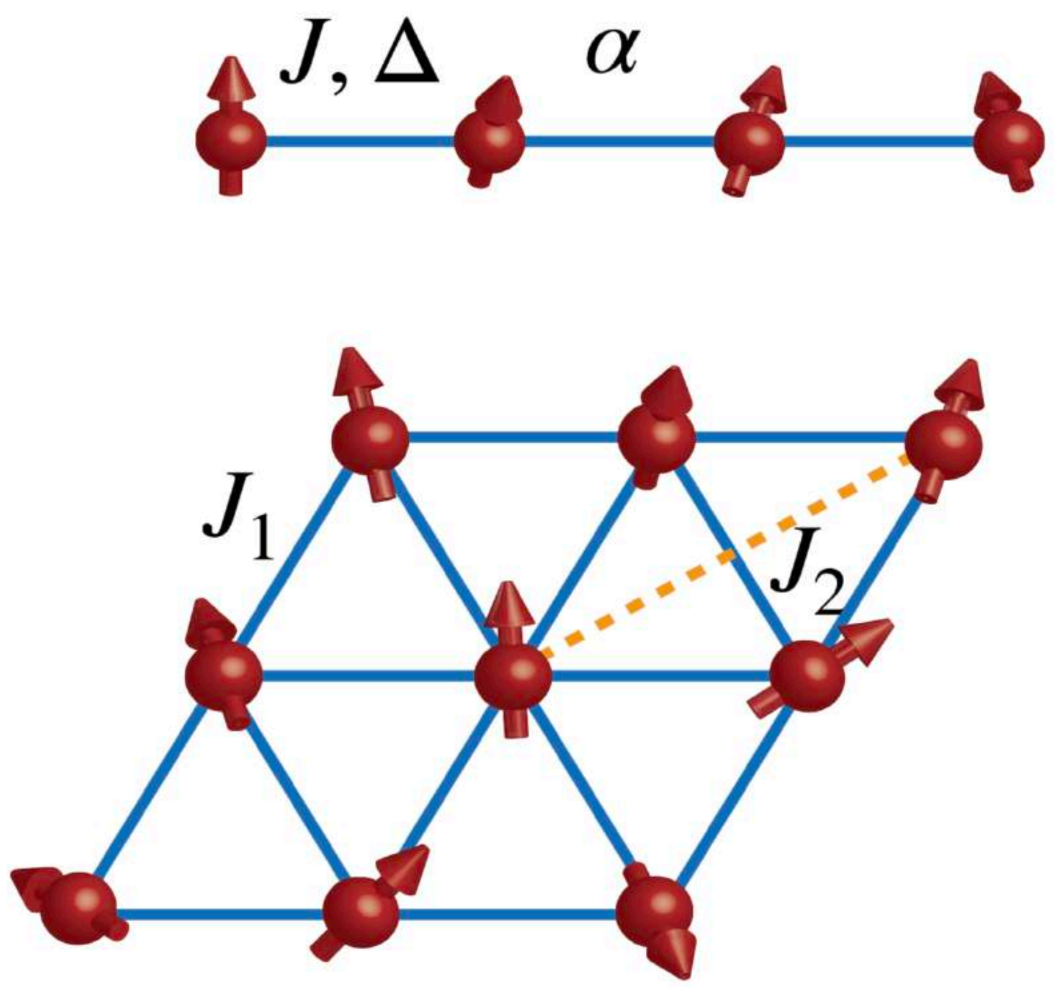
CQM² QMAGEN 北航物理学院 SCHOOL OF PHYSICS,BUAA 中国科学院理论物理研究所 Institute of Theoretical Physics, Chinese Academy of Sciences

