

Magnetic phase transitions and magnetoelastic coupling in *Ba₃CoSb₂O₉*

Ming Li^{1,2}

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Co-authors: J. Quilliam², H. Zhou³, Z. Dun³

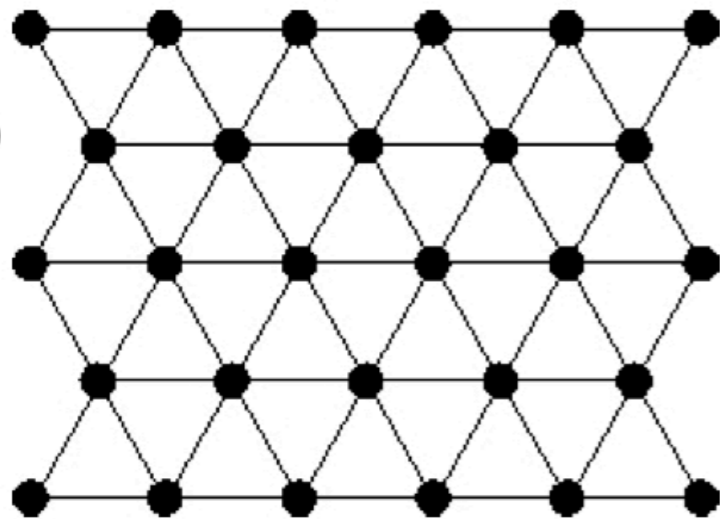
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²Département de physique, Université de Sherbrooke

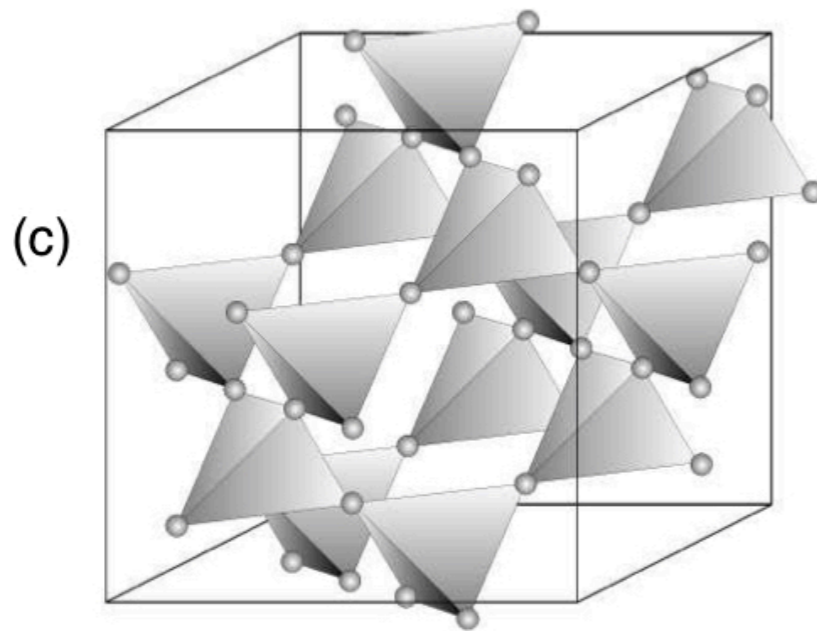
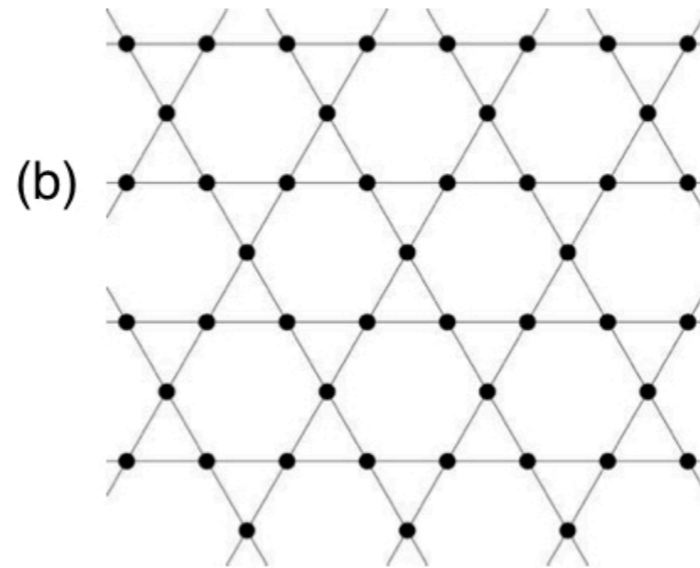
³Department of Physics and Astronomy, University of Tennessee

Degenerate ground states in frustrated antiferromagnets

Triangular

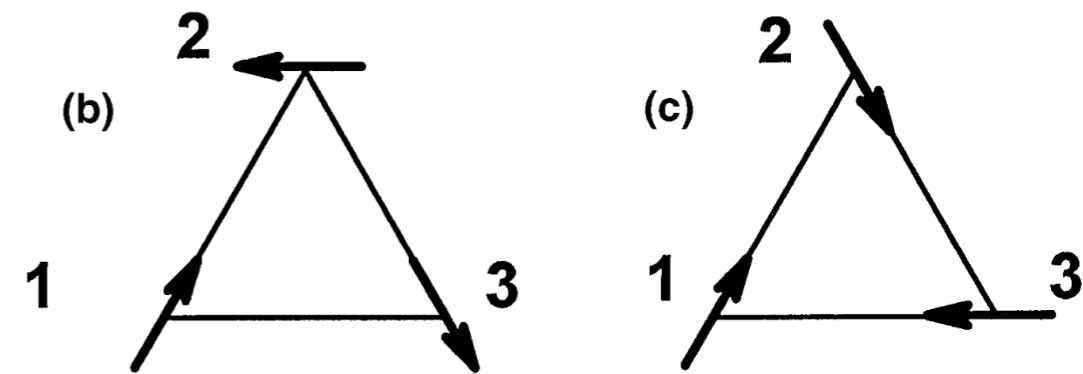
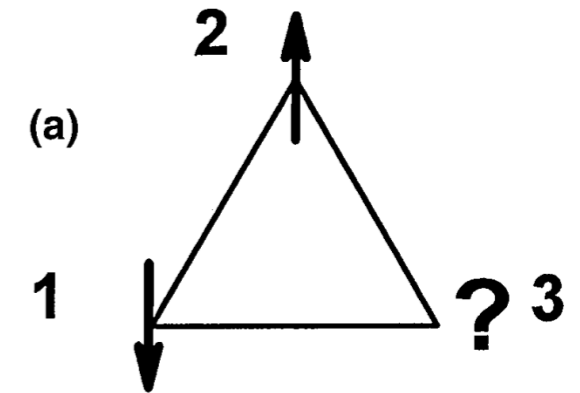


Kagomè



Pyrochlore

AF Frustration



Two 120° degenerate chiral states

Different properties from normal antiferromagnets
because of degenerate ground states

Properties of $Ba_3CoSb_2O_9$

Stacked equilateral triangular lattice
(Space group $P6_3/mmc$);

Magnetic ions Co^{2+} with
effective $1/2$ spin;

Quasi-2D crystal because of
 $J_c/J_{ab} \approx 0.027$;

Easy-plane anisotropy.

