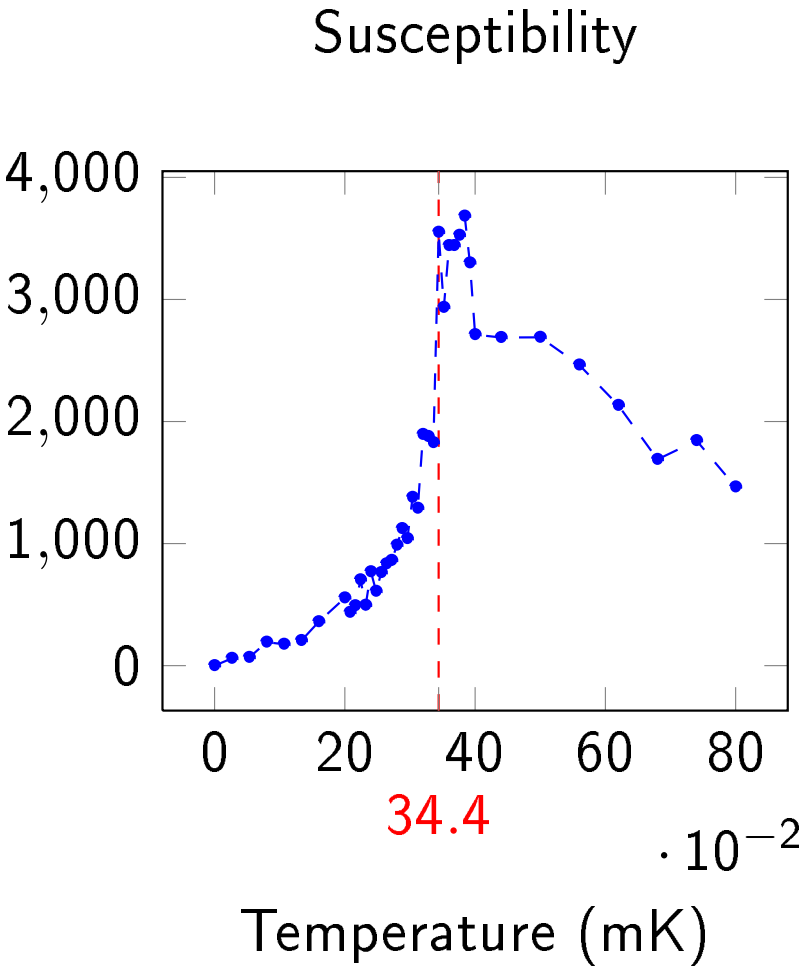

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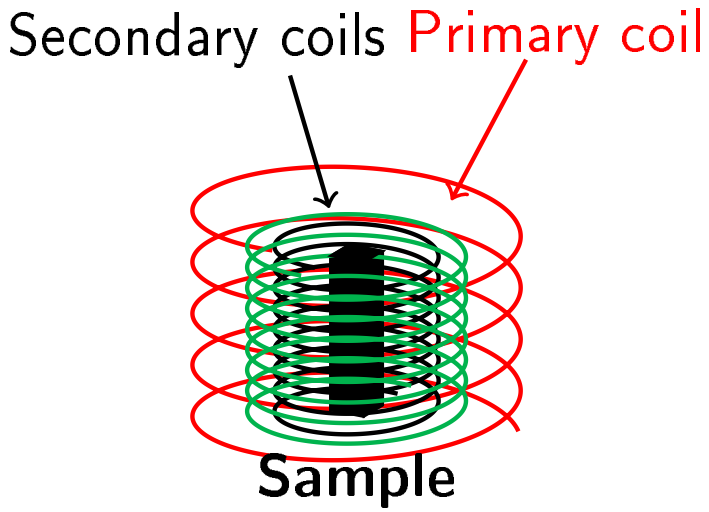
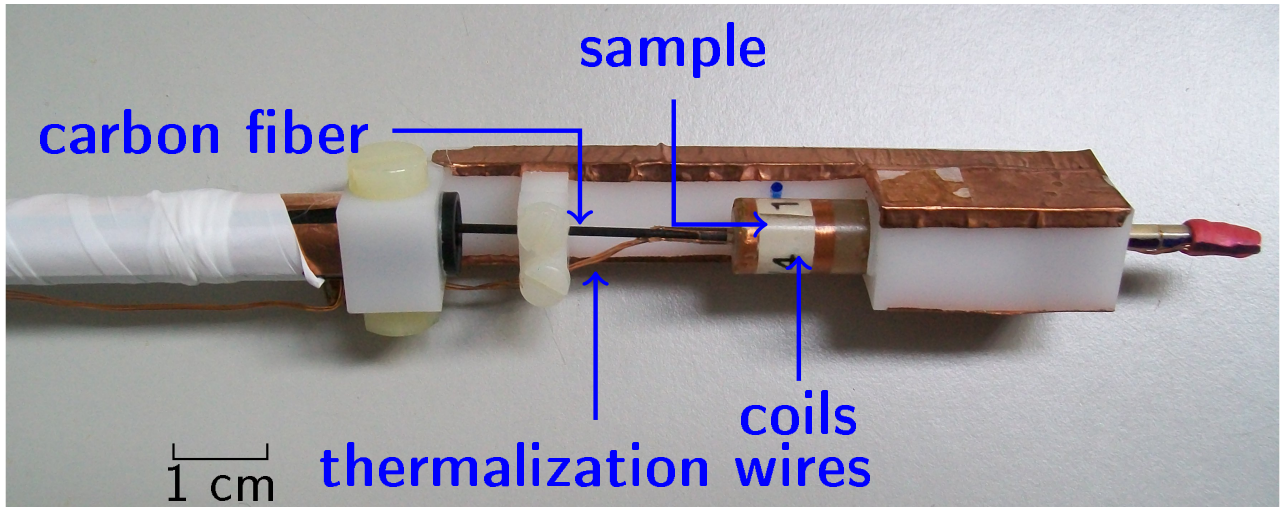
- H_C = 25 T Exp: 0.48 T
- α_{FDT} = 0.25
- α = 0.28