Decoding Quantum Magnetism Genome with Thermal Tensor Networks

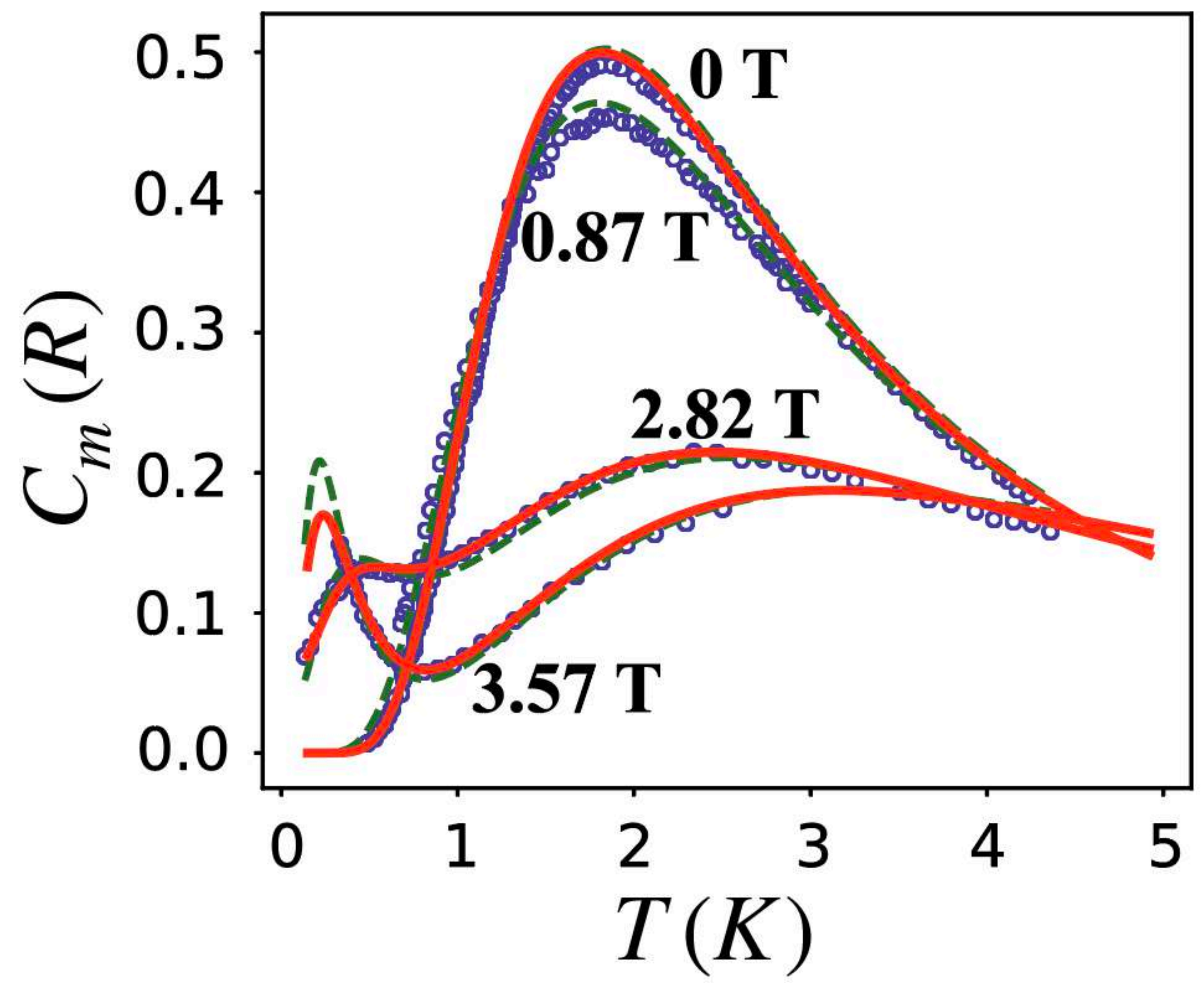