Properties and magnetic process of $Ba_3CoSb_2O_9$

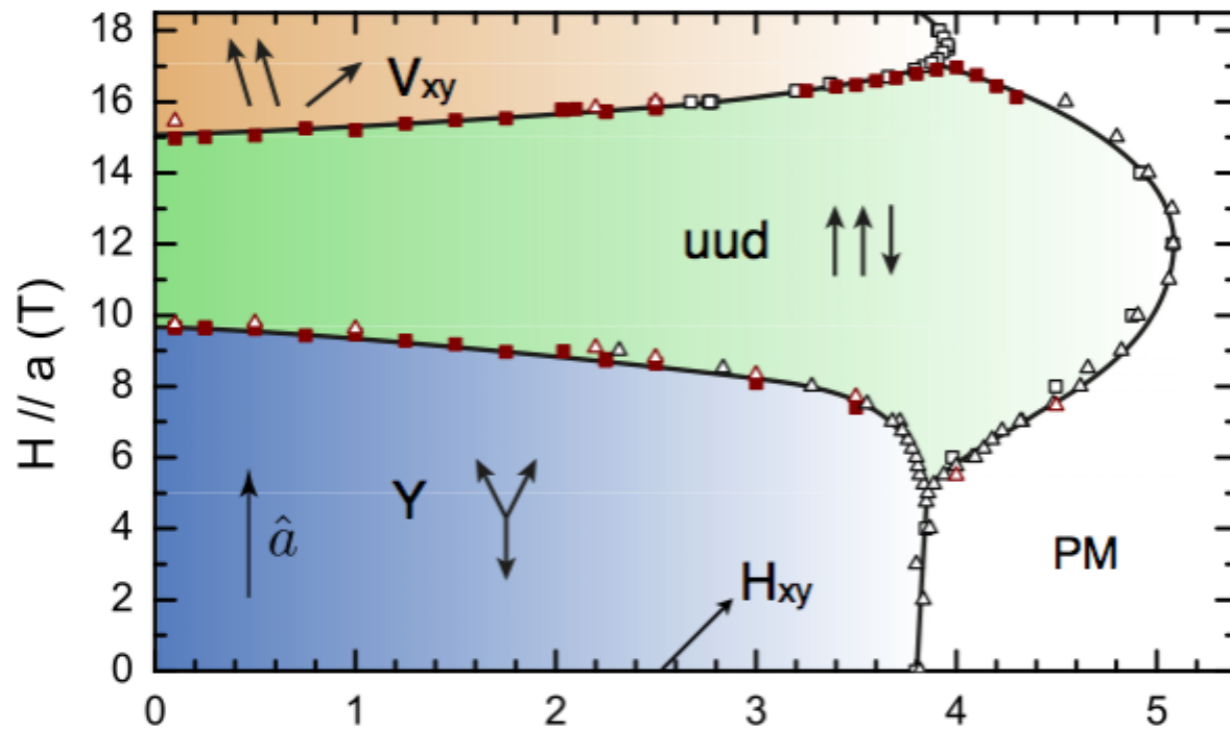
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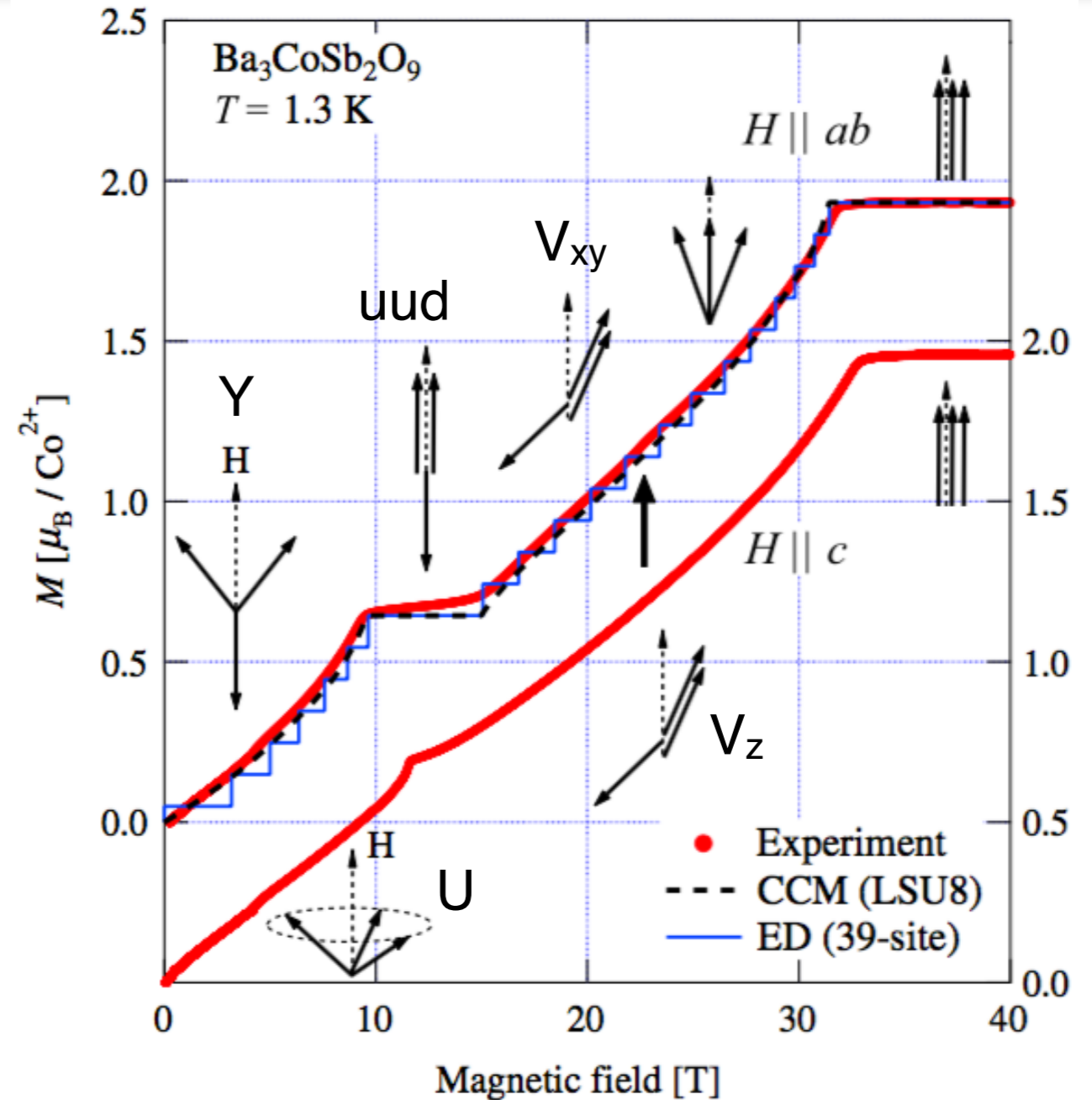
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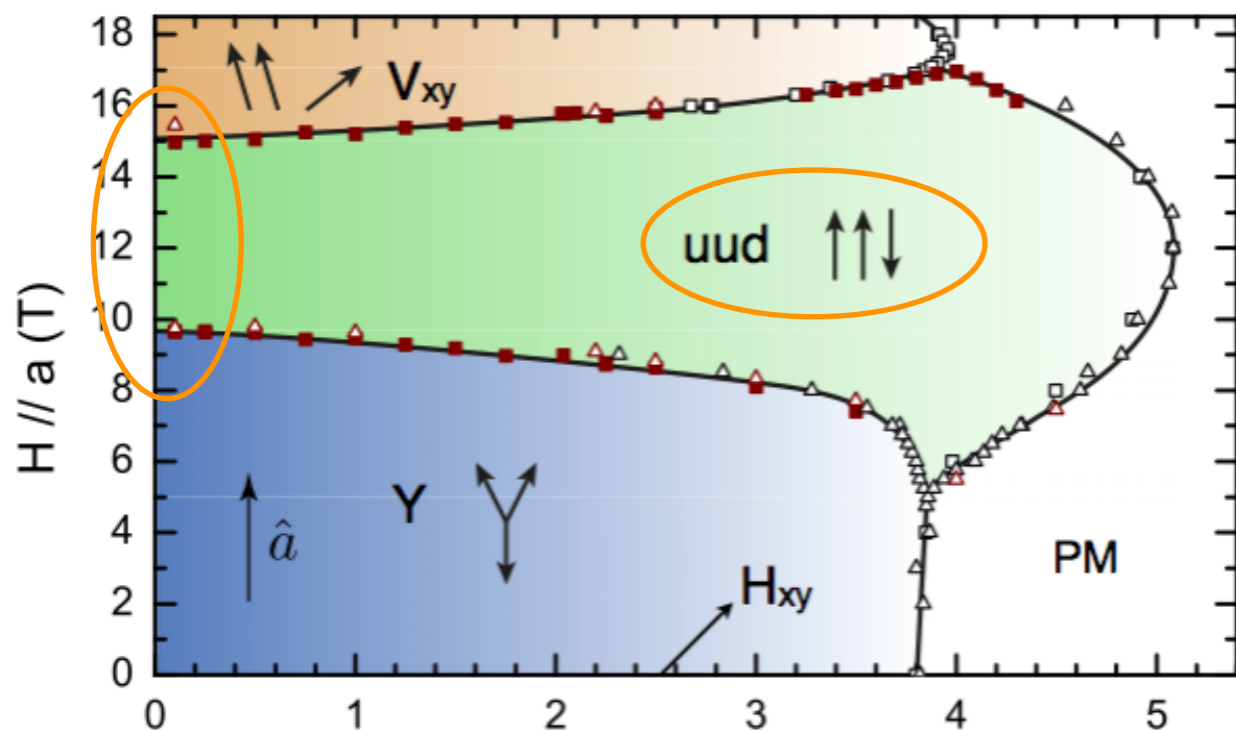
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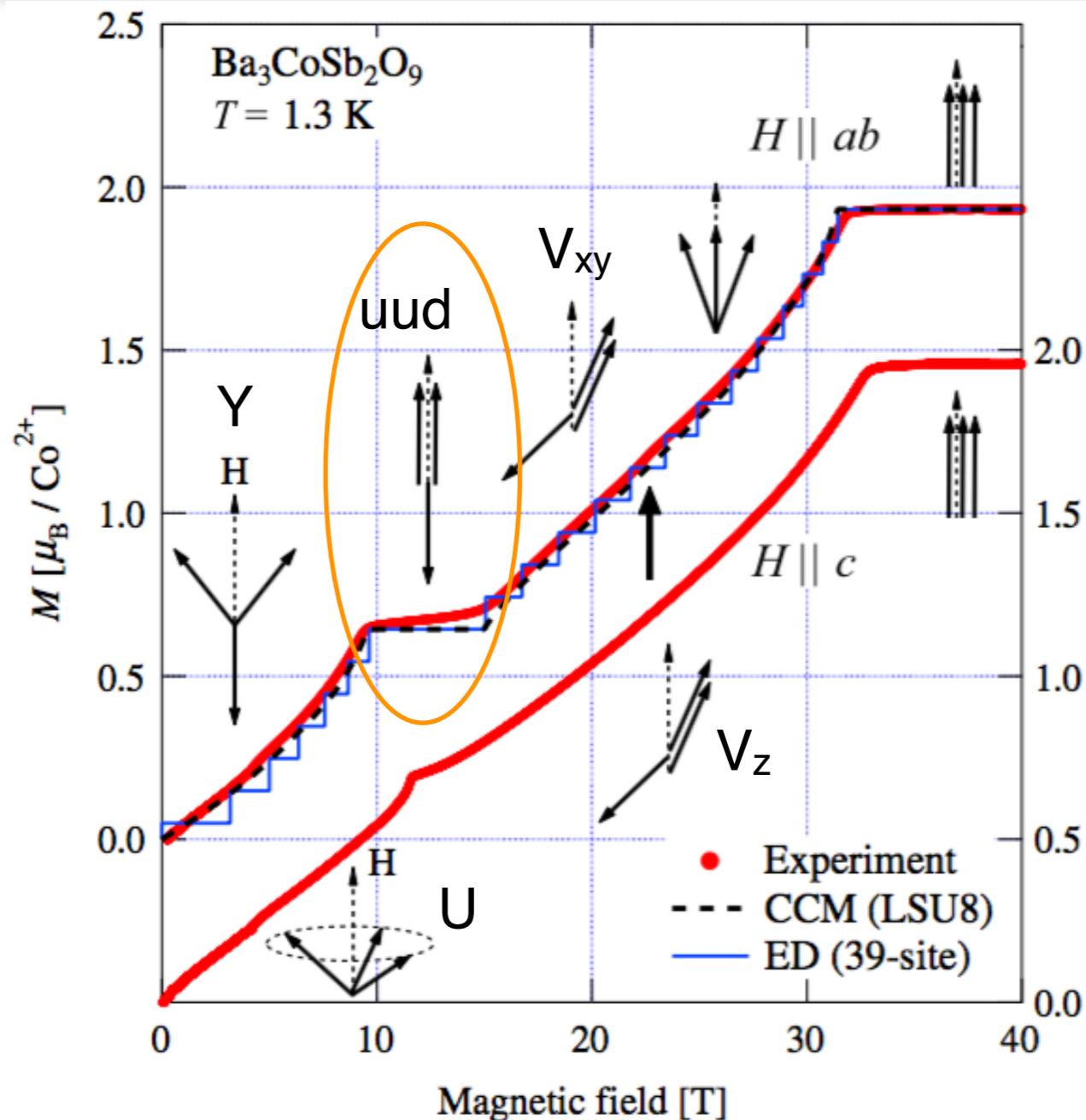
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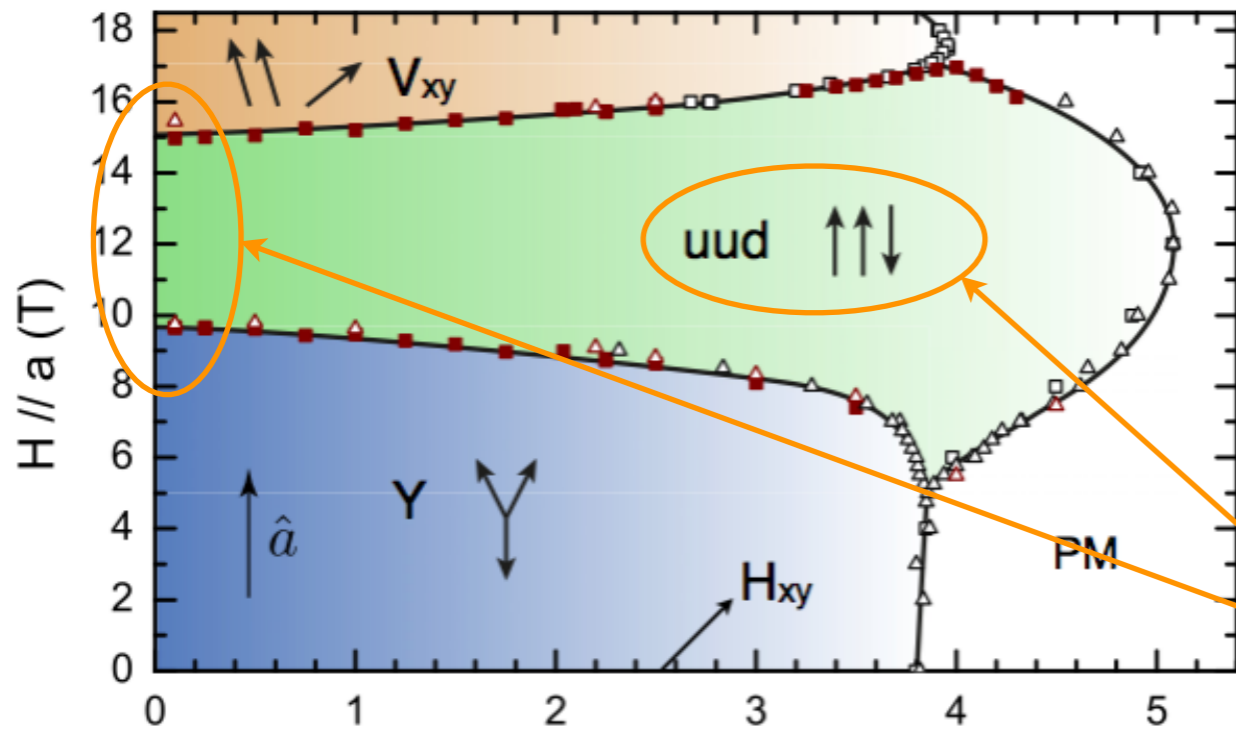
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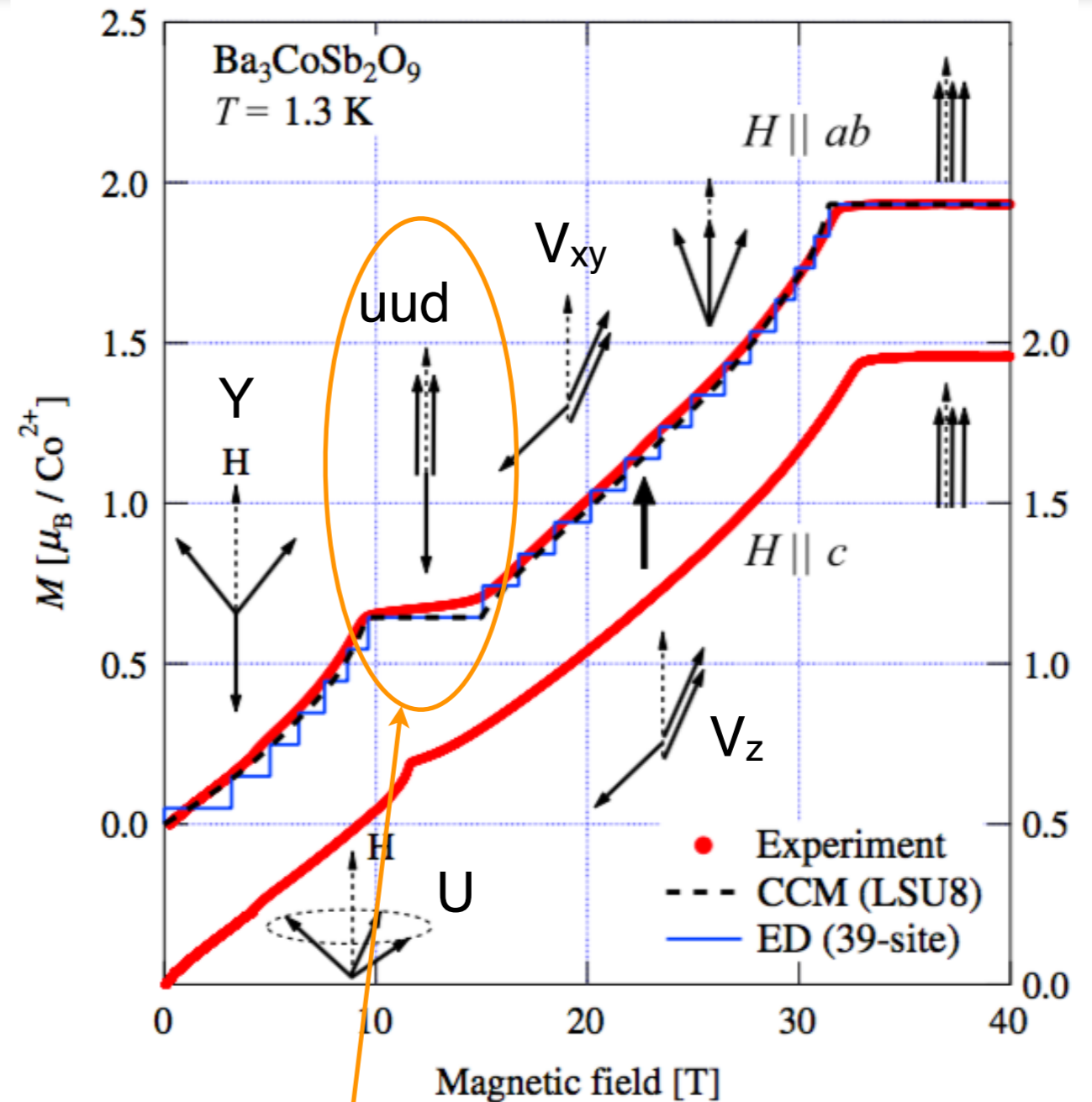
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Thermal and quantum fluctuation