- β = 0.18
- γ = 0.90

AC susceptibility measurements

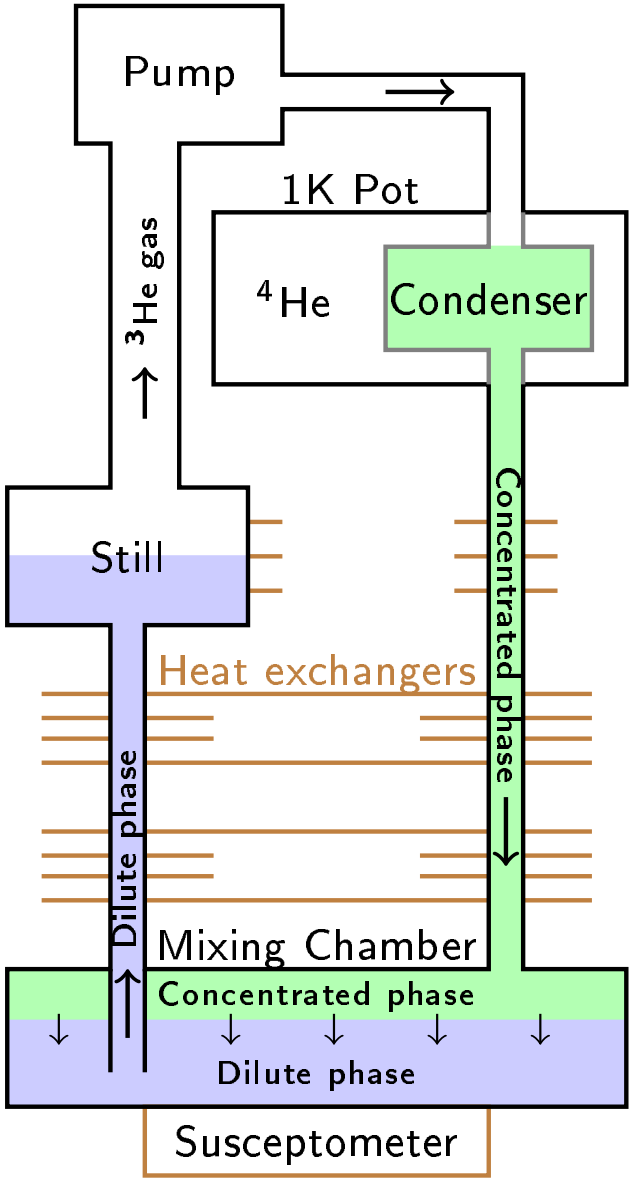
$$\chi' = \frac{\omega}{\mu_0 H_{a0} \pi} \int_0^{\frac{2\pi}{\omega}} \langle B \rangle \cos(\omega t) \mathrm{d}t \; - 1$$

