Co-existing long- and short-range magnetic order in the frustrated diamond antiferromagnet, $LiYbO_2$

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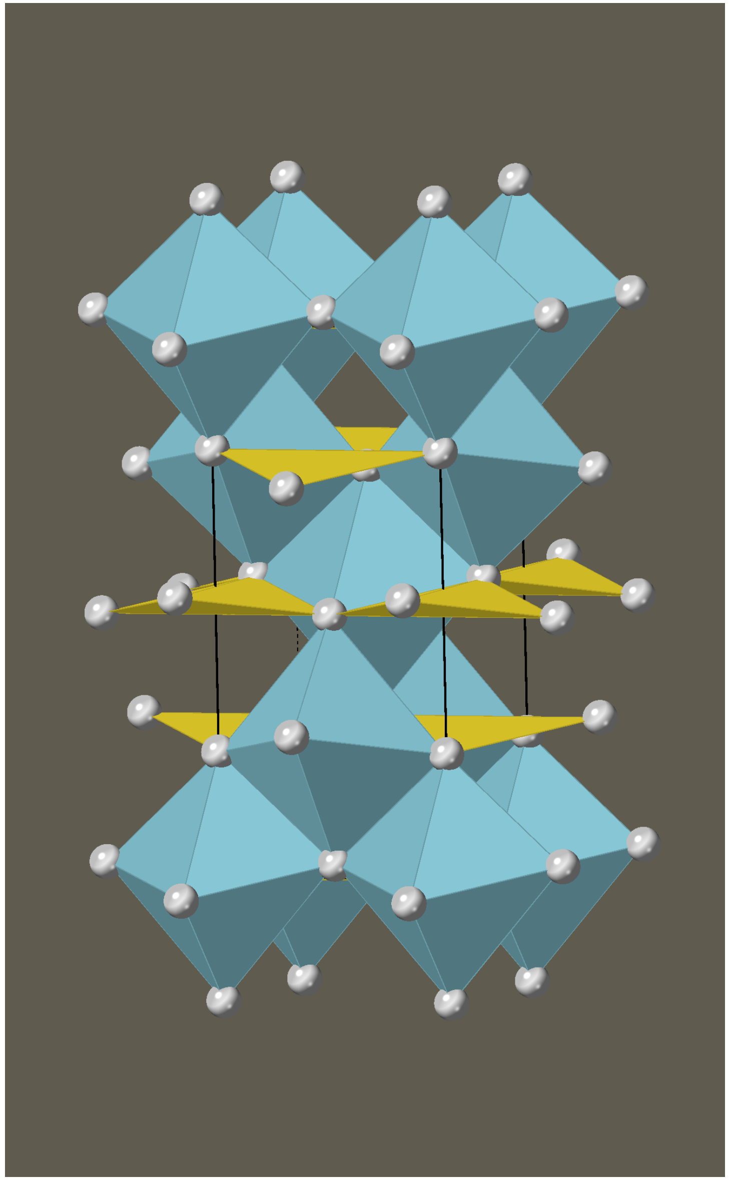
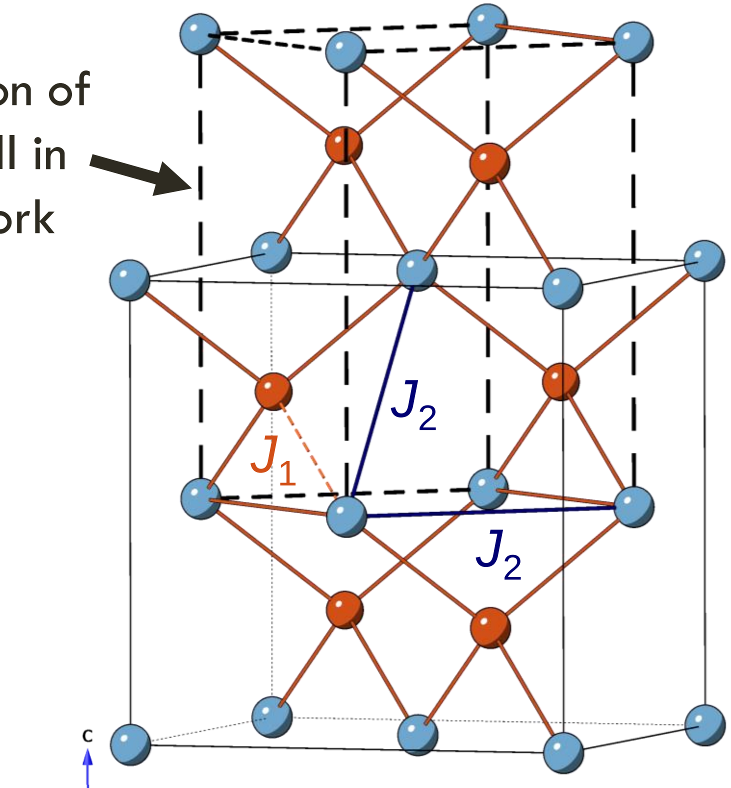