Wei Li, Beihang U. & ITP-CAS

IPAM virtual **Workshop II: Tensor Network States and Applications**



Many-body **solver!**

Inverse problem



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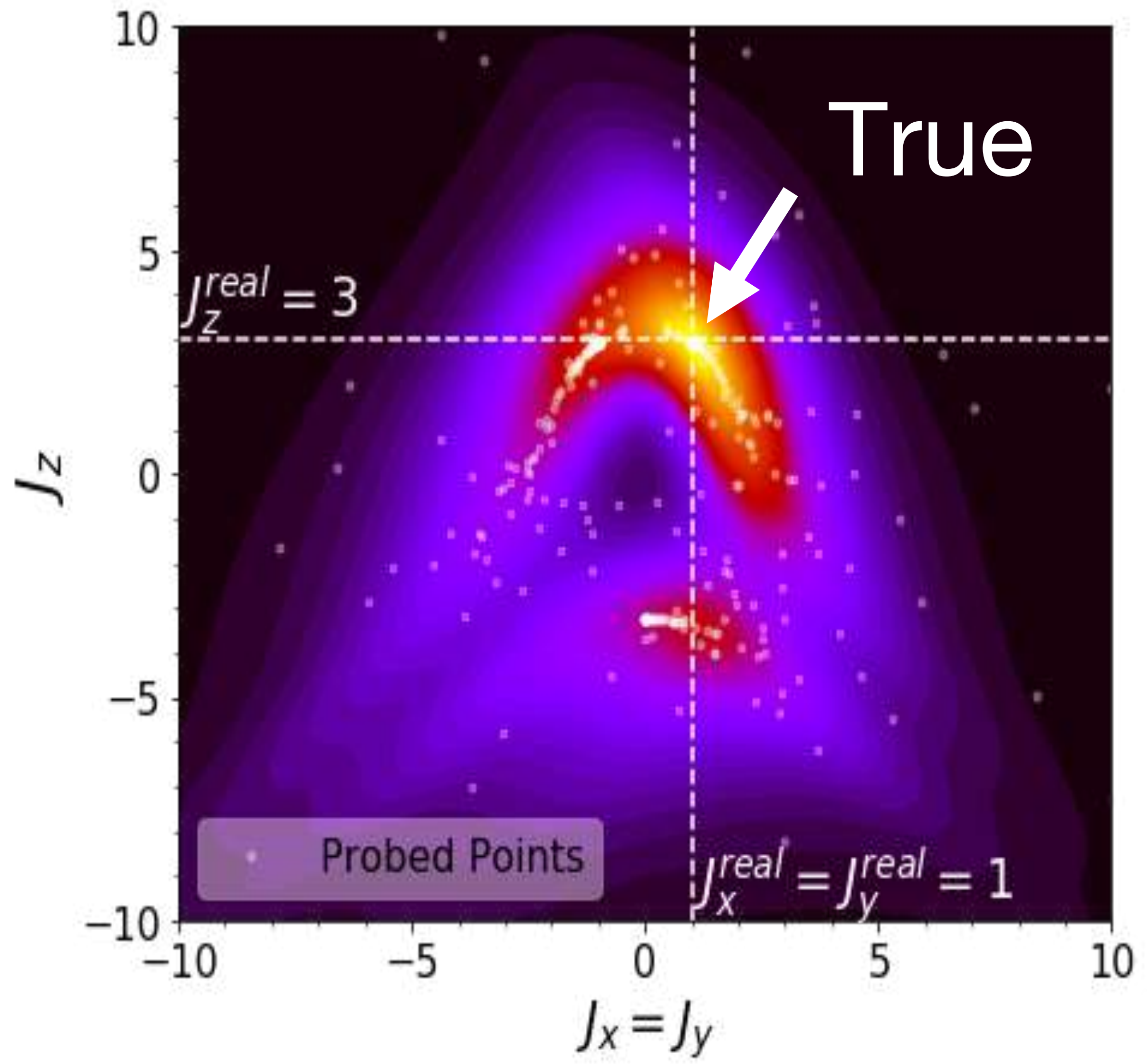