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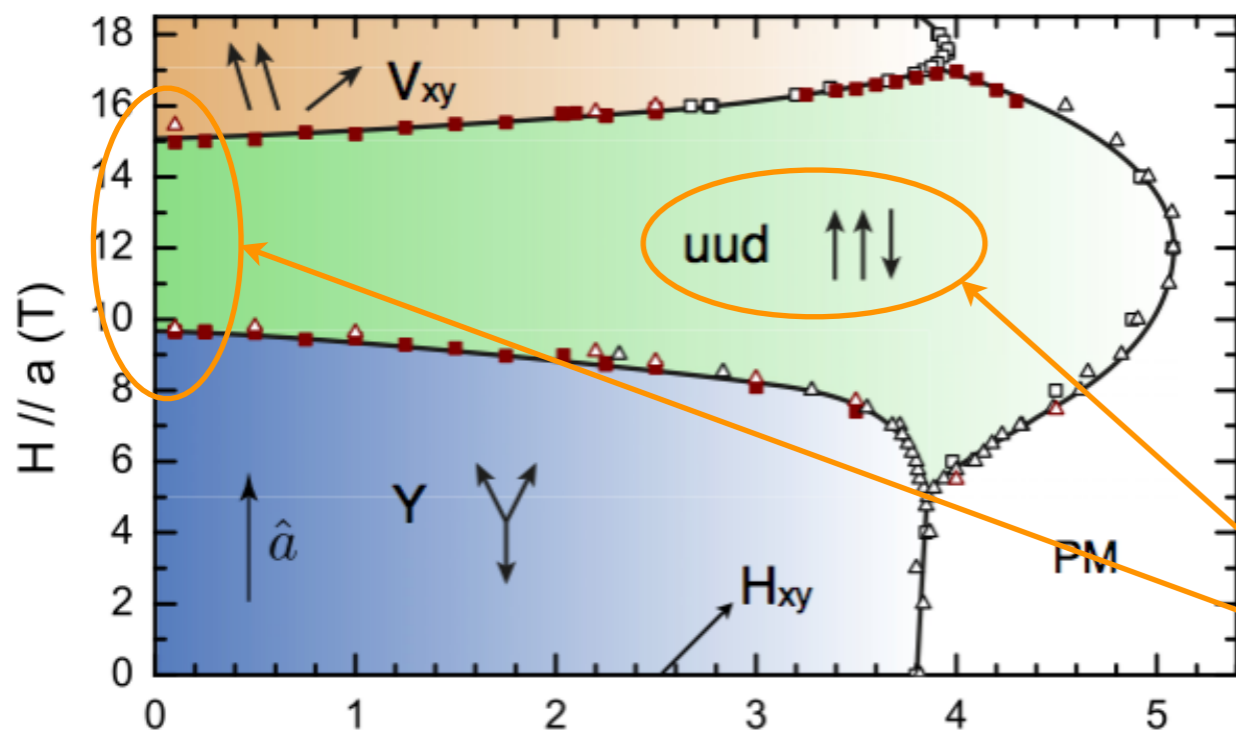
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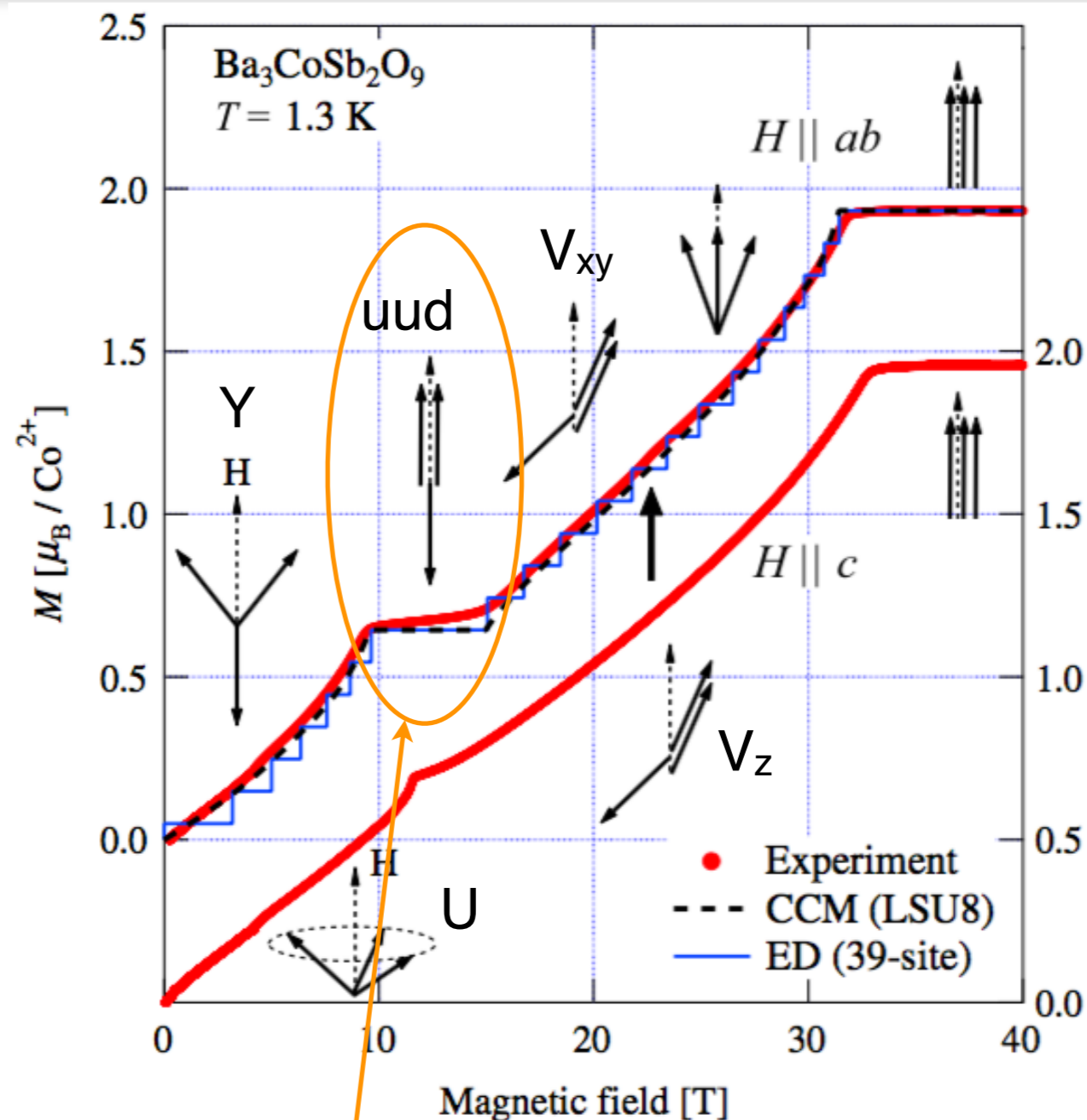
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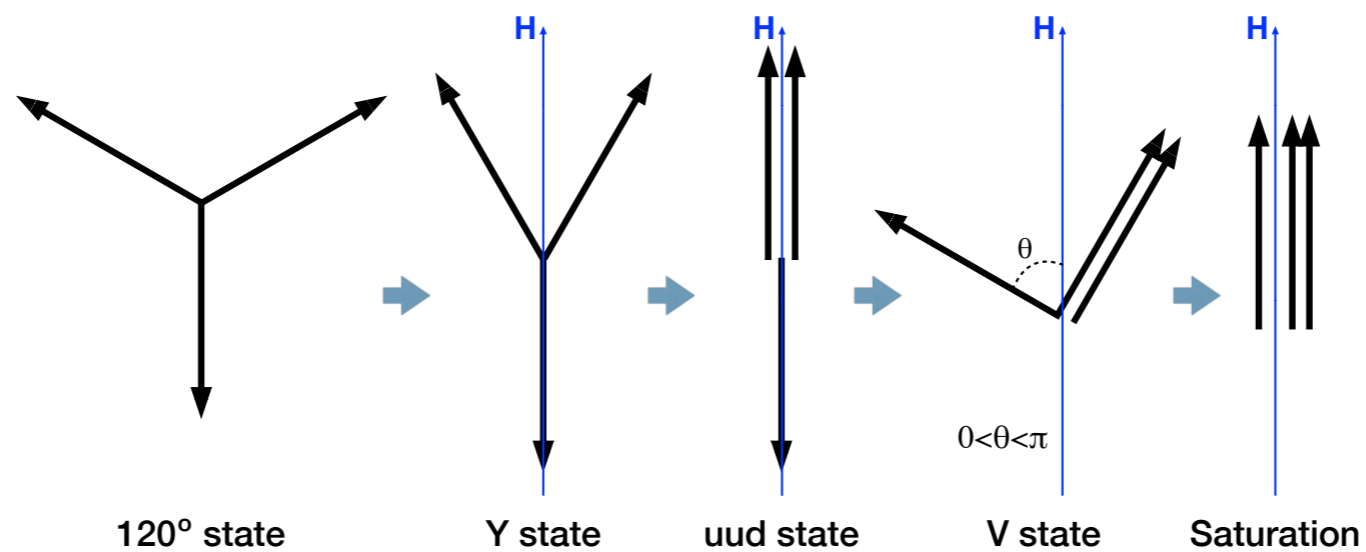
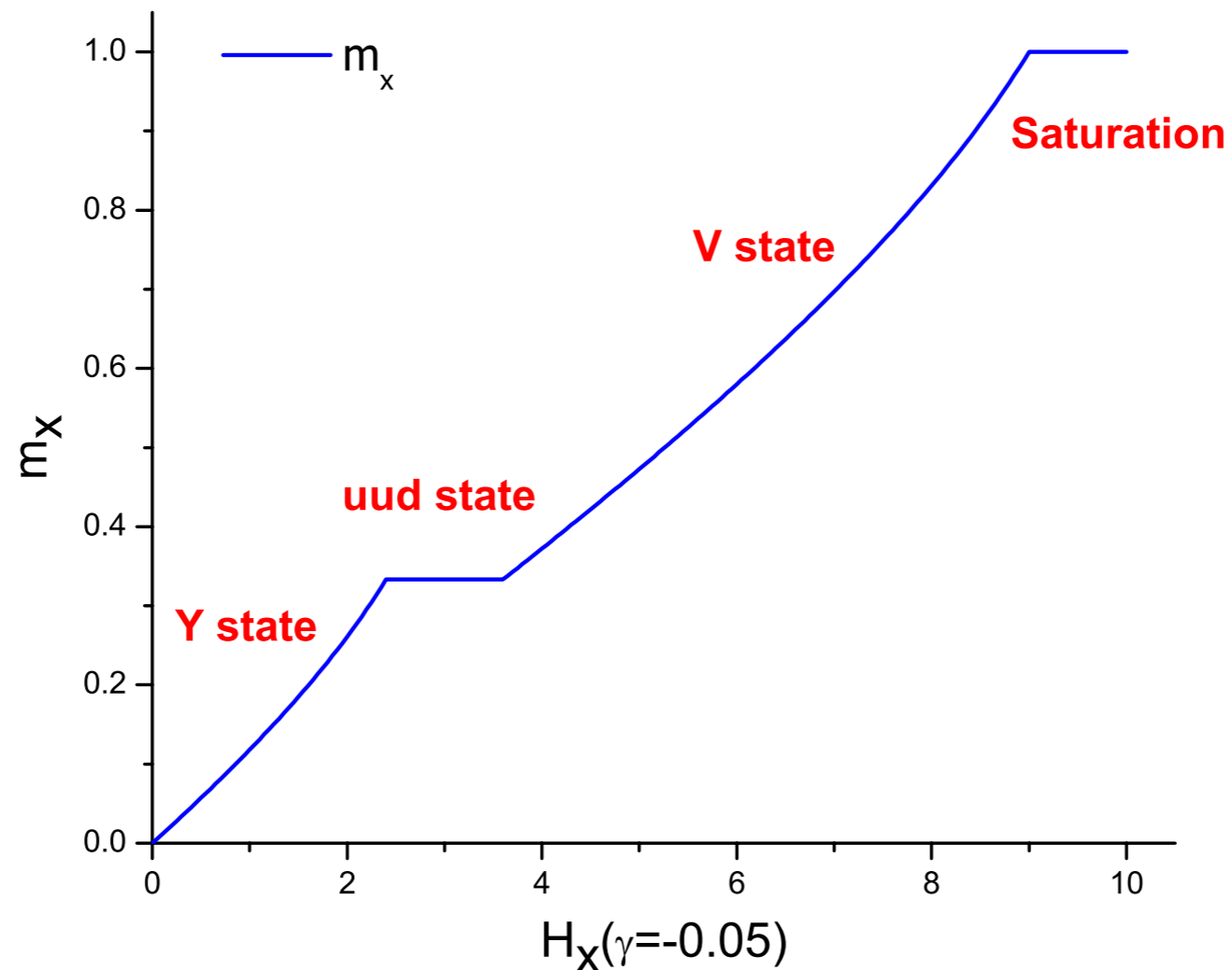
Thermal and quantum fluctuation

$$E \sim \sum_{ij} (S_i S_j)^2$$

M. E. Zhitomirsky, J. Phys.:
Conf. Ser. **592**, 012110(2015).

H_x dependence of magnetization

$$E/J = \sum_{i,j=A,B,C} \mathbf{S}_i \cdot \mathbf{S}_j + \gamma \sum_{\substack{i,j=A,B,C \\ i \neq j}} (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - \frac{1}{3} \mathbf{H} \cdot \sum_{i=A,B,C} \mathbf{S}_i$$