DIAMOND LATTICE

Definition of unit cell in this work



Sublattice 1

Sublattice 2

J_1-J_2 Heisenberg model on diamond lattice

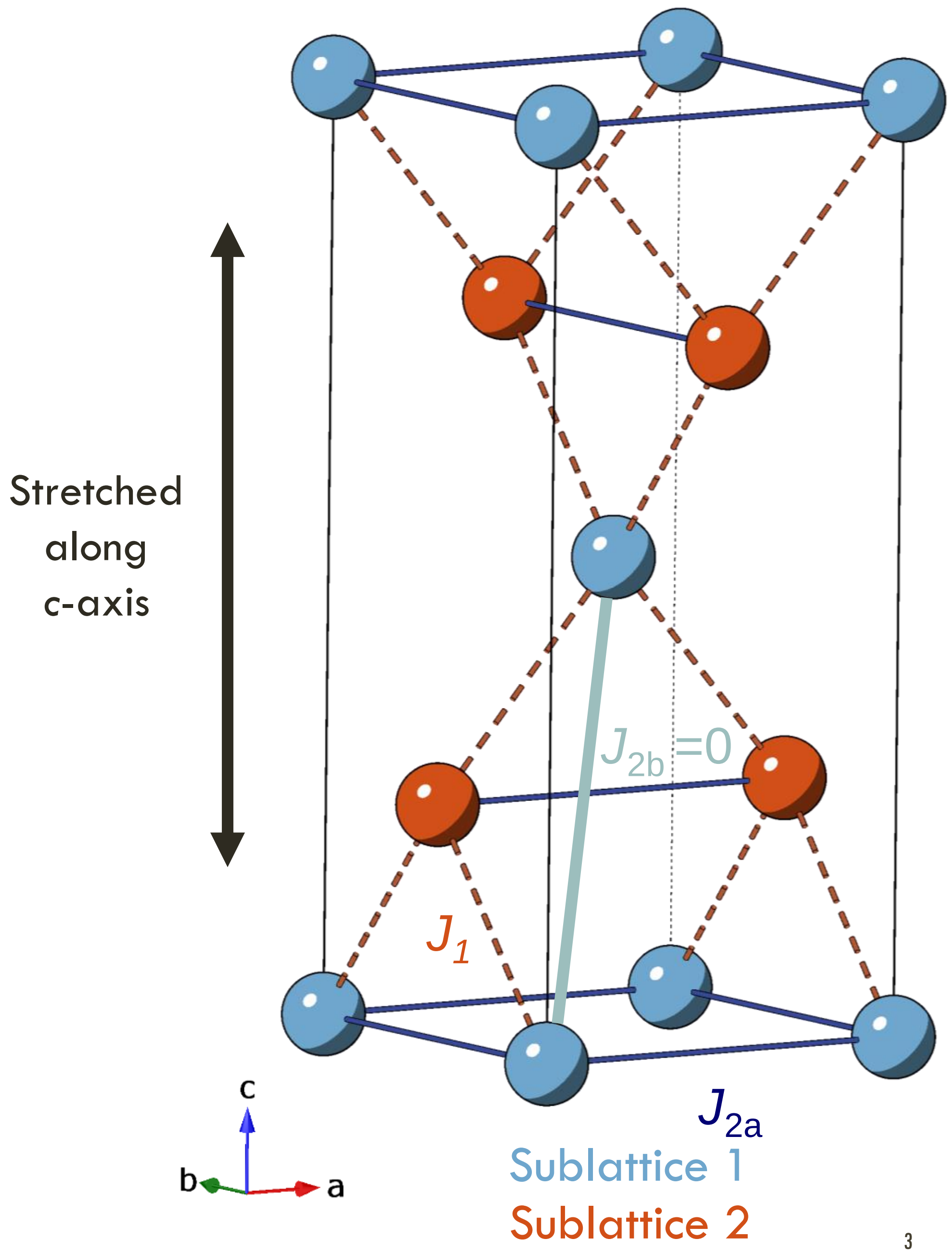
- Perturbing longer range couplings outside J_1-J_2
- Cubic-tetragonal distortion

What if the diamond lattice was not perfect to begin with?

STRETCHED DIAMOND LATTICE

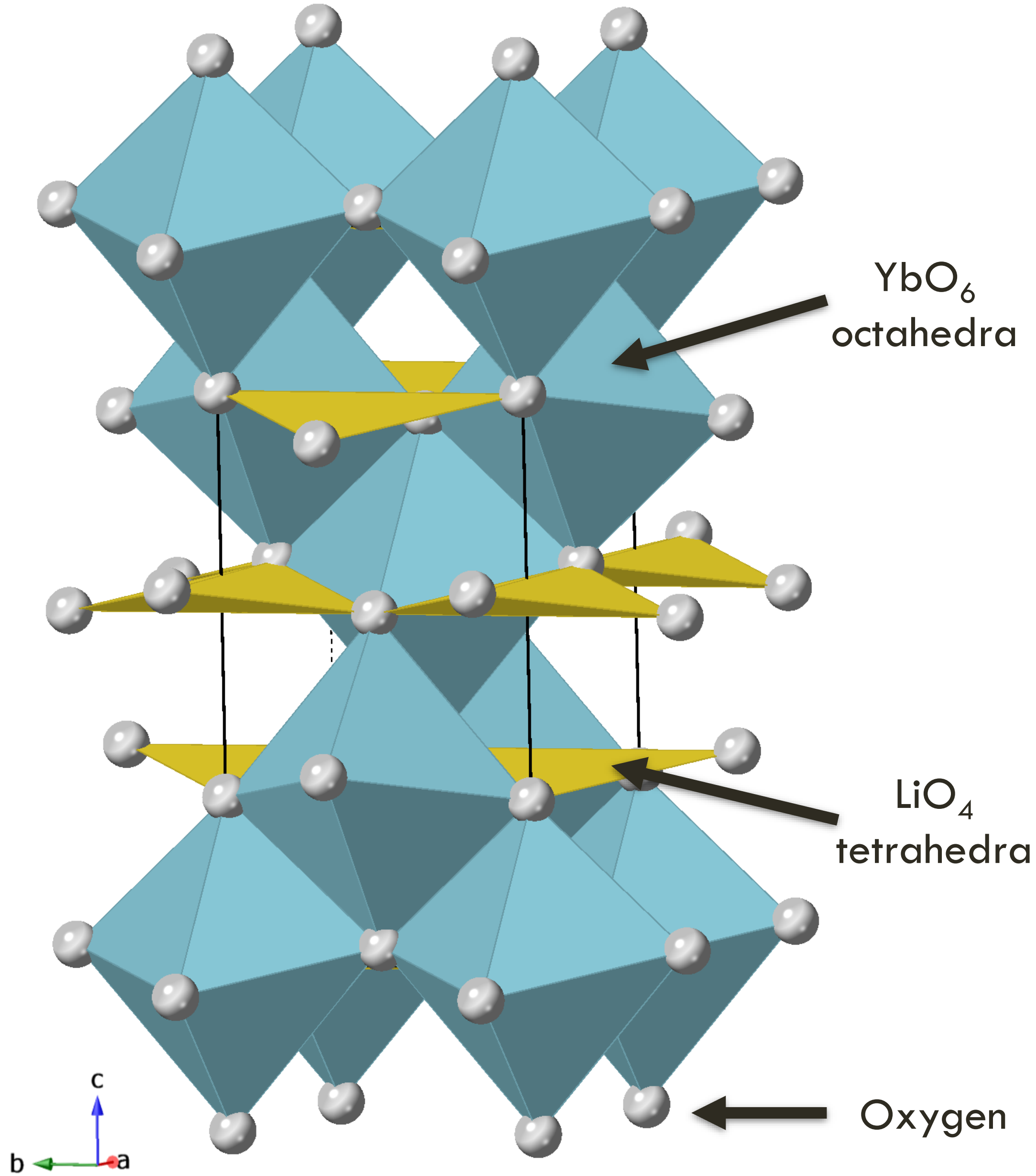
J_1-J_2 Heisenberg model on **stretched** diamond lattice