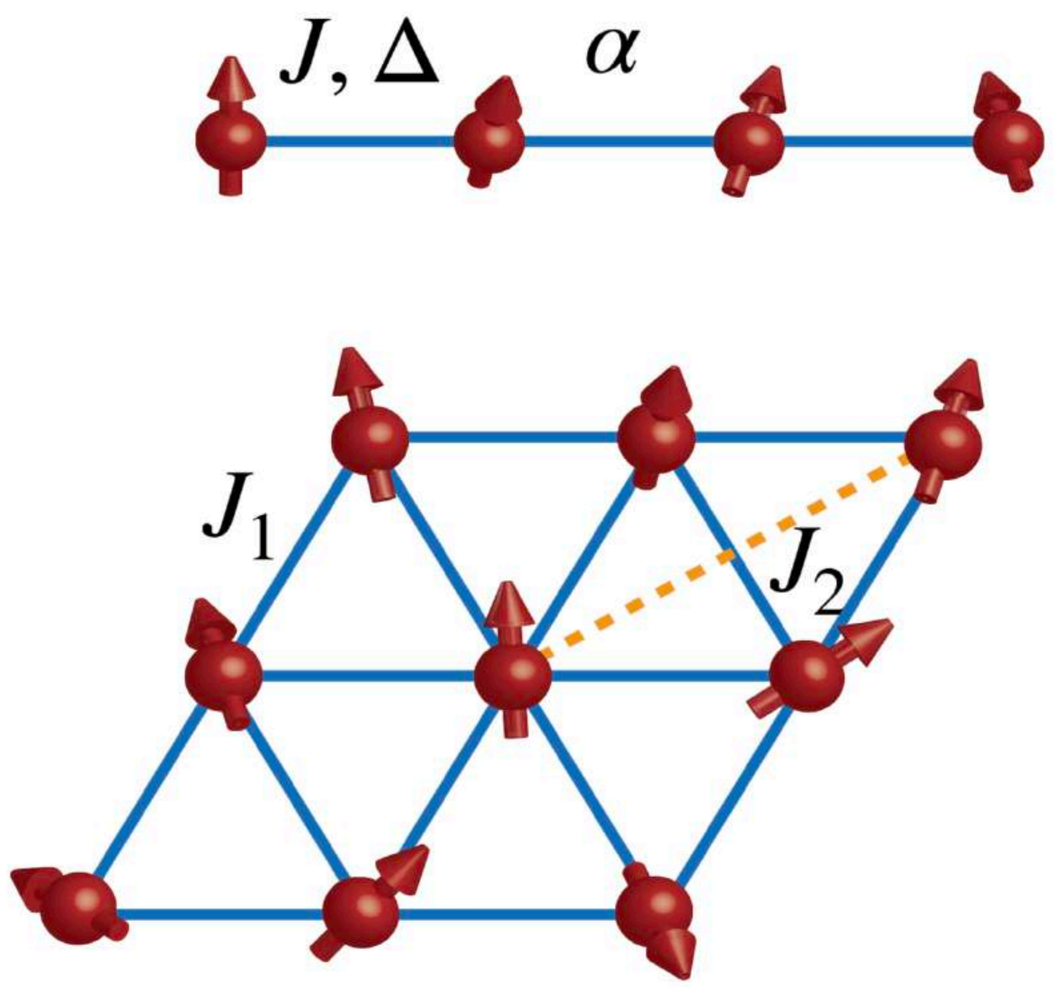
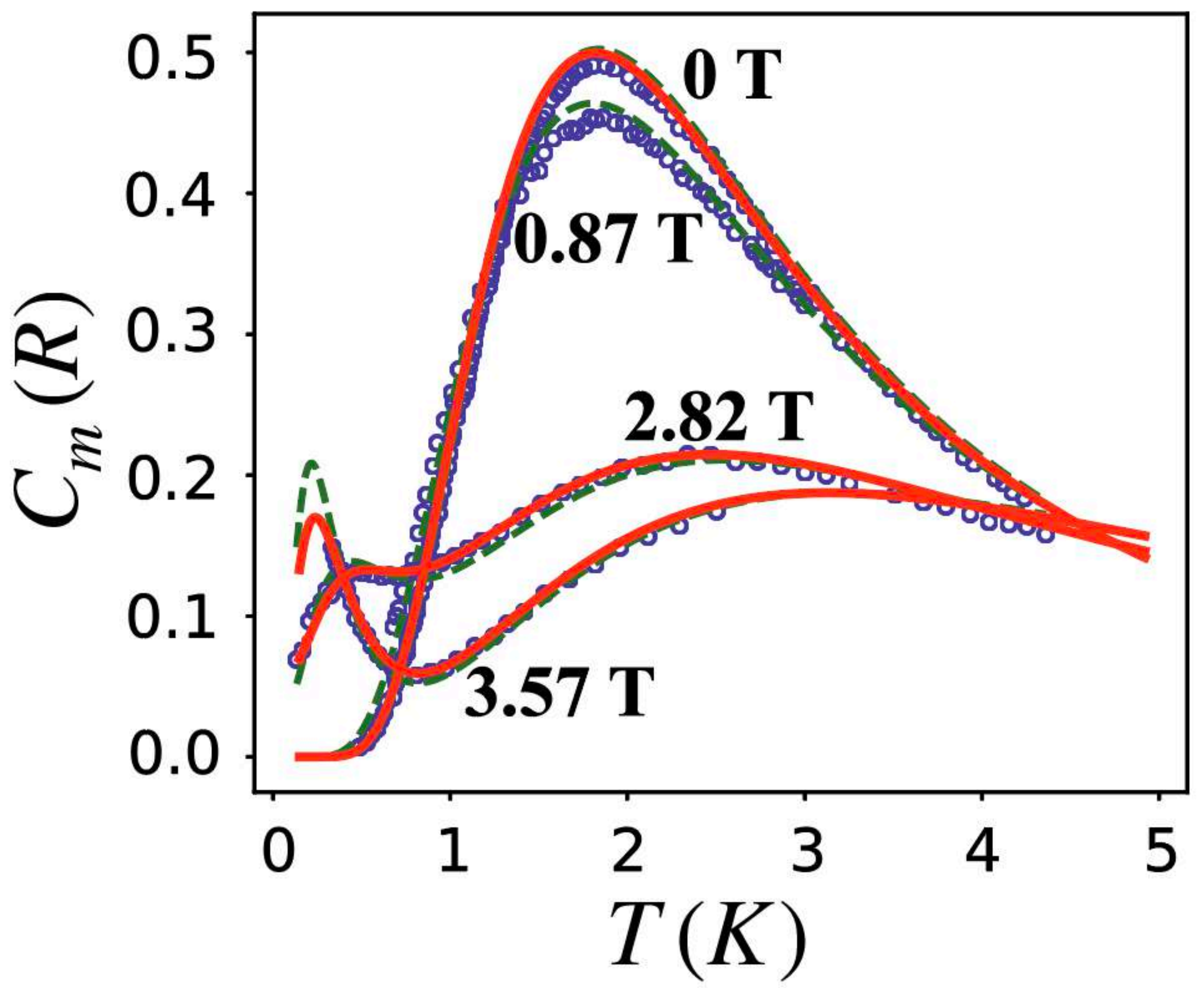
Find the Spin Model!