Magnetoelastic coupling and bi-quadratic exchange

Magnetoelastic coupling is accounted for the variation of exchange constant ($\delta J = Ke$, where e is strain). With elastic energy, we conclude

$$F \sim JS^2 \rightarrow F = (J + Ke)S^2 + \frac{1}{2}Ce^2$$

For equilibrium,

$$\frac{\partial F}{\partial e} = KS^2 + Ce = 0$$

so that

$$e = -\frac{K}{C}S^2$$

therefore,

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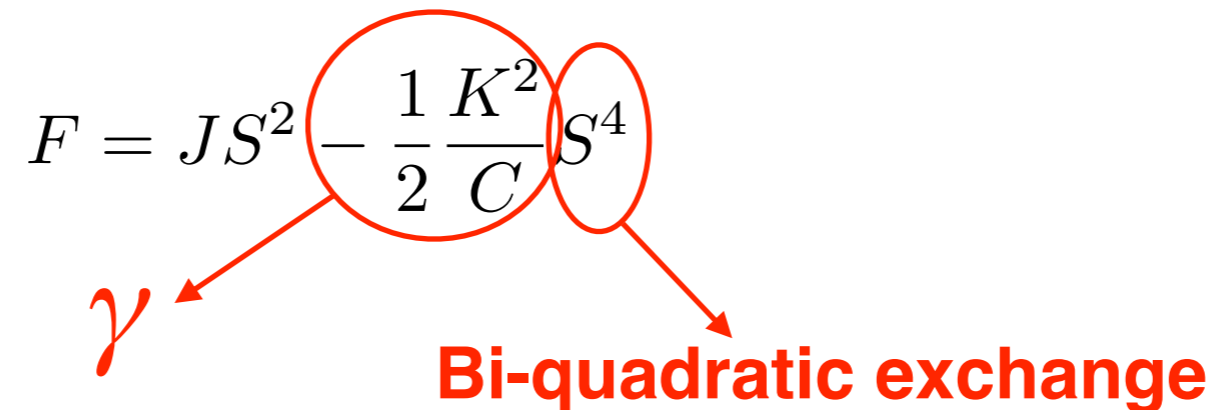
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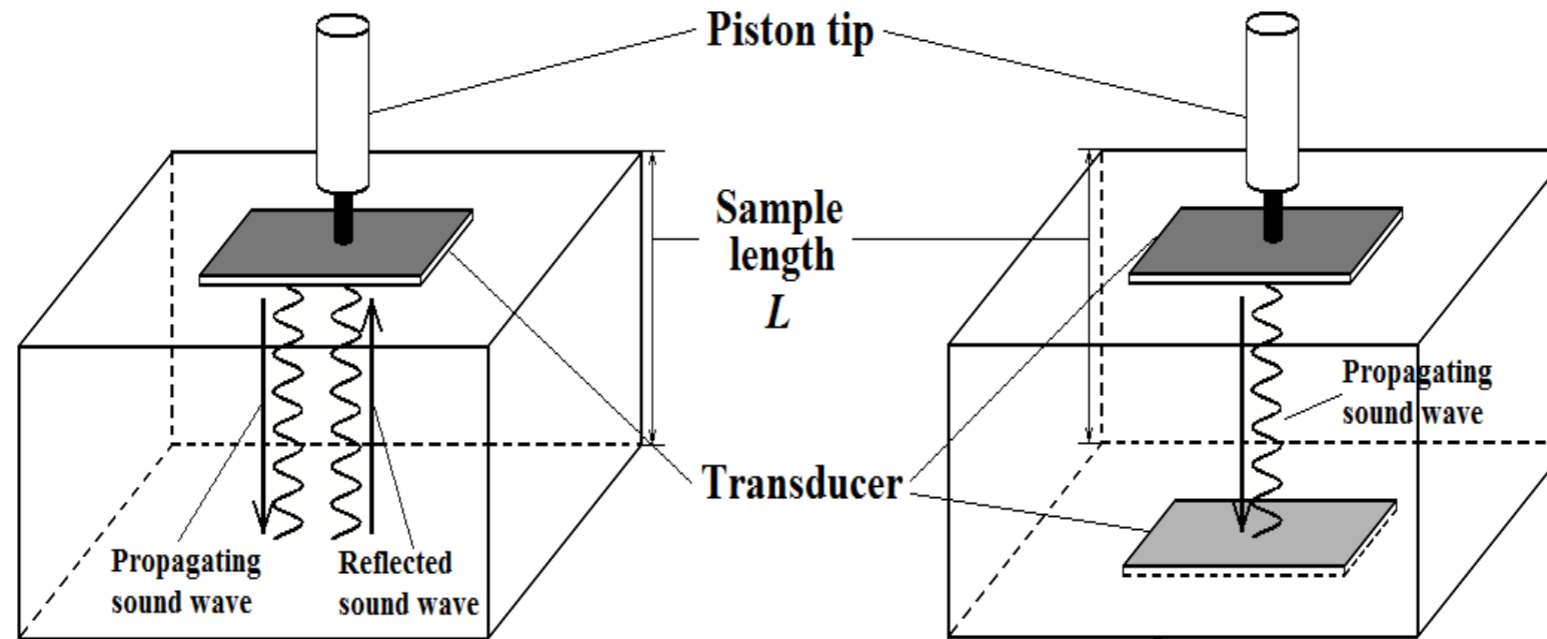
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Bi-quadratic exchange

Reflection and Transmission configuration



Phase difference Φ :

$$\Phi = \frac{2\pi t}{T} = \frac{2\pi L f}{v}$$

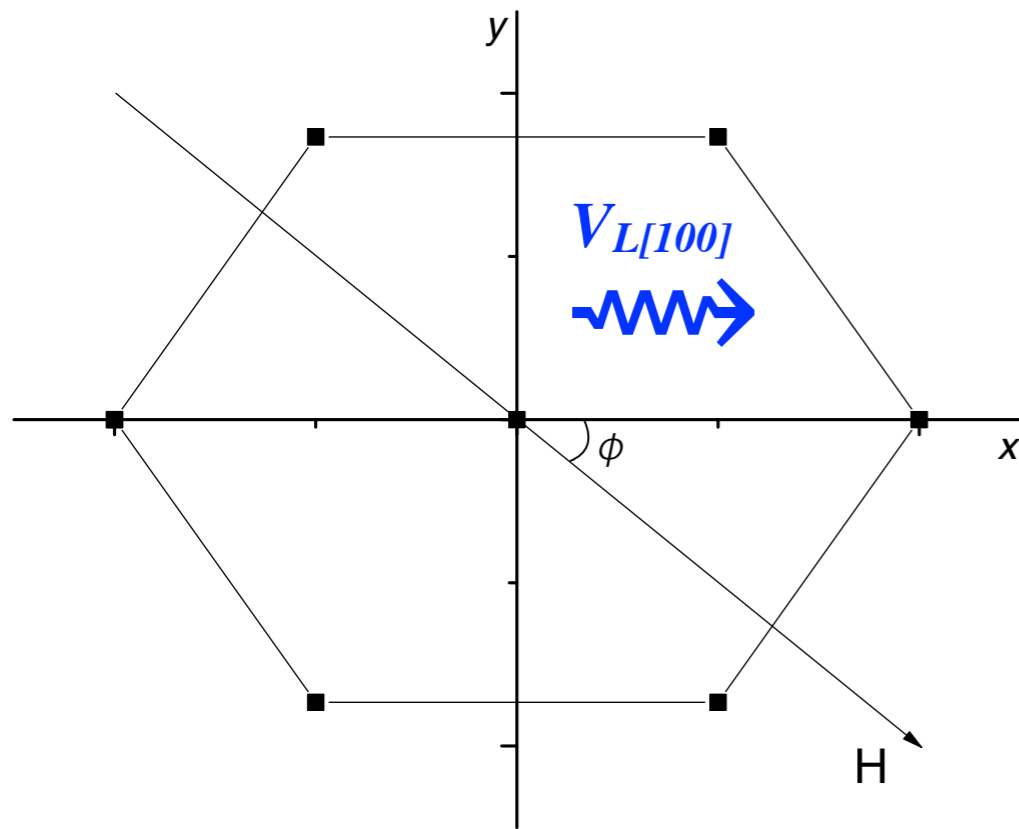
Ignoring thermal expansion and keeping the relative phase difference equal to zero:

$$\frac{\Delta\Phi}{\Phi} = \frac{\Delta f}{f} - \frac{\Delta v}{v} = 0.$$

With $v = \sqrt{\frac{C}{\rho}}$, where C is elastic constant, ρ is mass density,

$$\frac{\Delta C}{2C} = \frac{\Delta v}{v} = \frac{\Delta f}{f}.$$

Geometry of the experiment

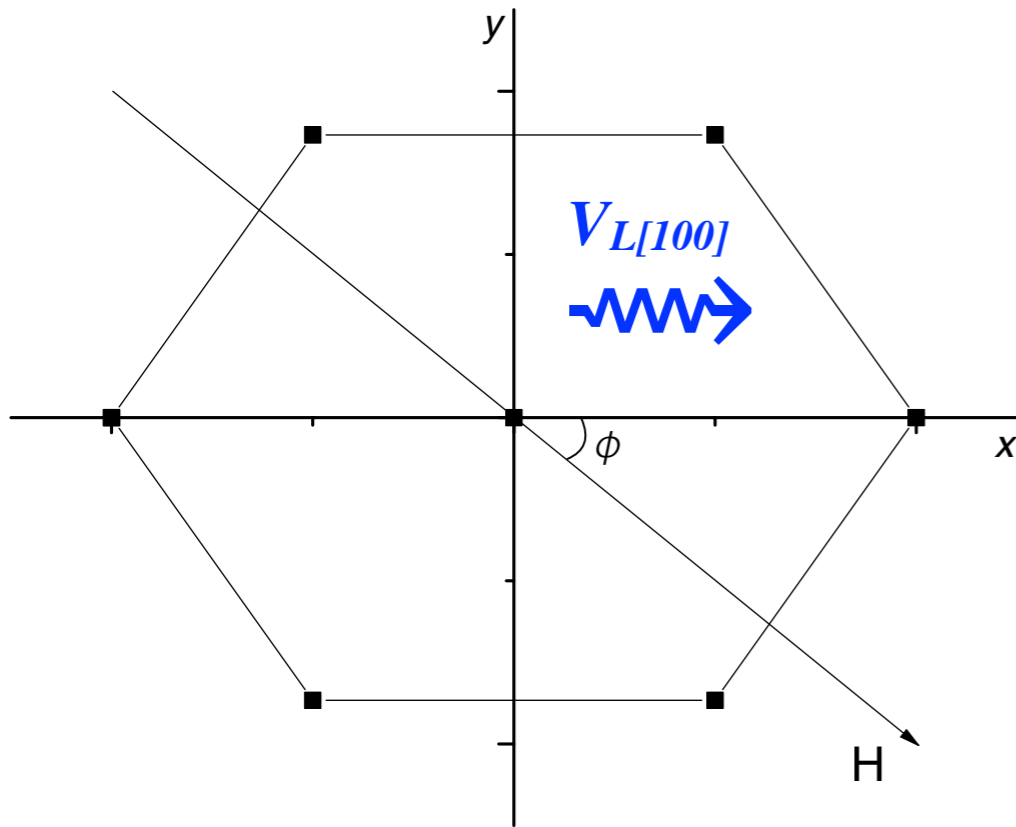


$V_{L[100]} = \sqrt{C_{11}/\rho}$ as function of ϕ
 $\phi = 0^\circ$ corresponds to $\mathbf{H} \parallel x$ -axis