- Superexchange pathways are equivalent in length through J_1 and J_{2a}
- J_{2b} pathway is significantly longer, $J_{2b} = 0$
- Frustration generated if $|J_1| \sim J_{2a}$



$LiYbO_2$

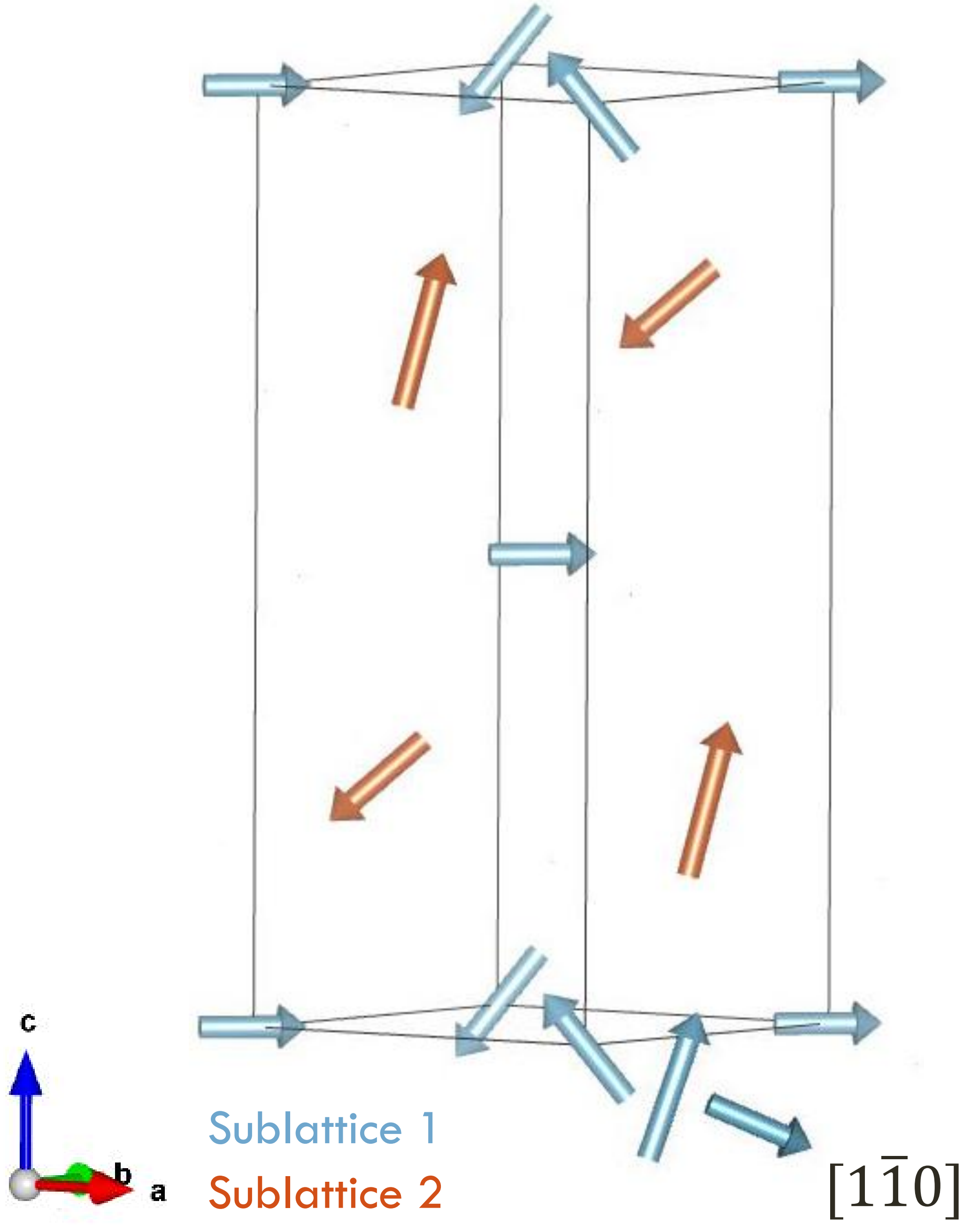
- $I4_1/amd$ space group



Y. Hashimoto *et al. Chem. Mater.* **14**, 8, 3245 – 3251 (2002),
M. M. Bordelon *et al. Phys. Rev. B* **103**, 014420 (2021)