Many-body **solver!**

Inverse problem



Collaborators

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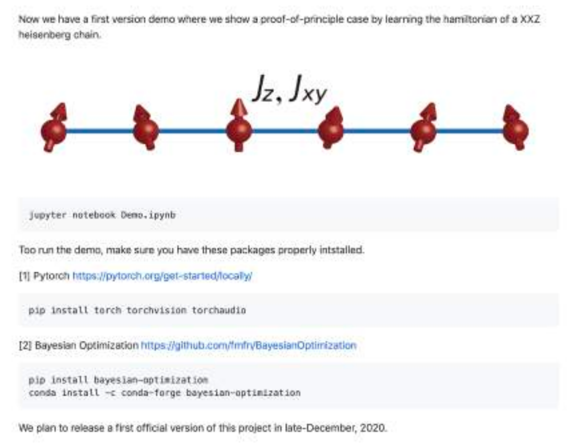
于思拙

Yuan Gao
高源

Bin-Bin Chen
陈斌斌

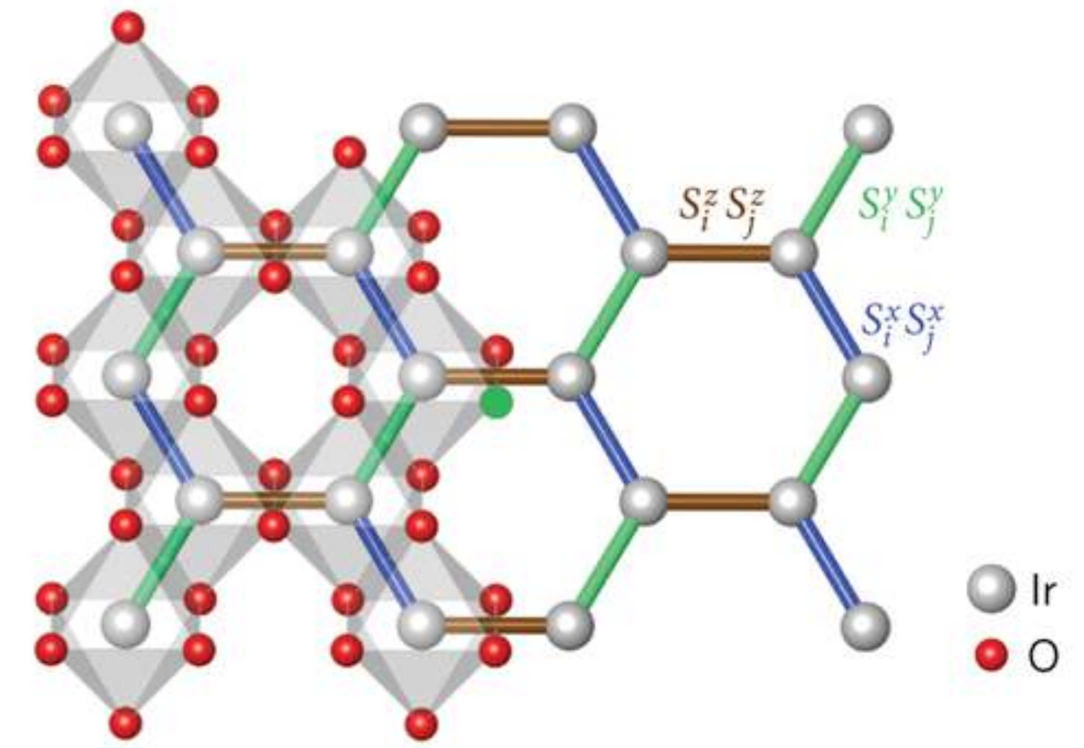


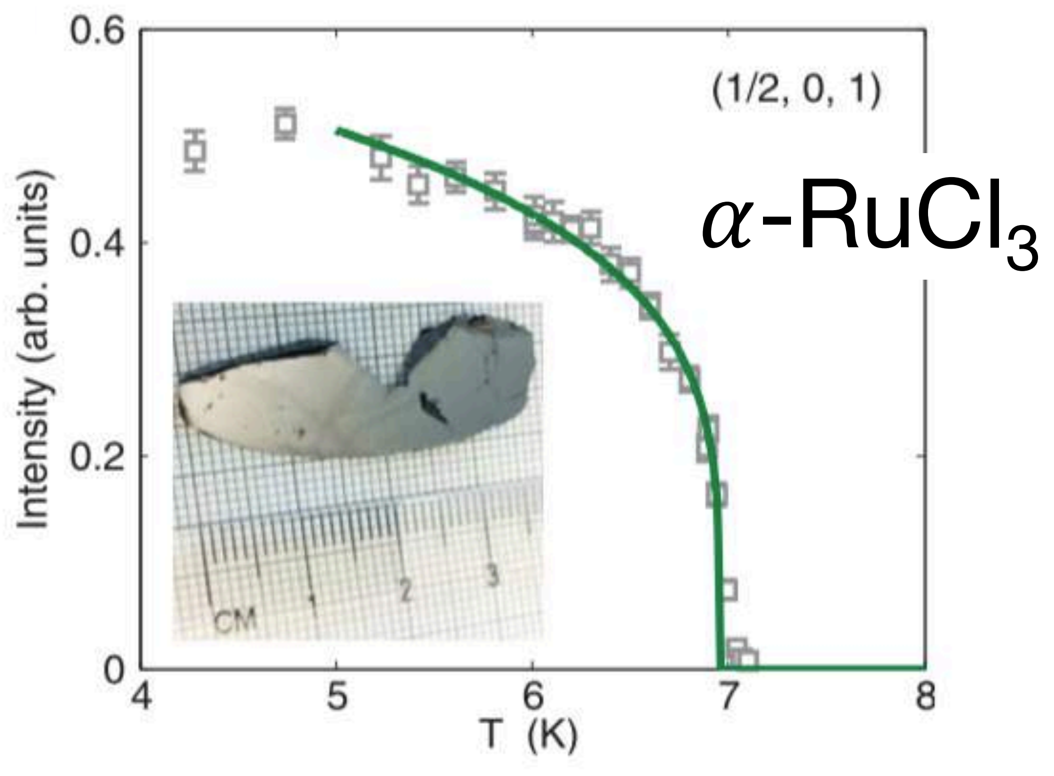
S. Yu, Y. Gao, WL, arXiv:2011.12282 (2020)