Period: 180° for hexagonal symmetry
without distortion

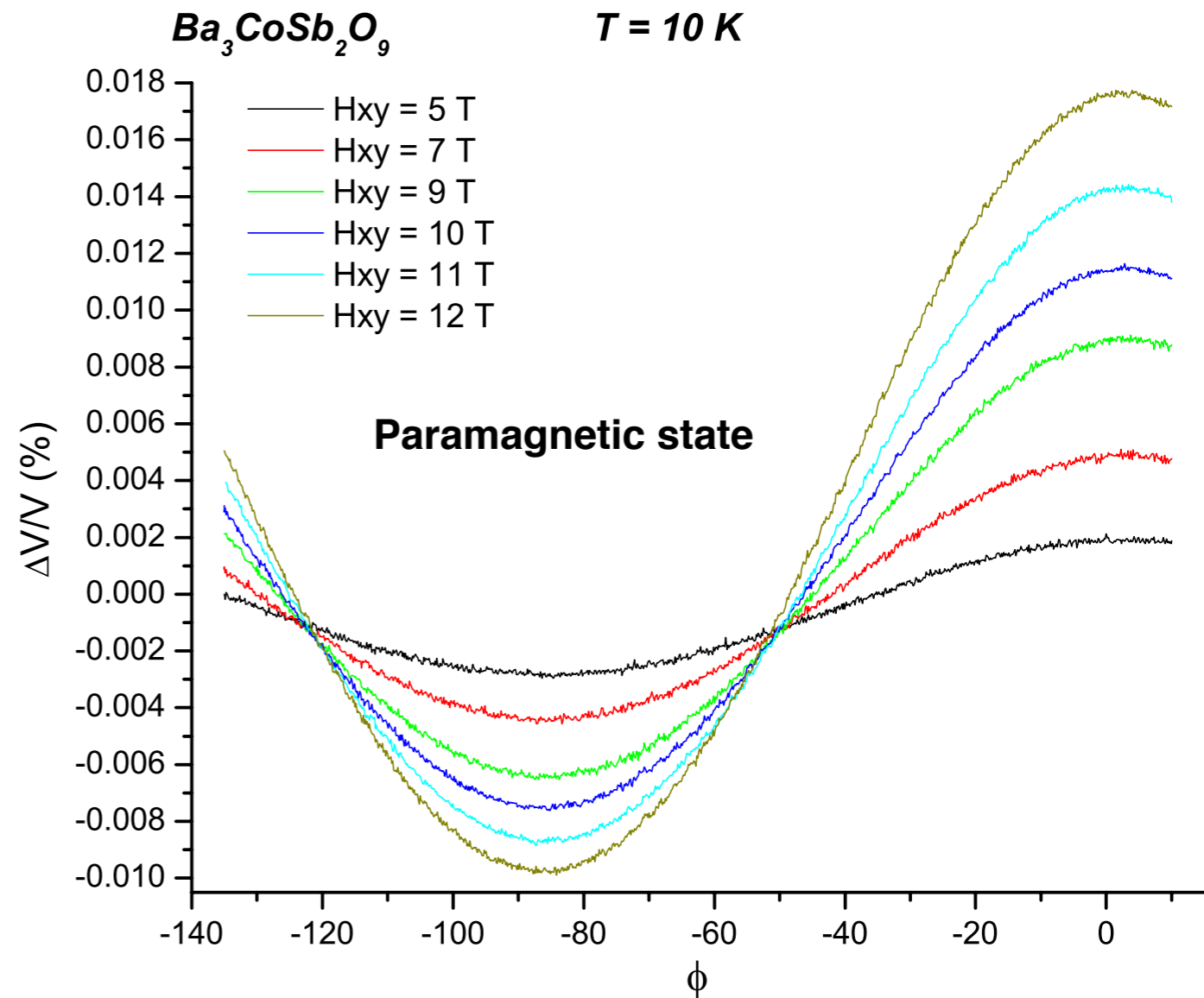
Angular dependence of $\Delta V/V$

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Linear-quadratic magnetoelastic coupling

The total free energy includes elastic coupling ($F(e)$), linear-quadratic magnetoelastic coupling ($F(m, e)$) and the magnetization contribution ($F(m)$):

$$F = F(e) + F(m, e) + F(m),$$

where (using the Voigt notation)

$$F(e) = \frac{1}{2} C_{\alpha\beta} e_{\alpha} e_{\beta},$$

$$F(m, e) = K_{\alpha\beta} \mathcal{M}_{\alpha} e_{\beta},$$

$$F(m) = A_Q \mathbf{m}^2 - \mathbf{m} \mathbf{H},$$

$$\begin{aligned} \mathcal{M}_{\alpha} &= \{ m_x^2, m_y^2, m_z^2, 2m_y m_z, 2m_z m_x, 2m_x m_y \}, \\ \alpha &= \{ 1, 2, 3, 4, 5, 6 \}, \end{aligned}$$

$C_{\alpha\beta}$ (elastic tensor) and $K_{\alpha\beta}$ (1-q tensor) remain invariant under the symmetry operations I^2 , C_y^2 , C_z^2 , C_z^3 .

The angular dependence of the new elastic tensor $C'(\phi)$ is obtained using

$$C'(\phi) = \frac{\partial^2 F}{\partial e_\alpha \partial e_\beta} - \frac{\frac{\partial^2 F}{\partial e_\alpha \partial m} \frac{\partial^2 F}{\partial e_\beta \partial m}}{\frac{\partial^2 F}{\partial m^2}}.$$

Therefore, the effect of linear-quadratic magnetoelastic coupling ($F(m, e)$) can be measured by

$$\begin{aligned} \frac{\Delta V_{L[100]}}{V_{L[100]}} &\simeq \frac{\Delta C'_{11}(\phi)}{2C_{11}} \simeq \frac{C'_{11}(\phi) - C'_{11}(0)}{2C_{11}} \\ &= A_{em} \sin^2(\phi) + B_{em} \sin^4(\phi), \end{aligned}$$

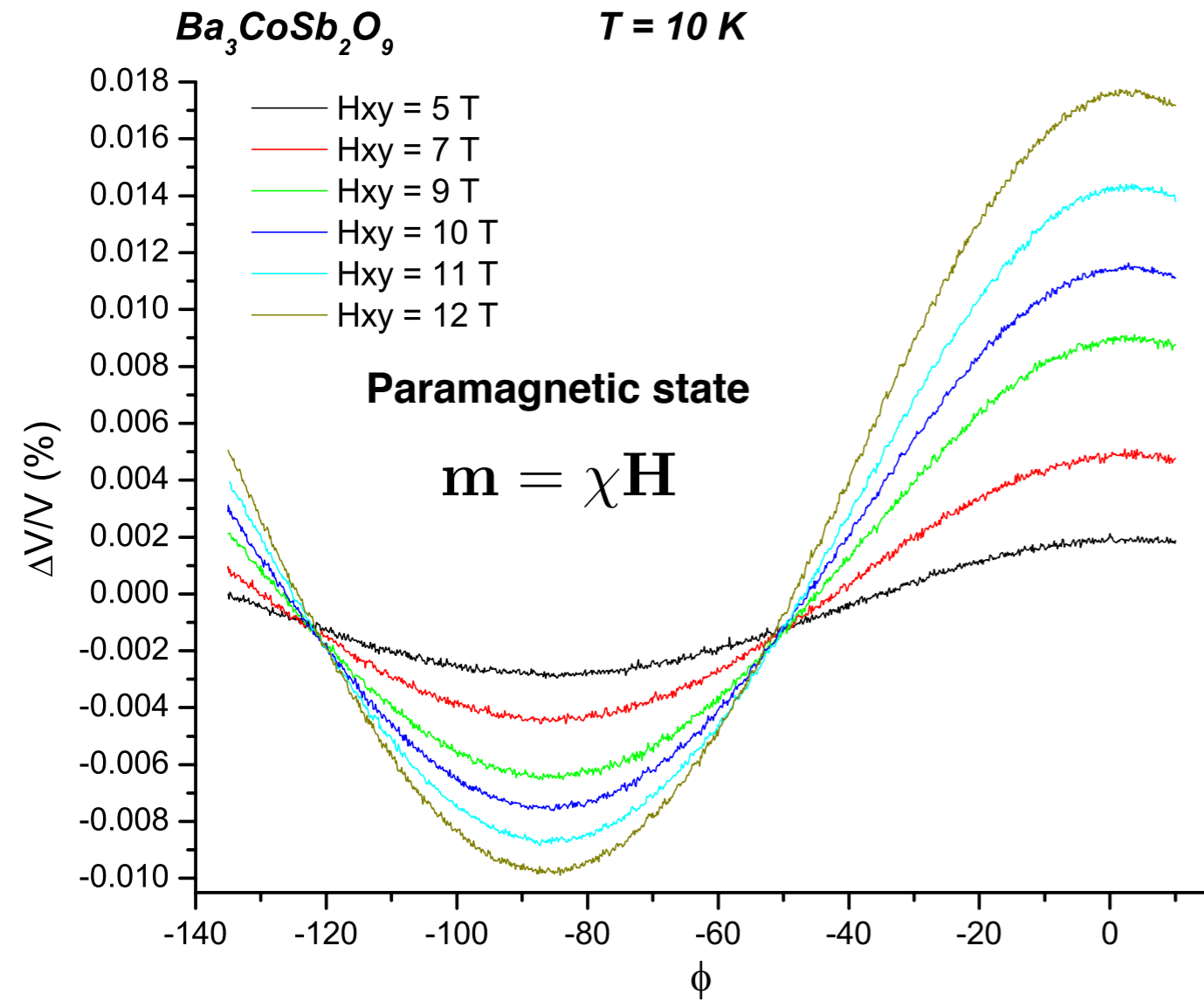
where

$$A_{em} = -\frac{8K_{m66}K_{m11}m^3}{C_{11}H}, \quad B_{em} = \frac{8K_{m66}^2m^3}{C_{11}H}$$

Strain:

$$e_1 - e_2 = -\frac{m^2 K_{m66} \cos(2\phi)}{C_{66}}, \quad e_6 = -\frac{m^2 K_{m66} \sin(2\phi)}{C_{66}}$$