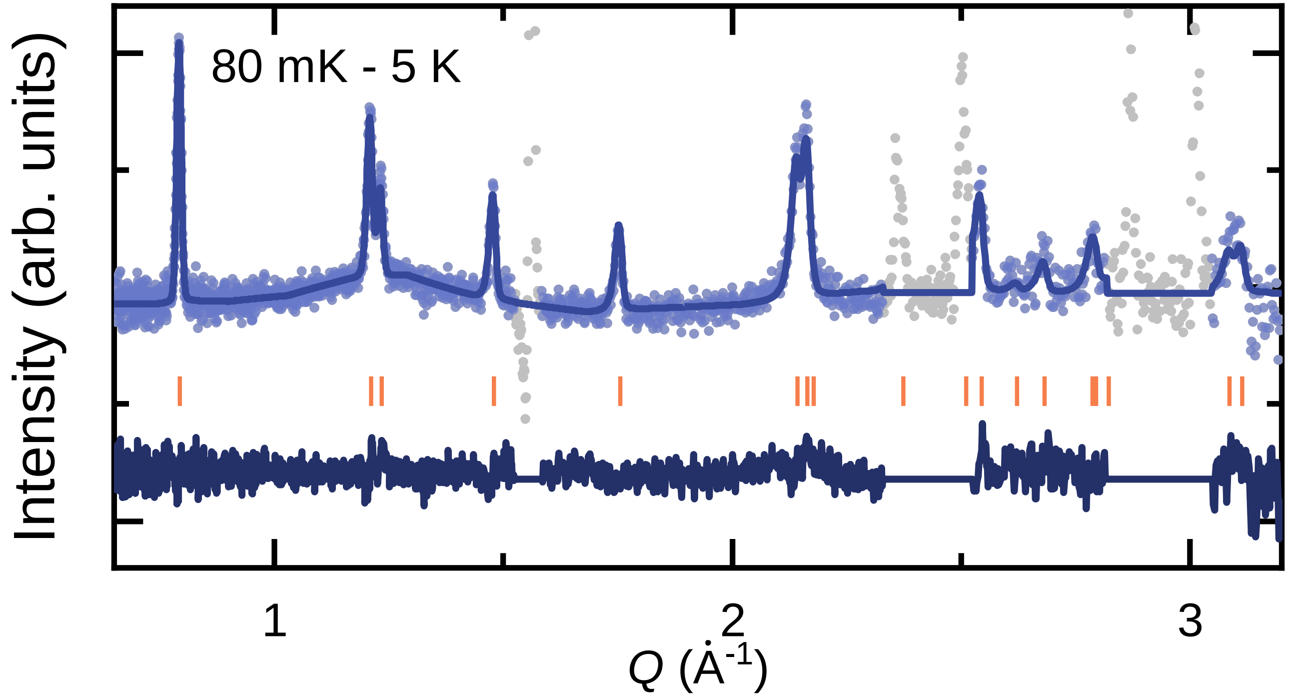
$LiYbO_2$

- $I4_1/amd$ space group
- Below 450 mK fully ordered incommensurate helix
- Helices related by fixed phase angle
  - Experiment = 0.58 π
  - Theory = π



Y. Hashimoto *et al.* *Chem. Mater.* **14**, 8, 3245 – 3251 (2002), M. M. Bordelon *et al.* *Phys. Rev. B* **103**, 014420 (2021)