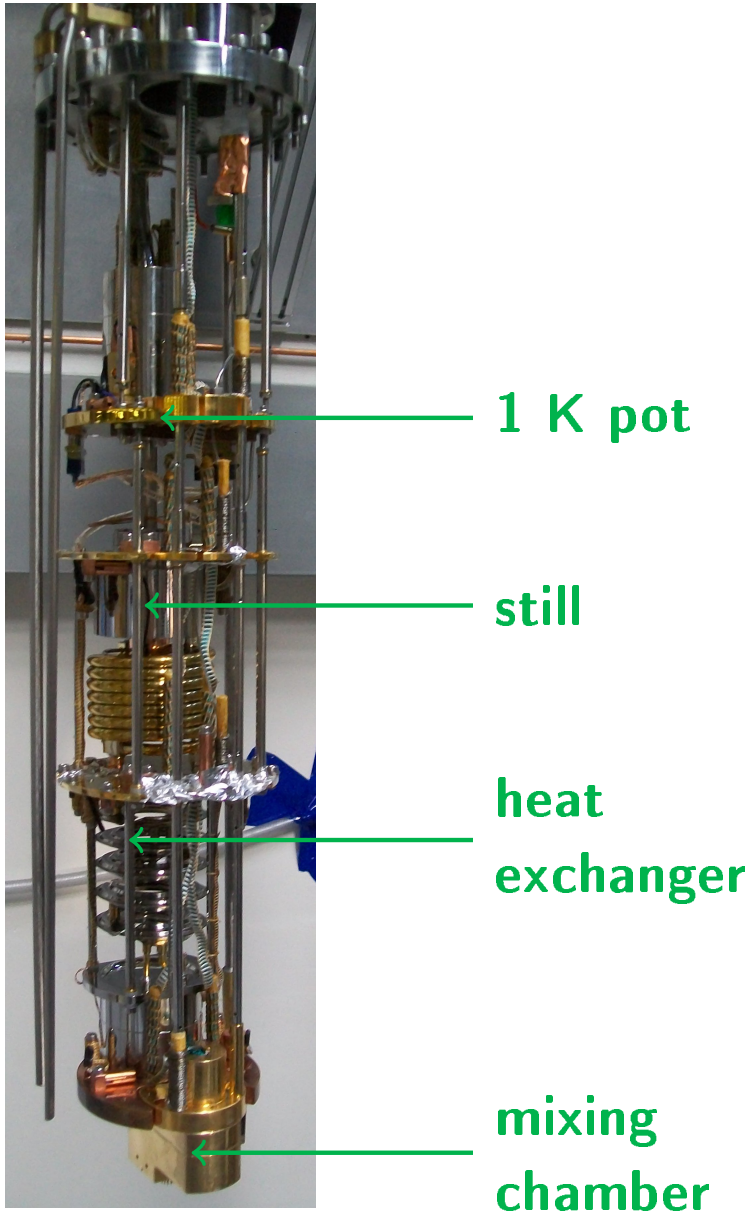
$$\chi'' = \frac{\omega}{\mu_0 H_{a0} \pi} \int_0^{\frac{2\pi}{\omega}} \langle B \rangle \sin(\omega t) \mathrm{d}t$$