Experimental results: angular dependence of $\Delta V/V$ at $T=10K$



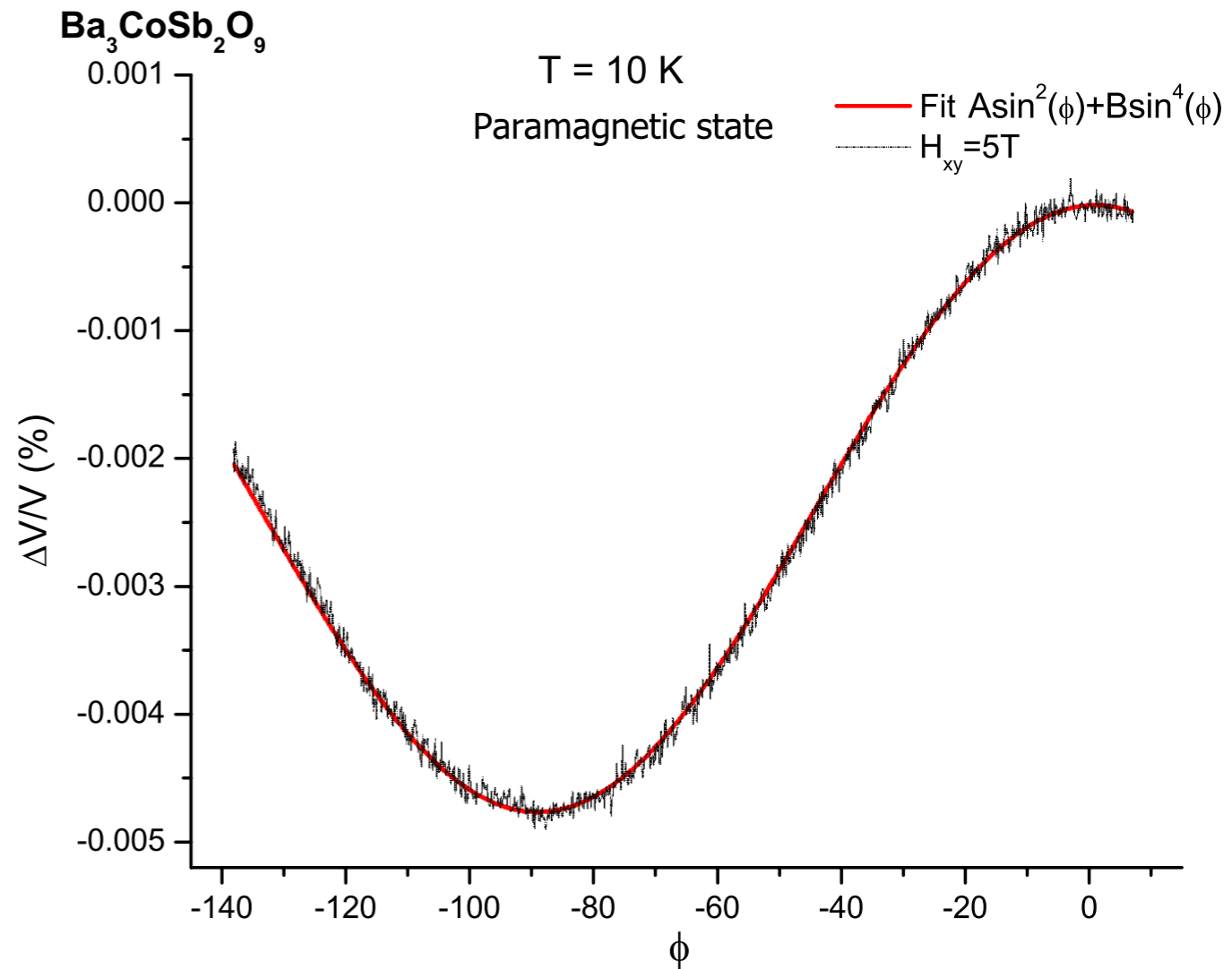
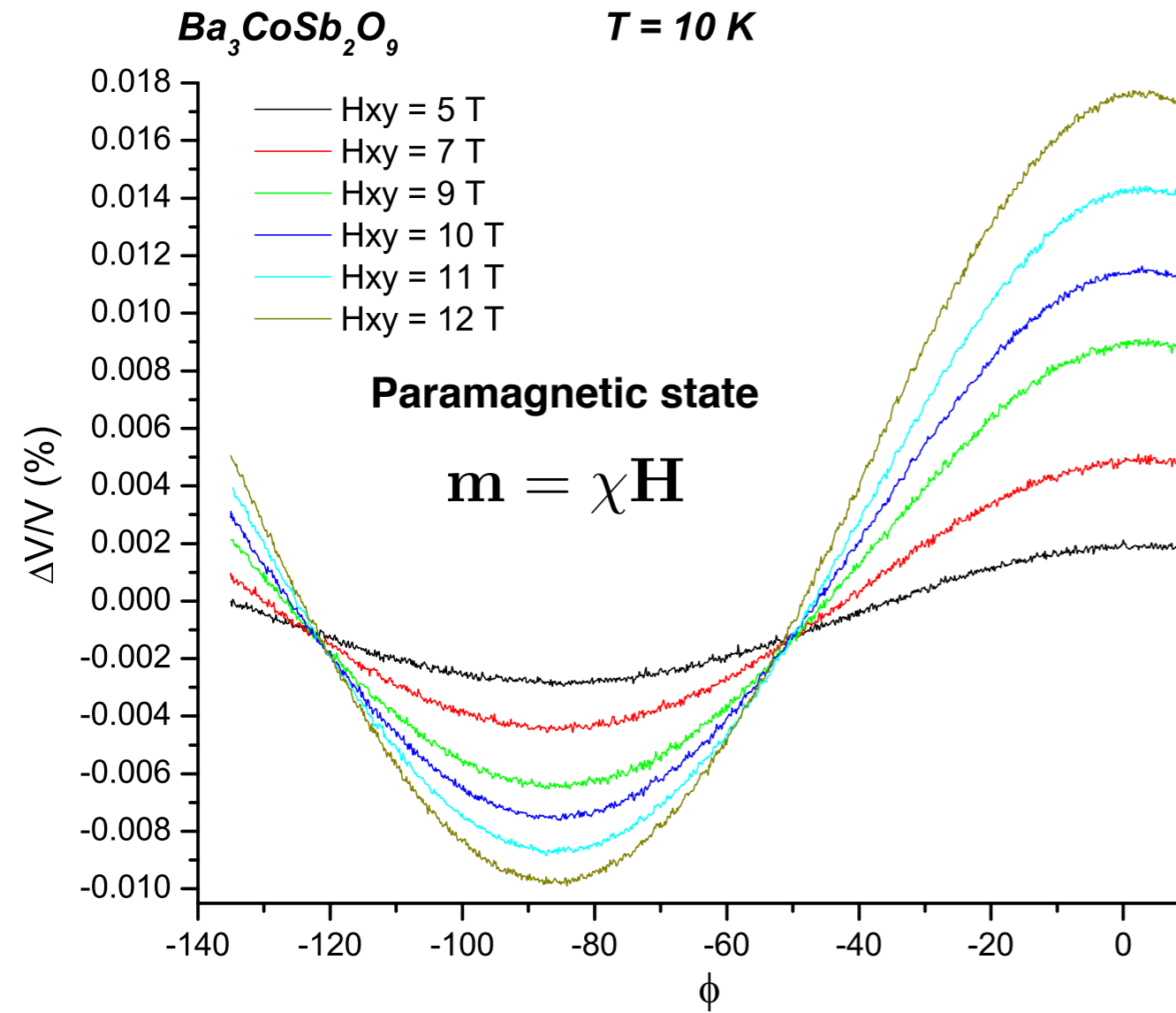
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$$e_1 - e_2 = -\frac{\chi^2 K_{m66}}{\mu_0 C_{66}} H^2 \cos(2\phi)$$