T < 450 mK

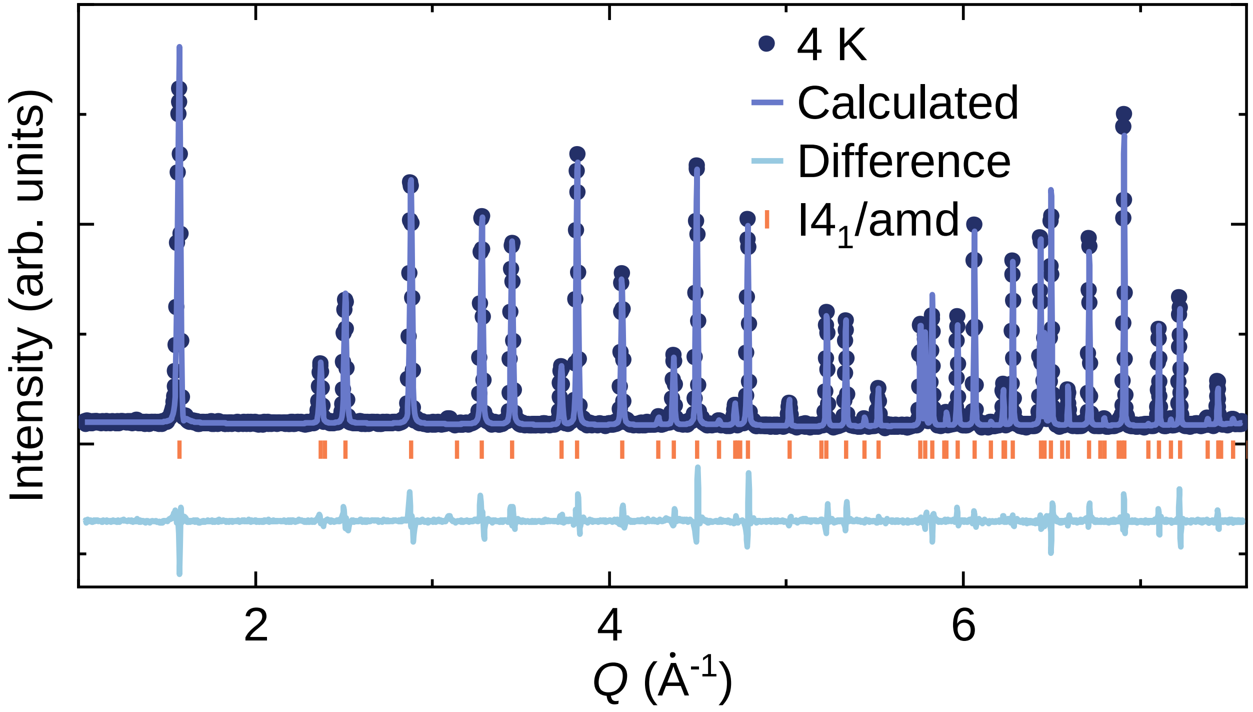


Magnetic scattering data from WISH, 80 mK – 5 K

R_{mag} = 13.1%, χ^2 = 3.06

k = (0.391, ±0.391, 0), μ_{order} = 0.63(1) μ_{B}, ϕ = 1.15(5)π

CHEMICAL STRUCTURE



High resolution NPD data from D2B at 4 K

R_F = 1.59%, χ^2 = 8.73

No preferred orientation

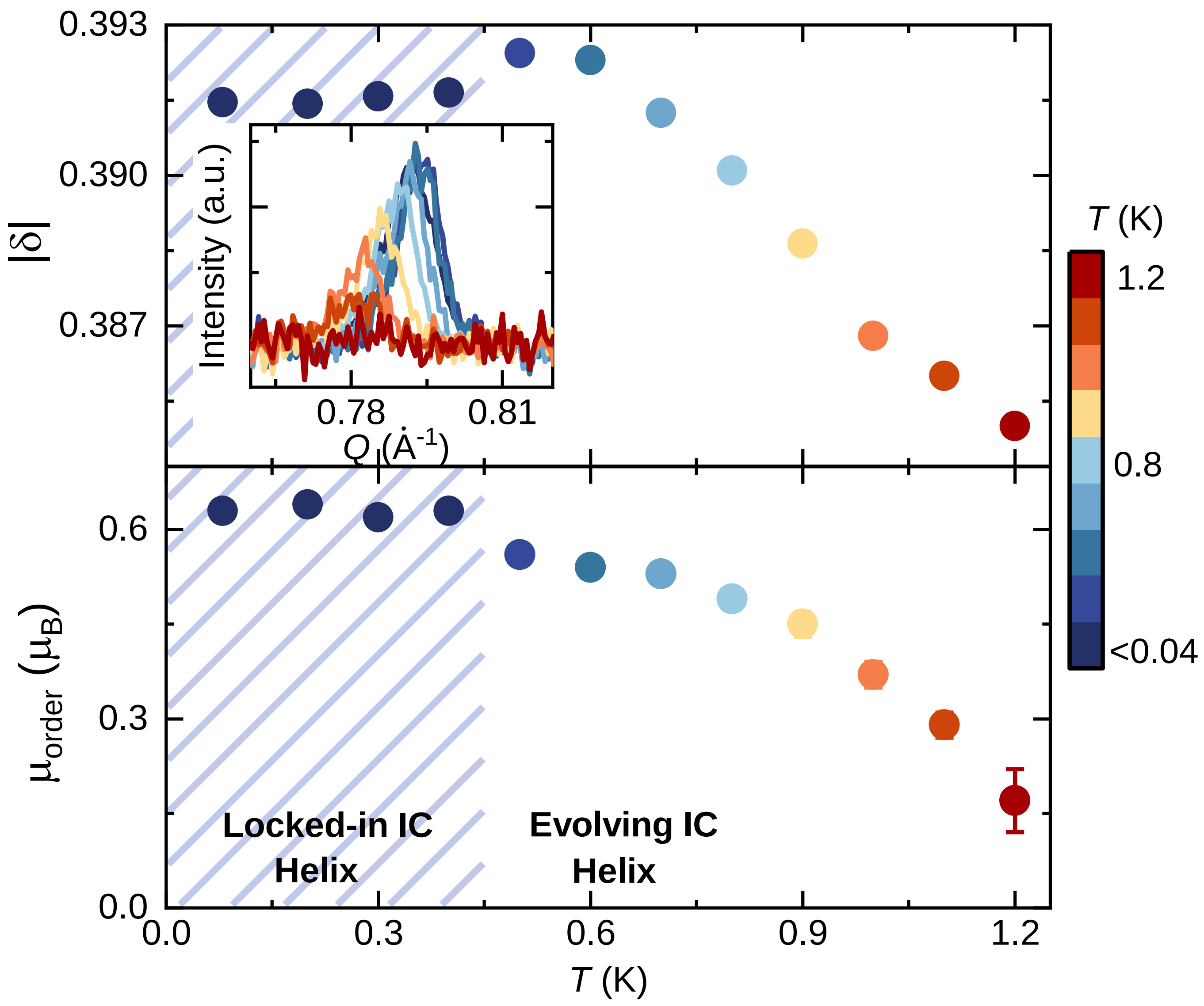
T EVOLUTION

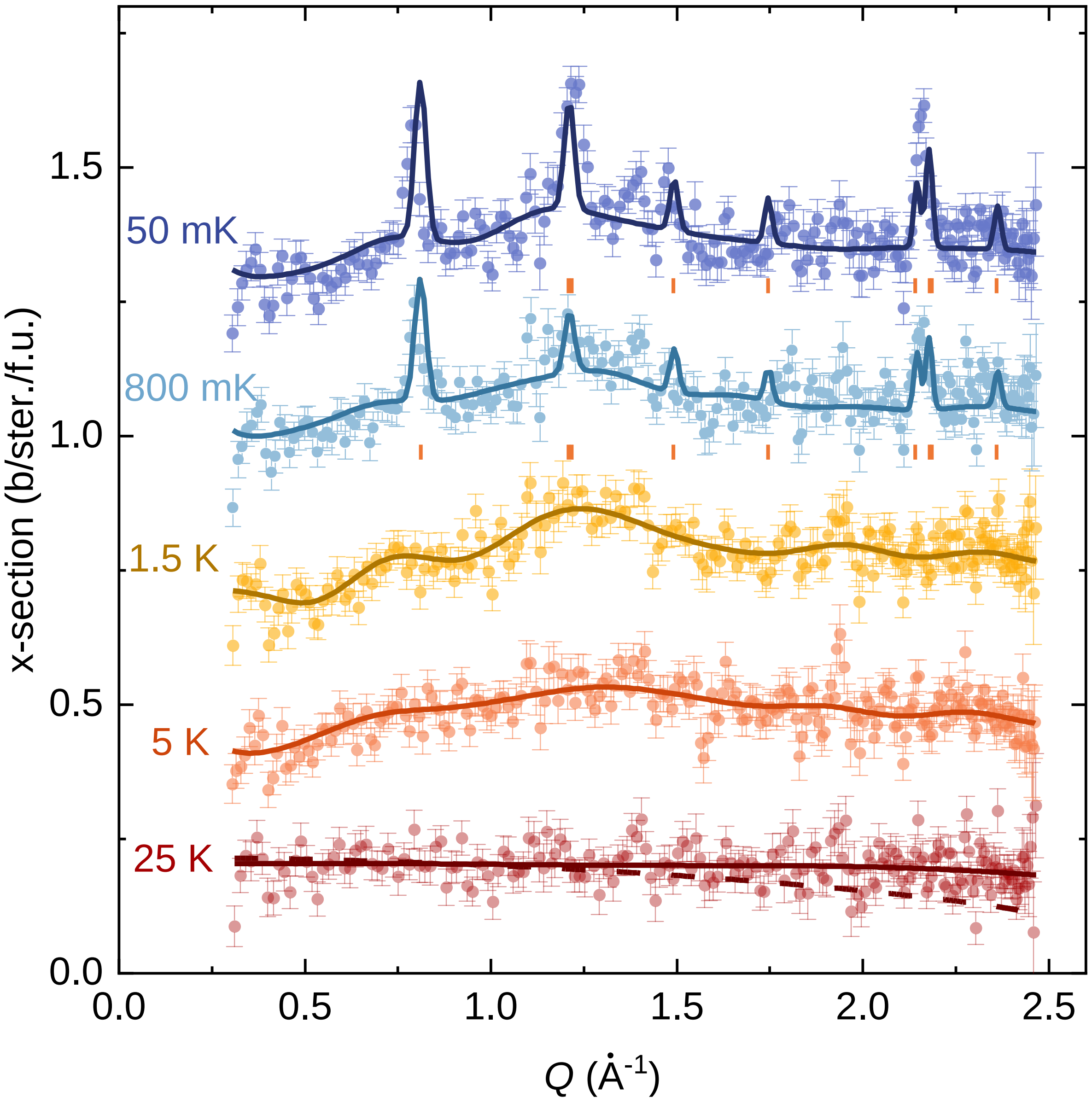
(0,0,0) magnetic satellite changes with T → Evolving incommensurate helix