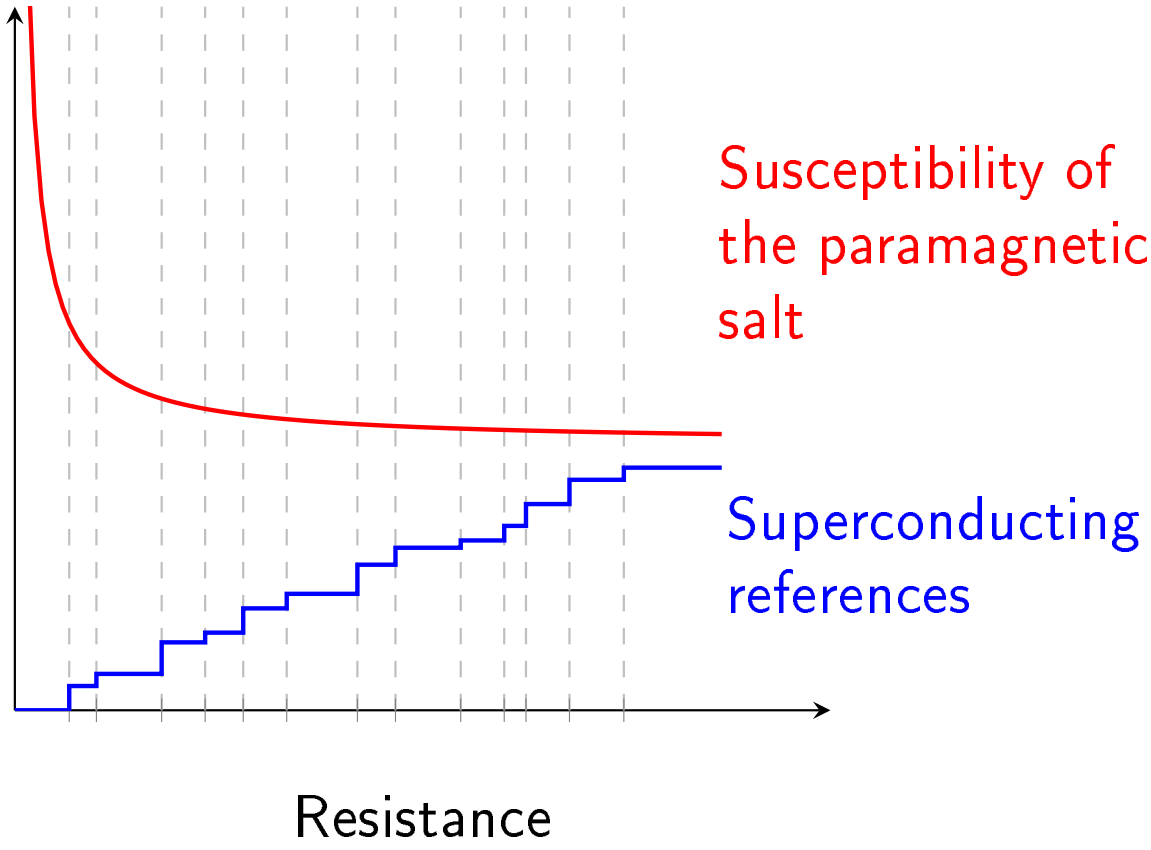
The dilution refrigerator



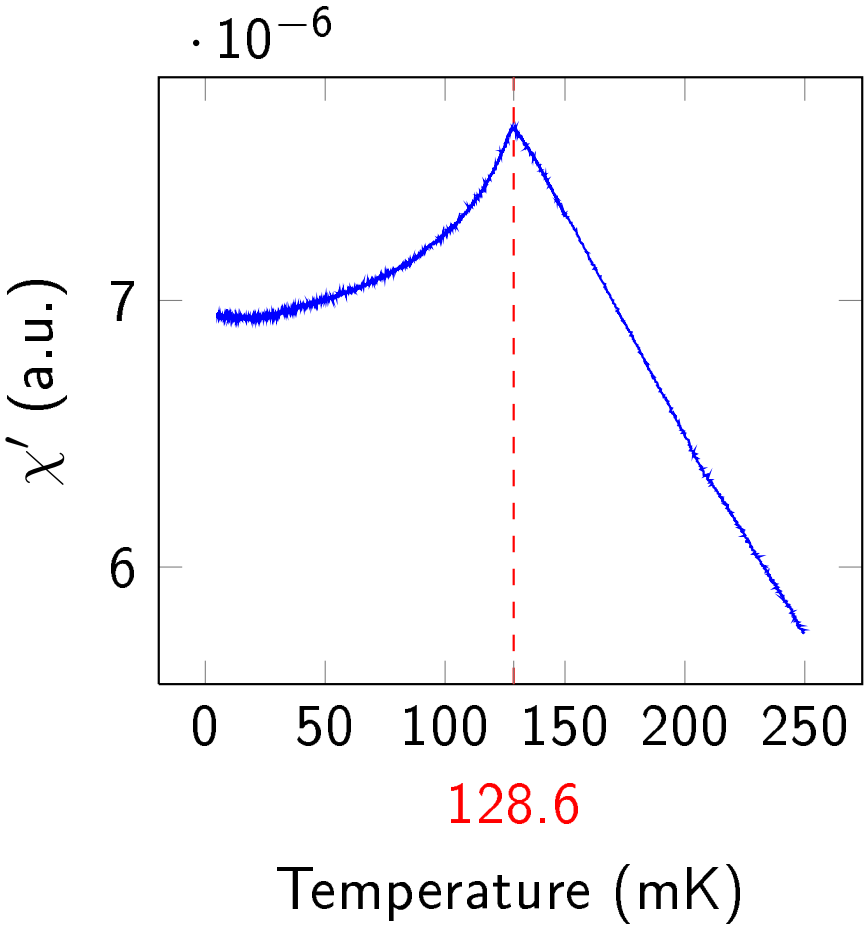


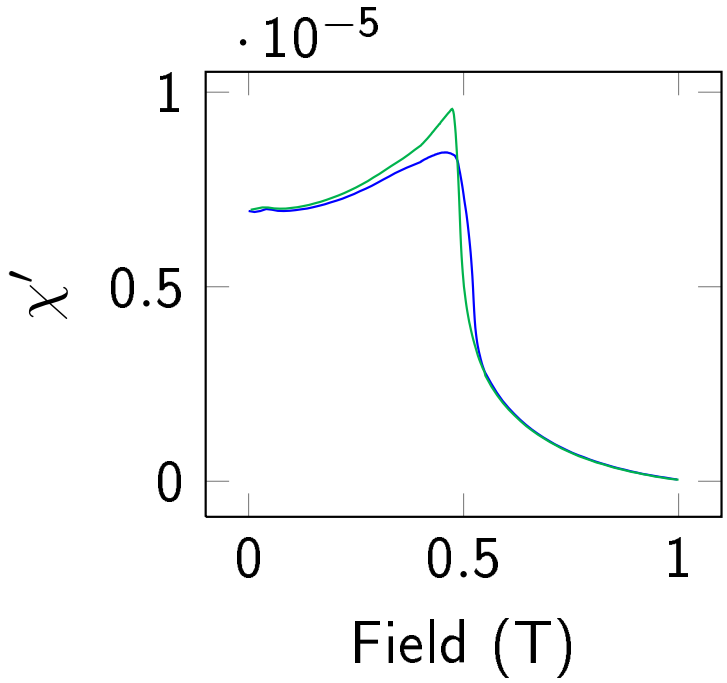