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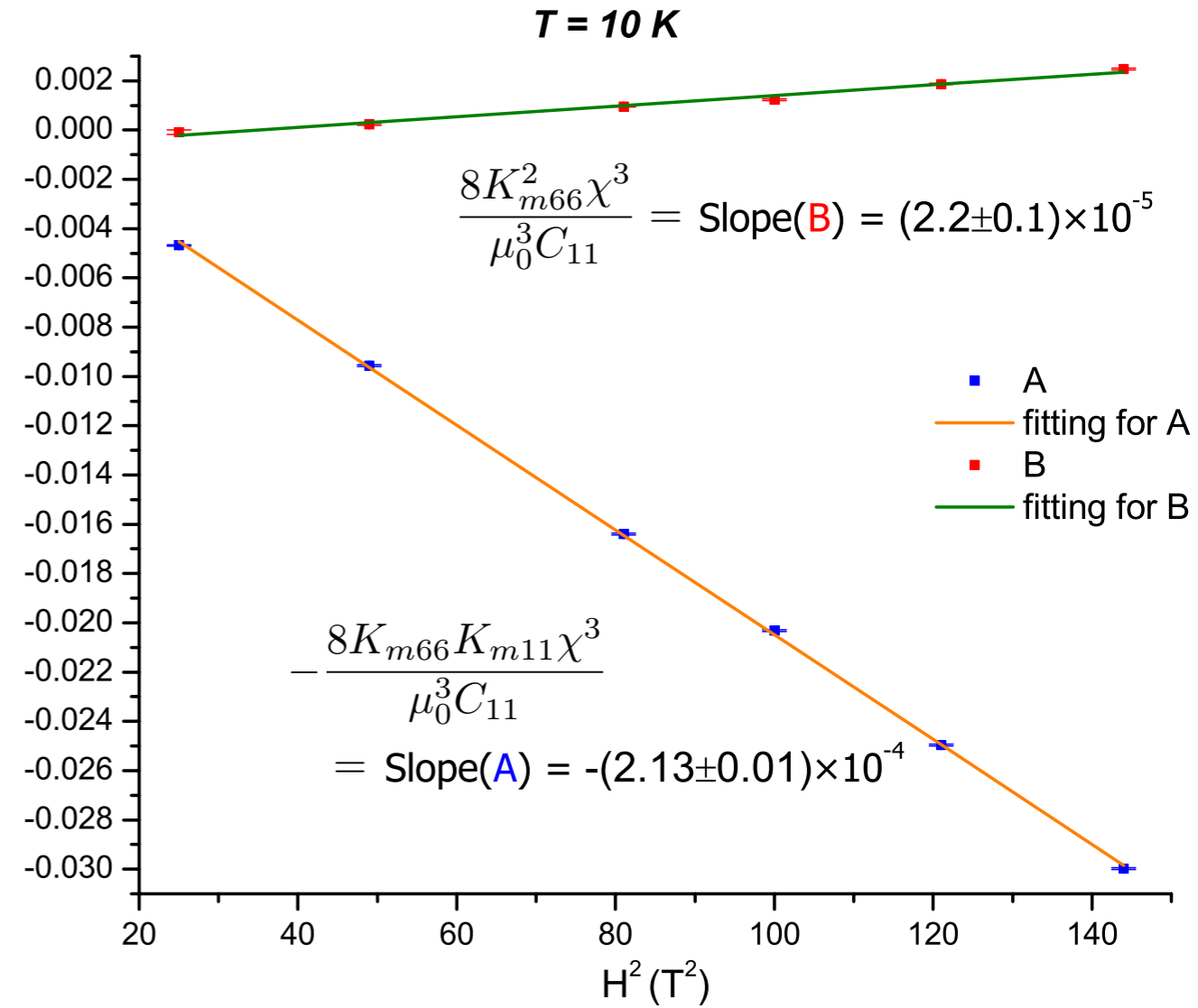
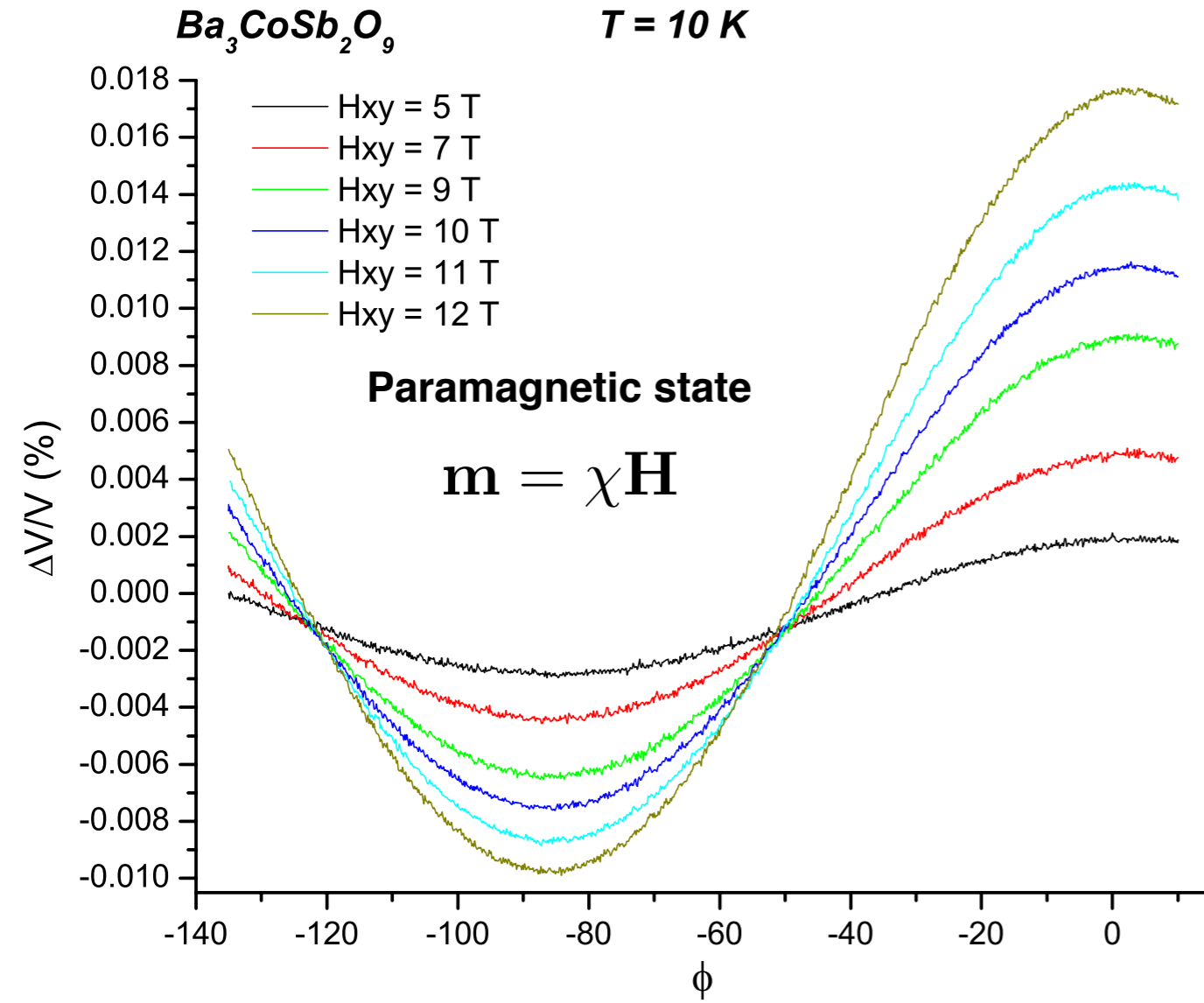
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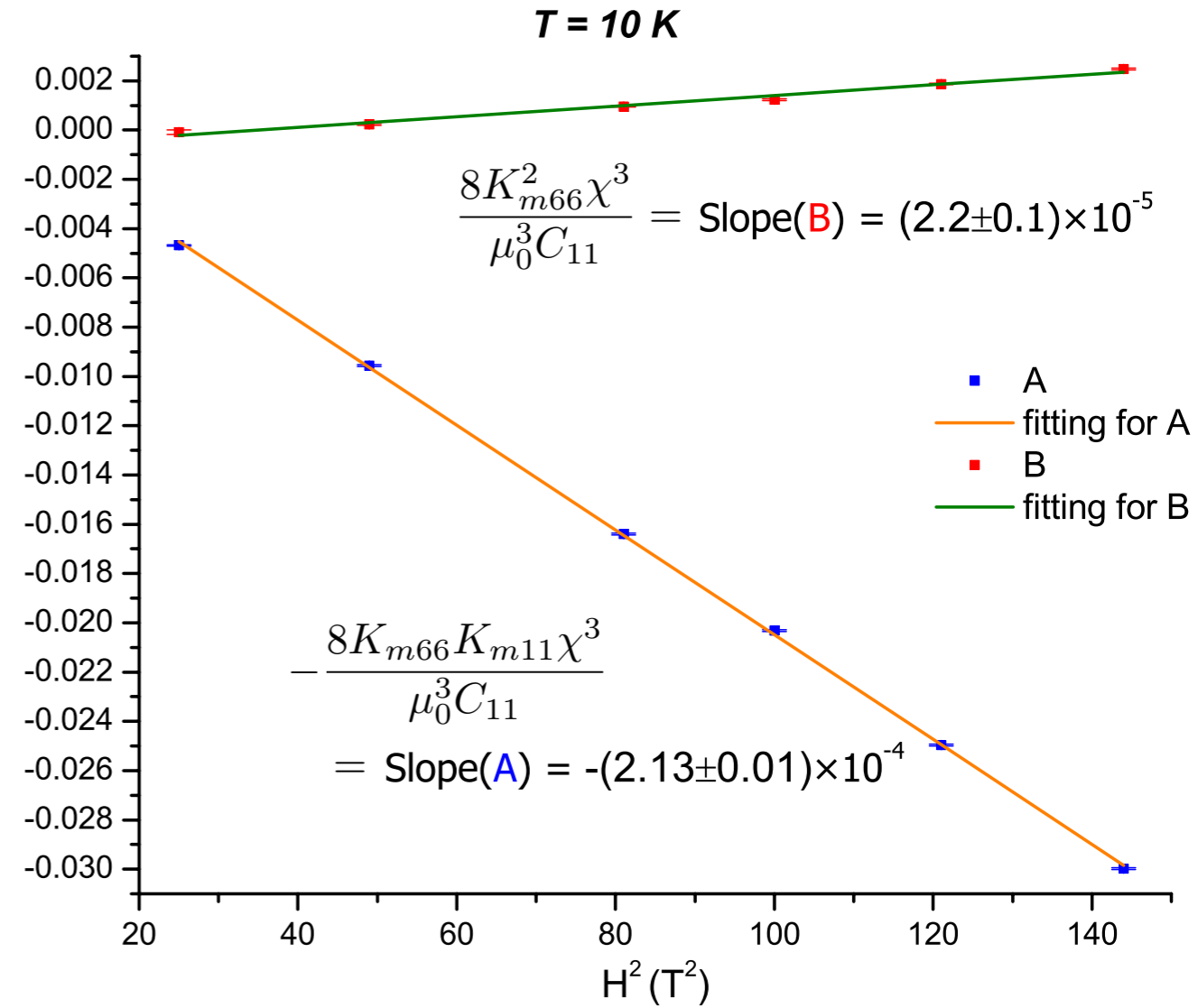
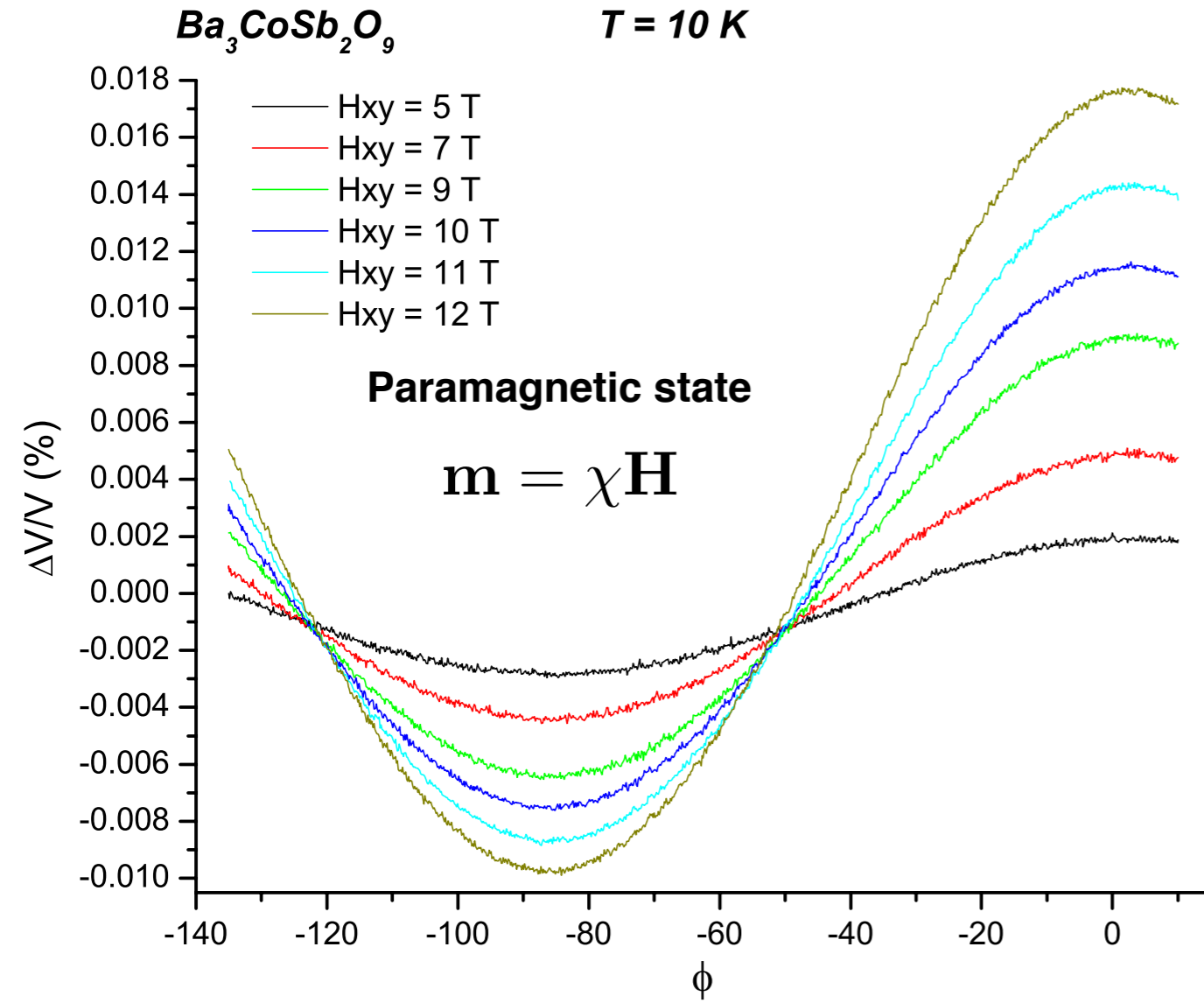
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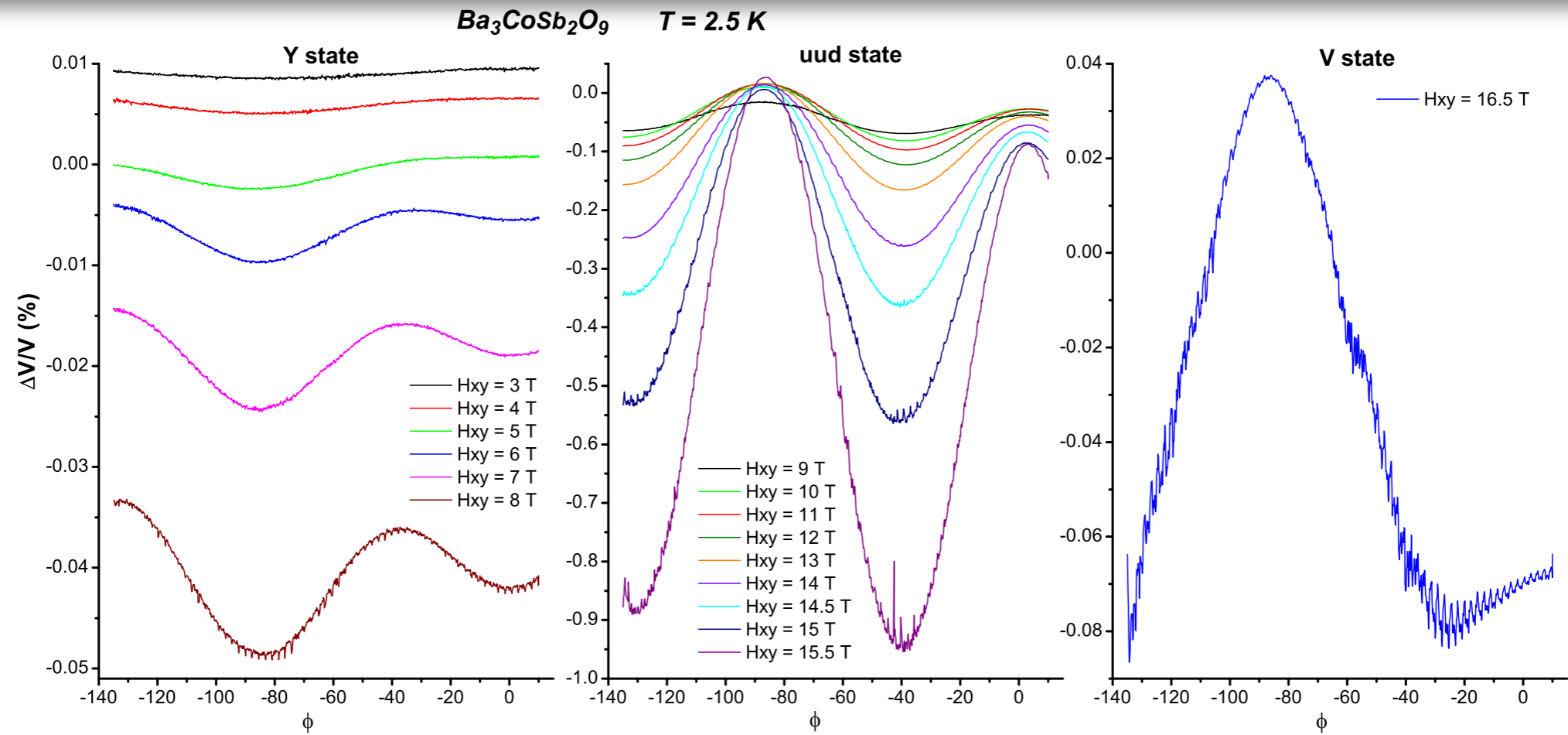
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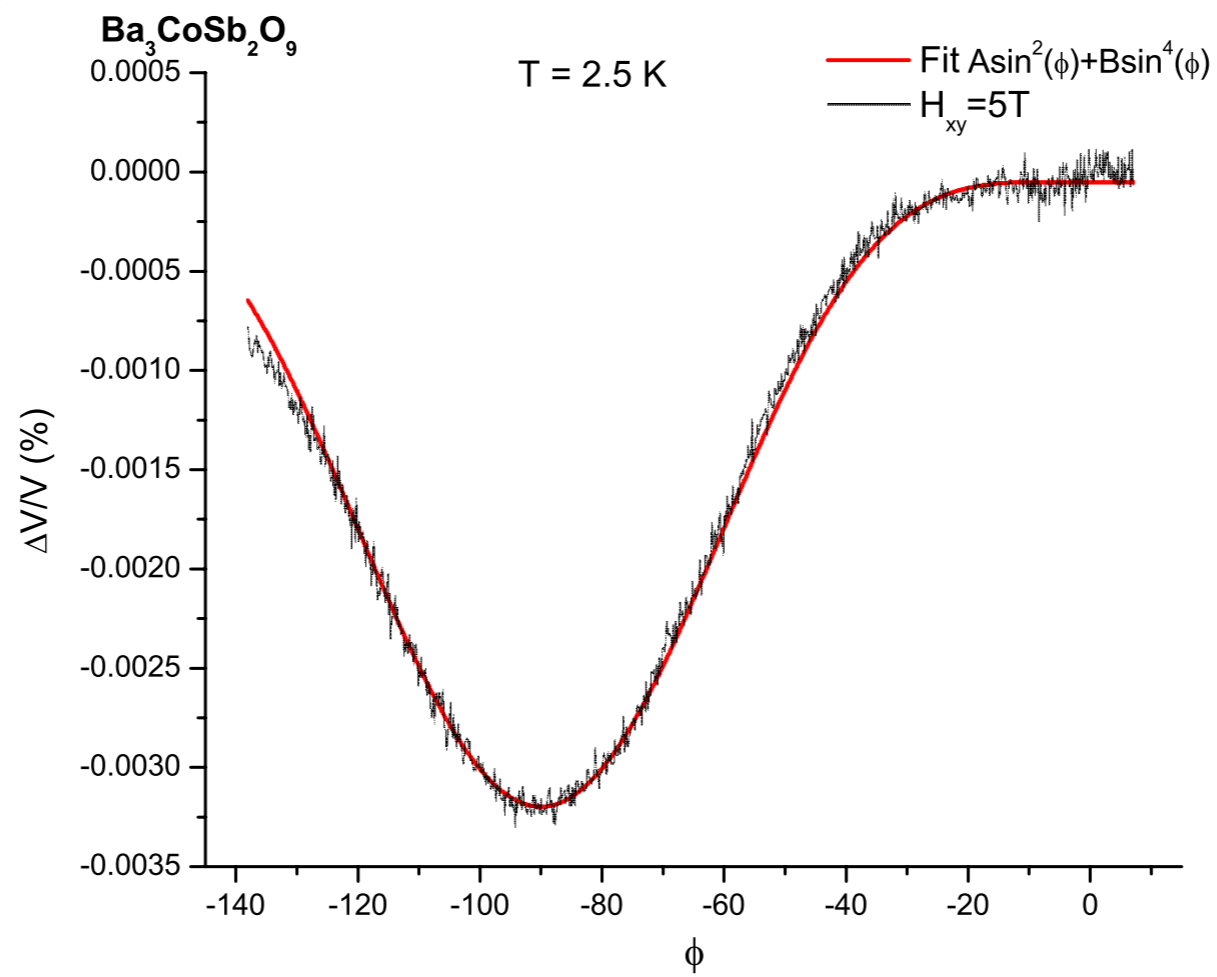
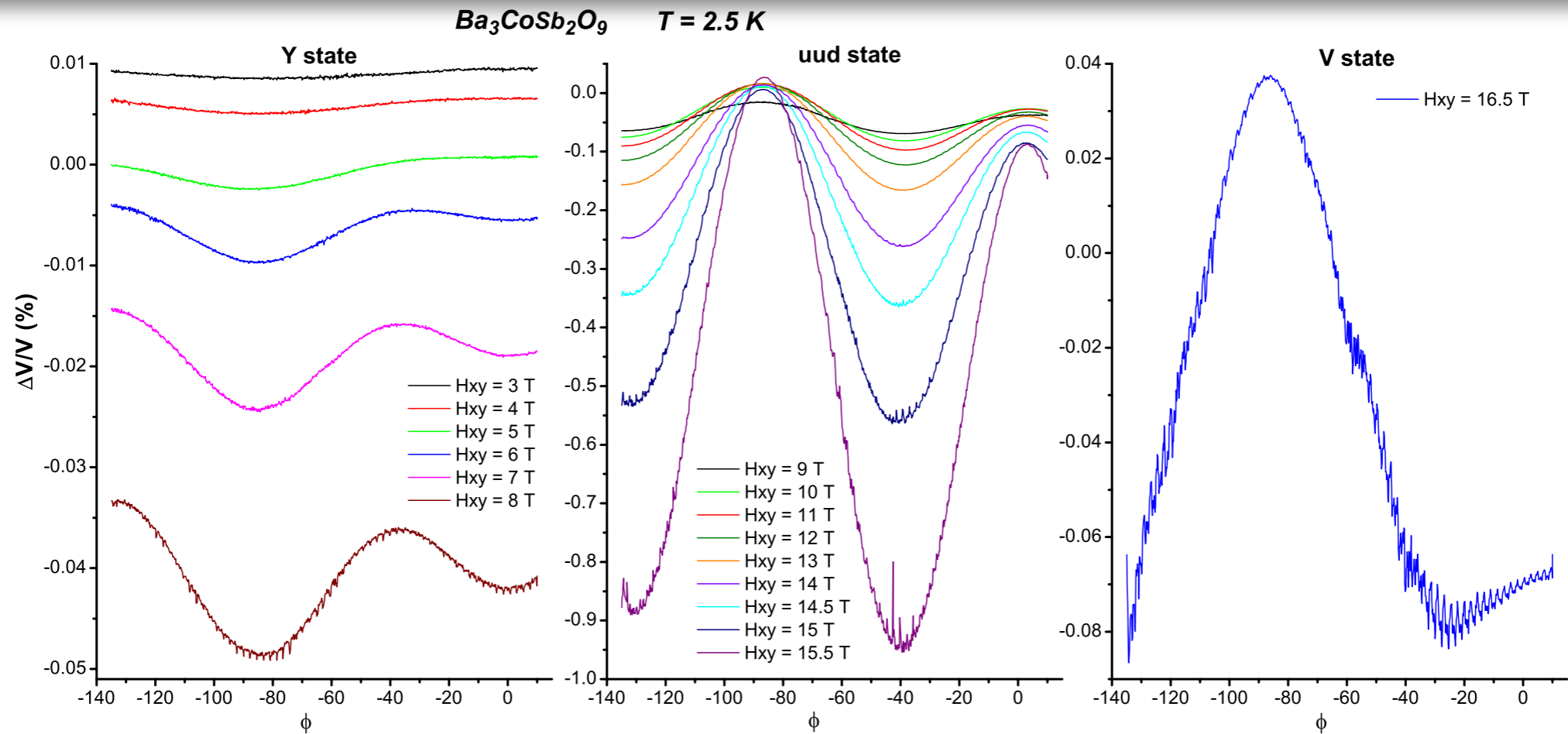
For $\mathbf{H} // \mathbf{x}$ and $1 T < H < 20 T$,
in paramagnetic state