1. **k** varies but always takes the form, **k** = (δ, ±δ, 0)

2. Moment size, μ_{order} gradually reduces to zero by 1.2 K

3. Phase angle, ϕ = 1.15(5)π





Diffuse scattering data measured on D7

Data have been vertically shifted by 0.3 b/ster./f.u. for clarity

DIFFUSE SCATTERING

SPINVERT + Bragg analysis – 50 mK and 800 mK [1,2]

- **k** = (0.4, ± 0.4, 0)
- 10 x 10 x 4 supercell

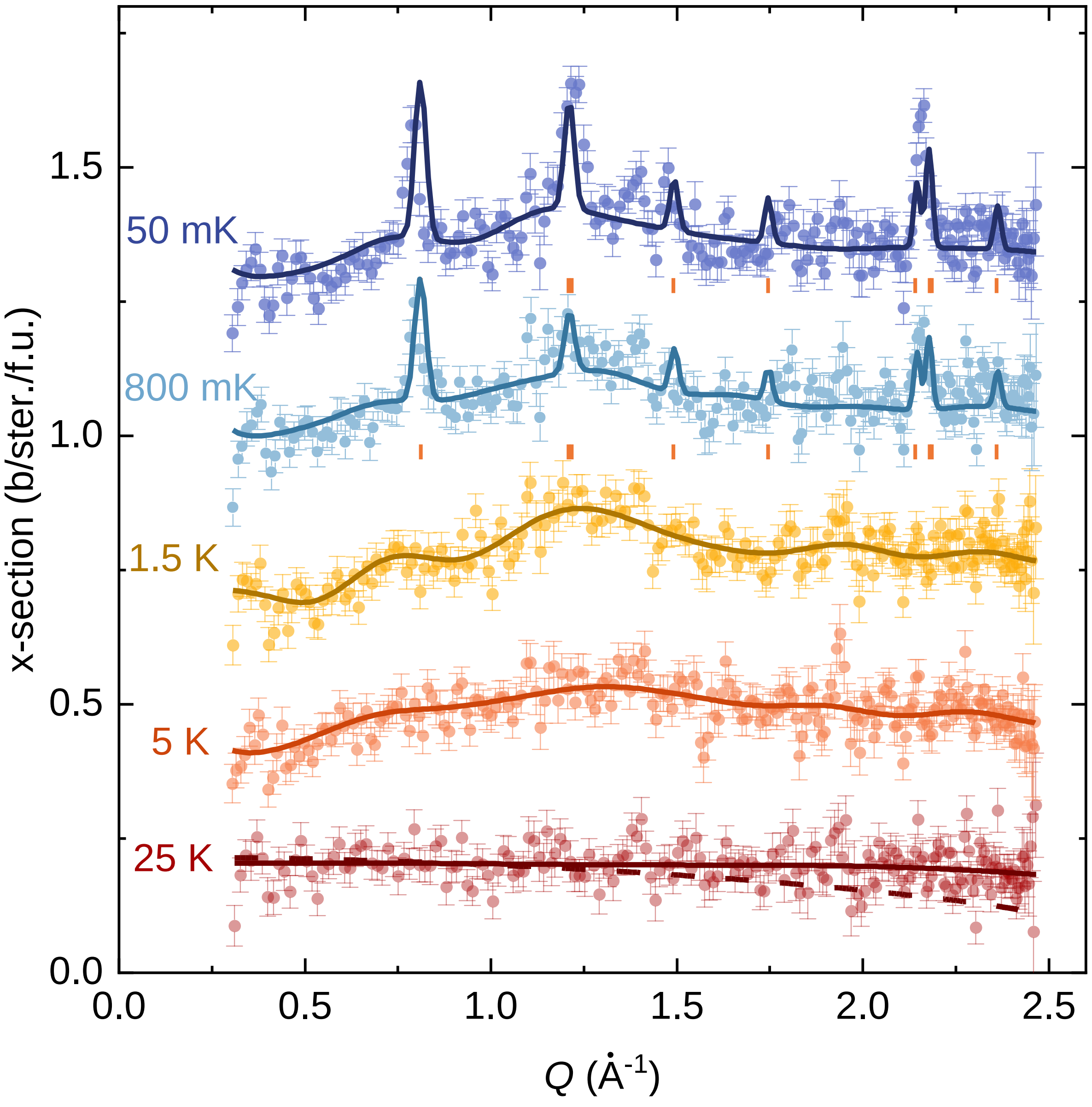
SPINVERT analysis – 1.5 K, 5 K and 25 K

- 6 x 6 x 3 supercell (25 K = 2 x 2 x 1)