Measurement of the temperature

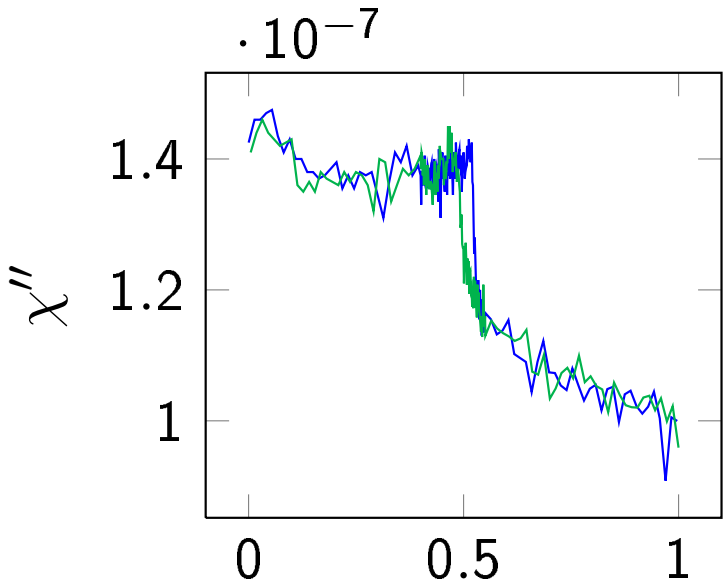
- Thermometer: thick film of RuOx
- Calibration with 13 superconducting references and a paramagnetic salt.