$$10^{-6} \lesssim e_1 - e_2 \lesssim 10^{-4}$$

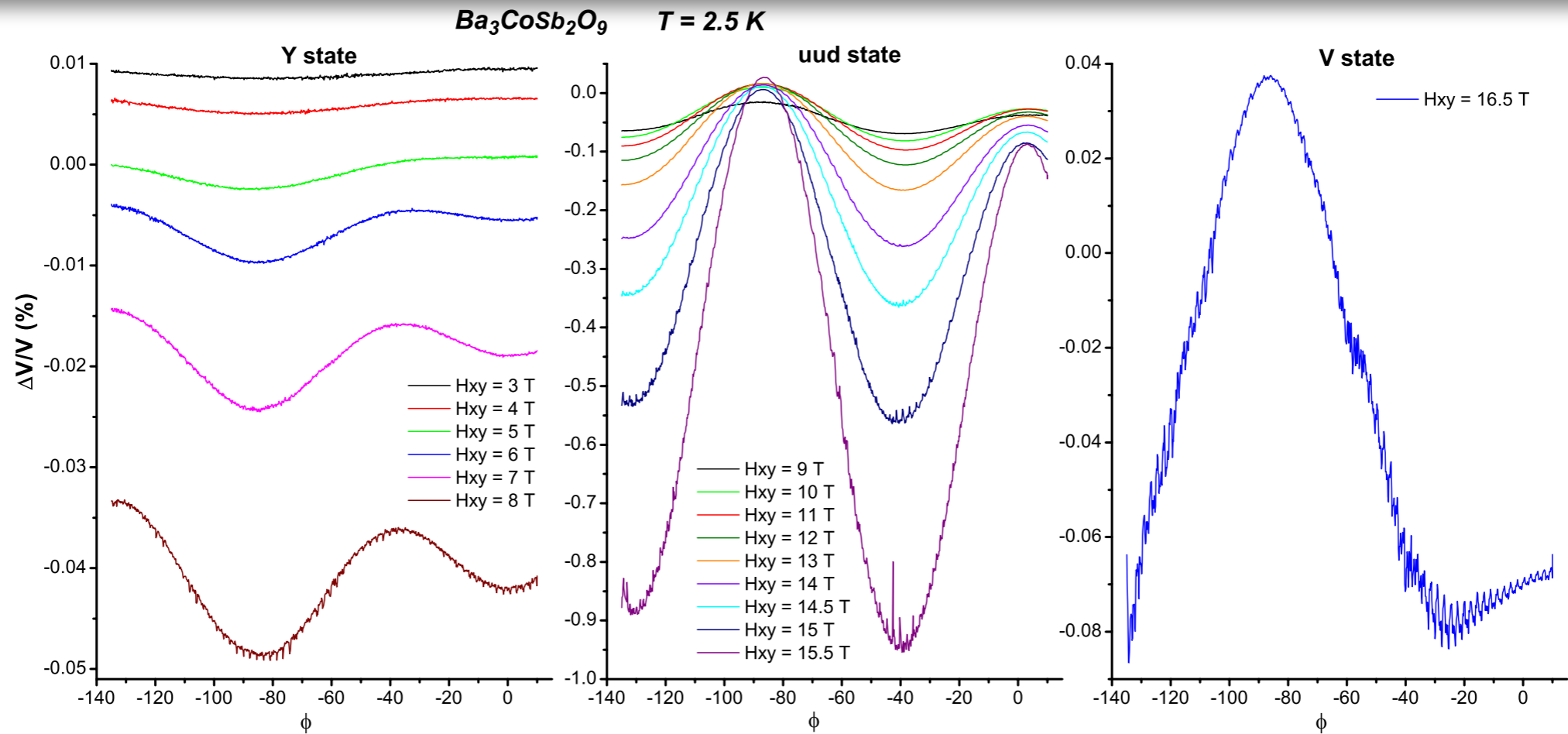
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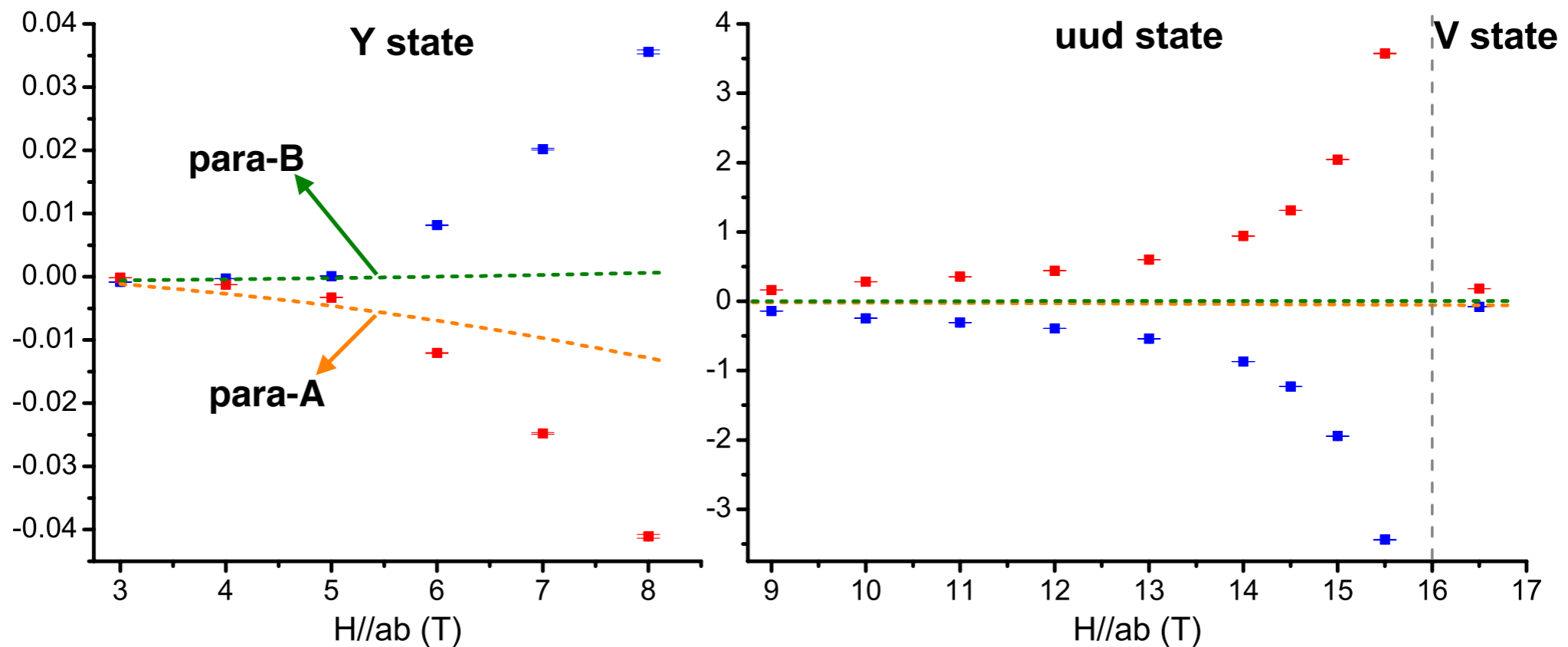


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$T = 2.5 K$

■ A — para-A
 ■ B — para-B



Conclusion and future work

1. Significant lattice distortions are included in paramagnetic state and ordered states as a function of the field;
2. The distortion is much larger in the ordered states than in paramagnetic state, especially in up-up-down state (magnetization plateau);
3. The direction of distortion might change from Y state to uud state;
4. Maintaining the magnetization plateau, lattice distortion works together with fluctuations, and some energy might be transferred from exchange coupling to elastic energy of lattice via spin-strain coupling;
5. A model is needed to analyze the spin-strain coupling in ordered states to explain the magnetization plateau;
6. Measurement of the distortions of $Ba_3CoSb_2O_9$ in paramagnetic state and ordered states as function of field is needed to confirm our conclusion.