Paramagnetic fit of Yb^{3+} ions – 25 K (dashed line)

- S = ½, g = 3

J. A. M. Paddison *et al.* J. Phys.:Condens. Matter **25**, 454220 (2013)
J. A. M. Paddison *et al.* Nature Commun. **7**, 13842 (2016)



Diffuse scattering data measured on D7

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DIFFUSE SCATTERING

T (K)	WISH	D7		
	μ_{order} (μ_B)	μ_{order} (μ_B)	$\mu_{disorder}$ (μ_B)	μ_{eff} (μ_B)
Base	0.63 (1)	0.80(1)	1.80(1)	2.60(1)
0.8	0.49(1)	0.67(2)	1.92(2)	2.59(2)
1.5	-	-	2.73(2)	2.73(2)
5	-	-	2.74(2)	2.74(2)
25	-	-	2.76(2)	2.76(2)

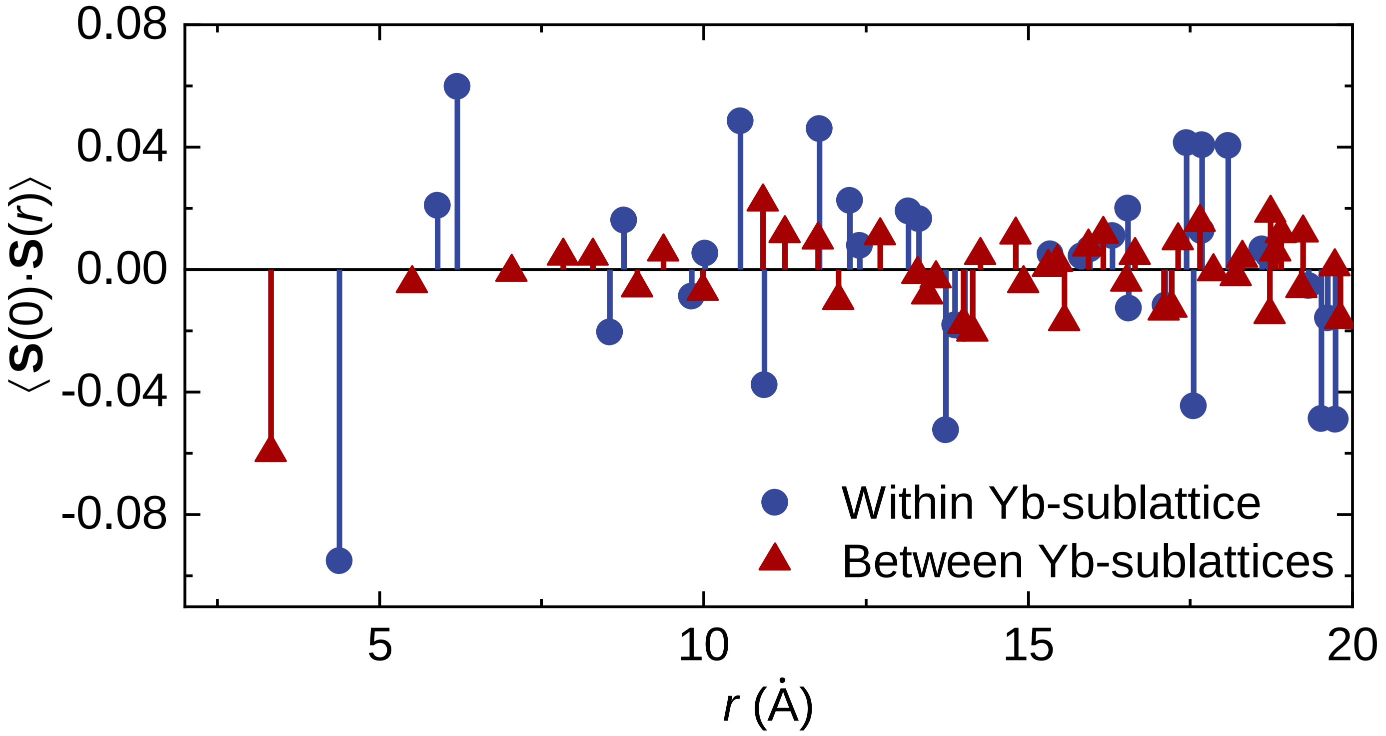
$\mu_{eff} = gS\ \mu_B$ $\mu_{eff} = g\sqrt{S(S+1)}\ \mu_B$

Full effective moment size:

WISH: 1.5 μ_B (40 % at base)

D7: 2.64 μ_B (30% at base)