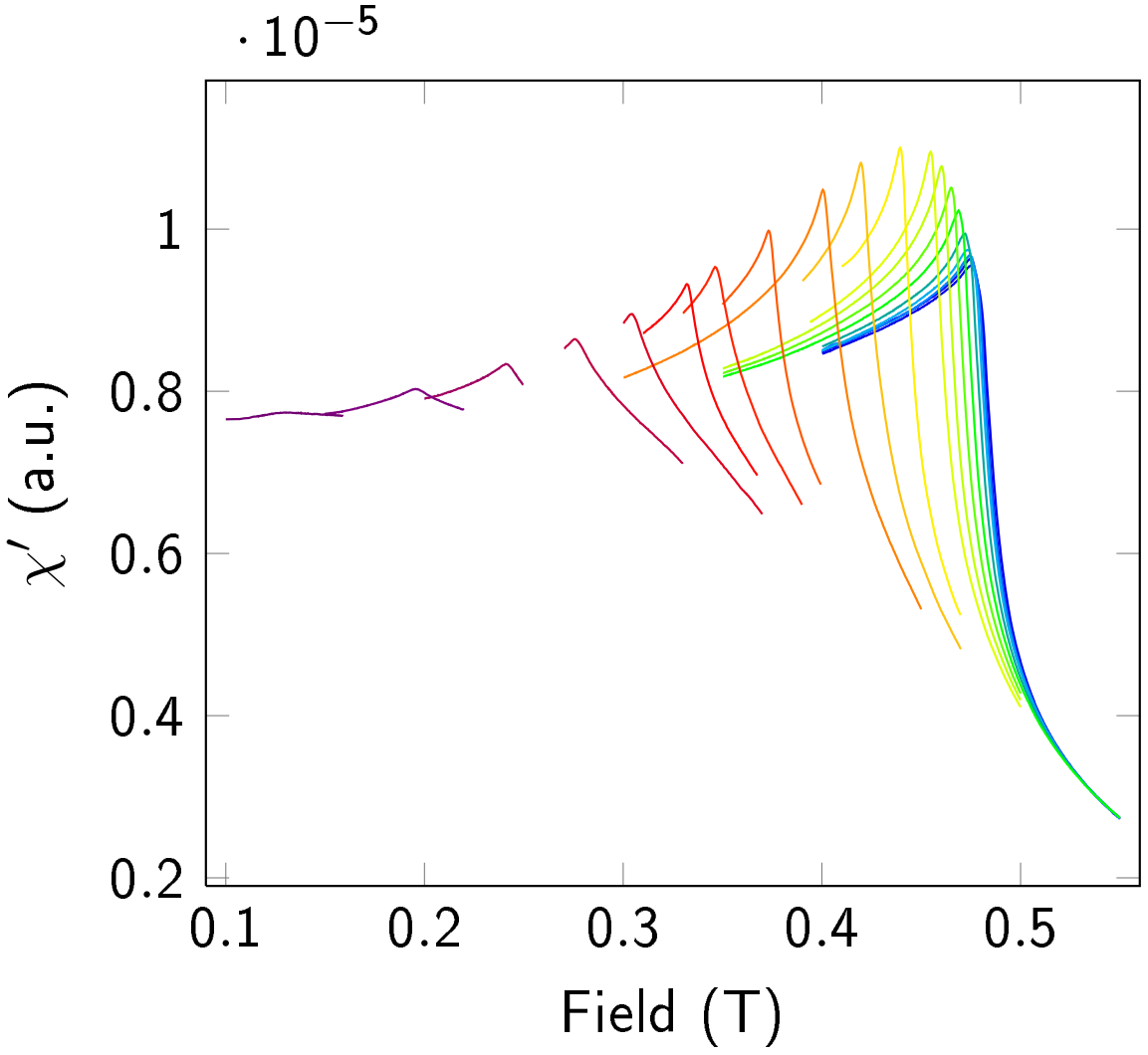
Critical field and temperature



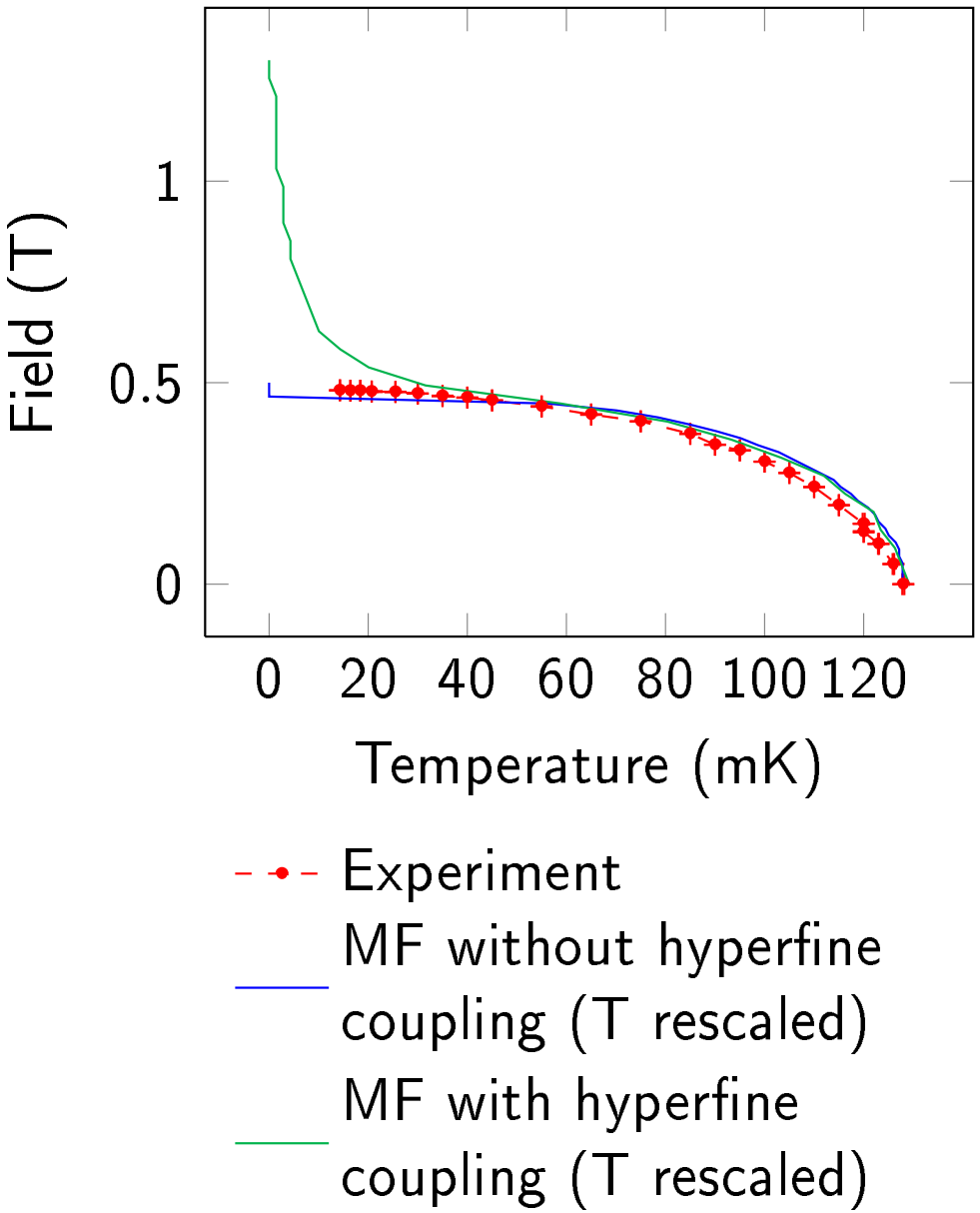




Field scans



Phase diagram



	T_N (mK)	exp.
Experiment	128	0.32
MF no hyp	186	0.24
MF hyp	182	

	H_C (T)	exp.
Experiment	0.48	0.54
MF no hyp	0.46	0.52
MF hyp	1.2	0.5

Future work

- Monte Carlo simulation for $LiYbF_4$ with the new parameters
- Study of the disordered compounds $LiHo_{1-x}Yb_xF_4$
  - Monte Carlo simulation
  - Measurement of the T_C-x phase diagram