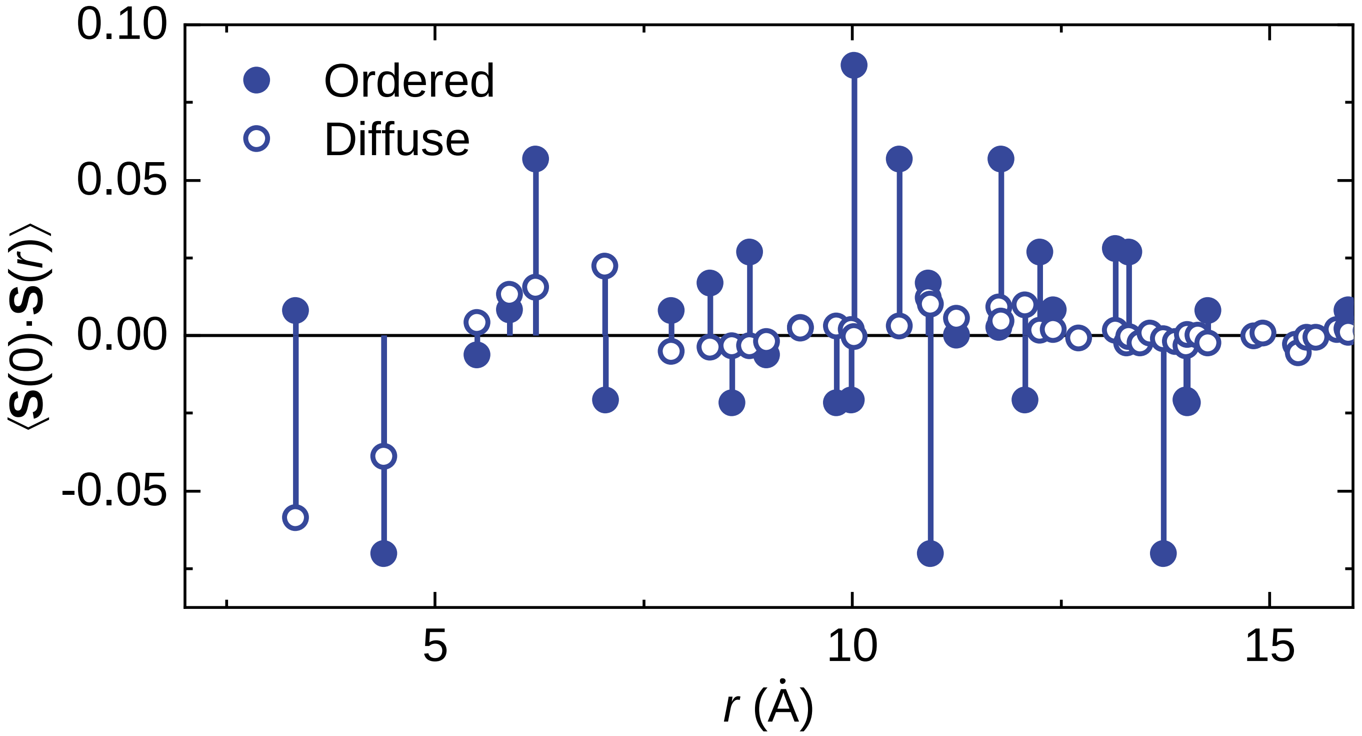
CORRELATIONS



Radial spin correlations calculated by SPINCORREL* at 50 mK

J. A. M. Paddison *et al.* J. Phys.:Condens. Matter **25**, 454220 (2013)

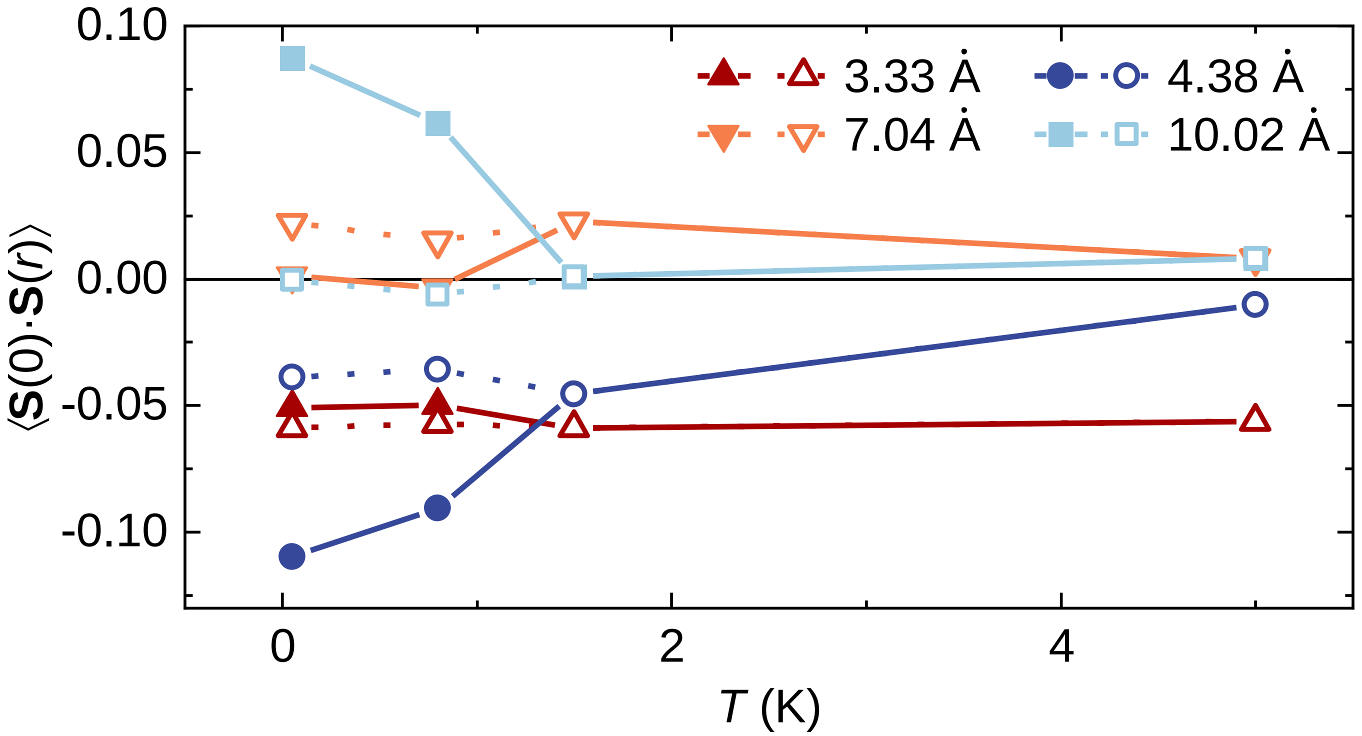
CORRELATIONS BREAKDOWN



Ordered contribution = **long**-range helical structure

Diffuse contribution = **short**-range order

T DEPENDENCE



Open markers = **diffuse** contribution = ***T* independent**

Closed markers = **ordered** correlation = ***T* dependent**

SUMMARY

$\mathbf{k} = (0.391, \pm 0.391, 0)$
$\mu_{order} = 40\ \%\ \mu_{eff}$
$\boldsymbol{\phi = 1.15(5)\pi}$

$\mathbf{k} = (\delta, \pm\delta, 0)$
μ_{order} reduces to zero
$\boldsymbol{\phi = 1.15(5)\pi}$

Persistent short-range correlations down to 50 mK
= partially disordered magnetic ground state

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Thank you all for listening!

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