https://github.com/QMagen

❑ Quantum Spin Liquid Candidates

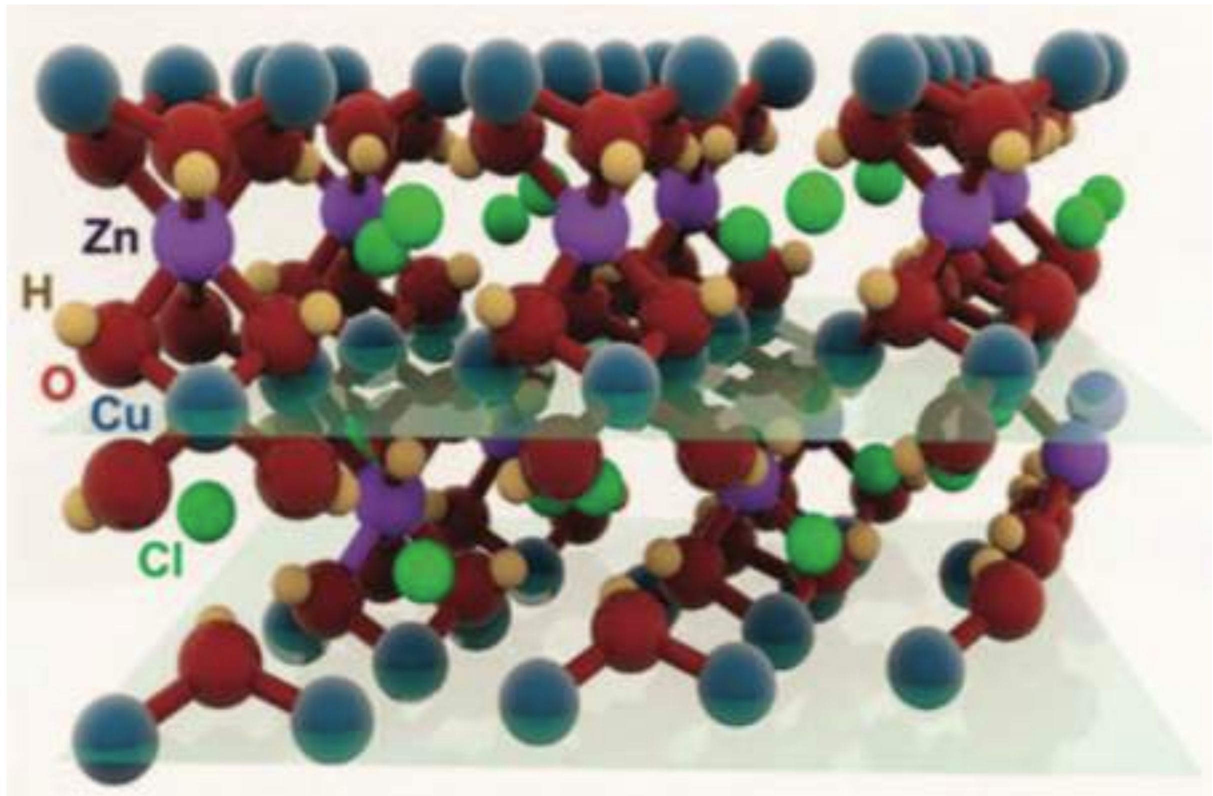
Kitaev materials





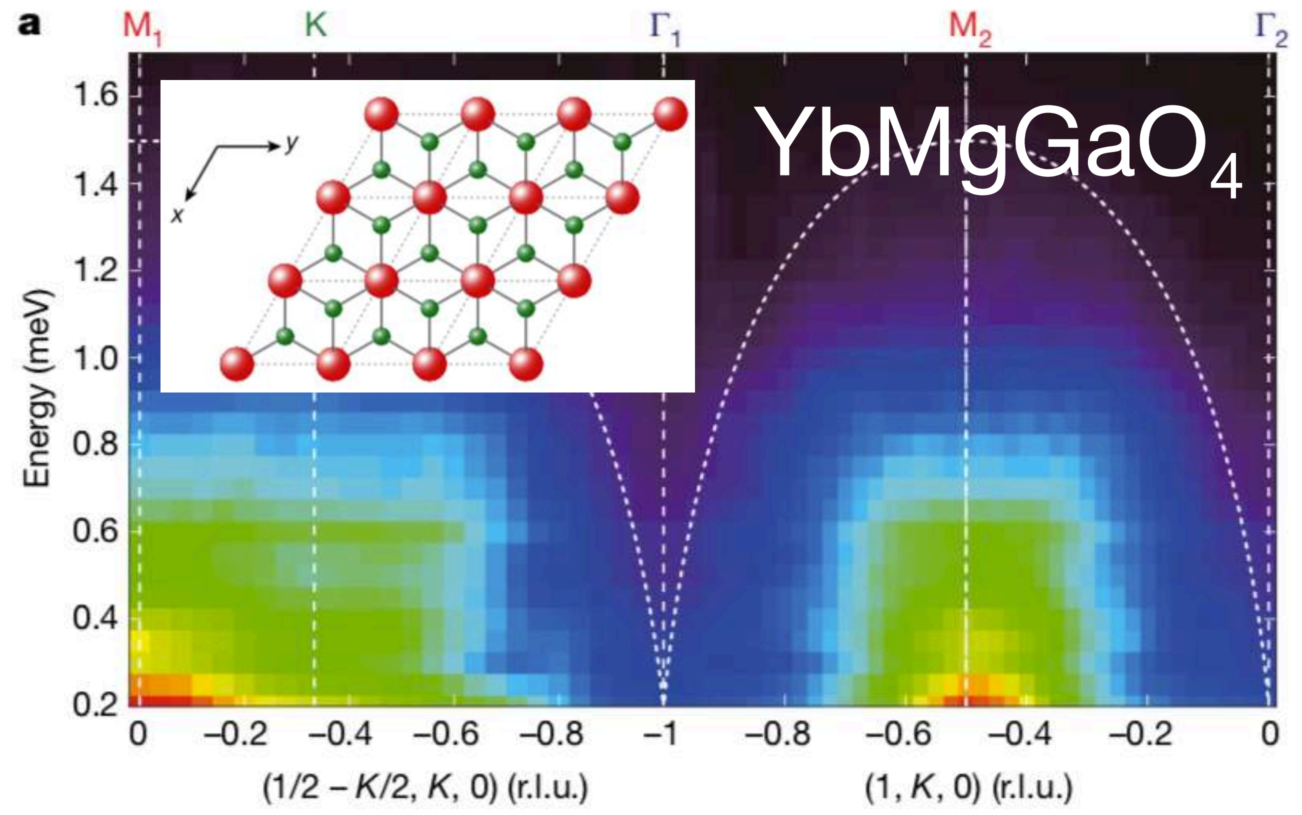
J. A. Sears **PRB** 2015; A. Banerjee, *et. al.*, **Science** 2017;

kagome magnets



Fu, *et. al.*, **Science** 2015
$Cu_3Zn(OH)_6FBr$, **CPL** 2018

triangular-lattice

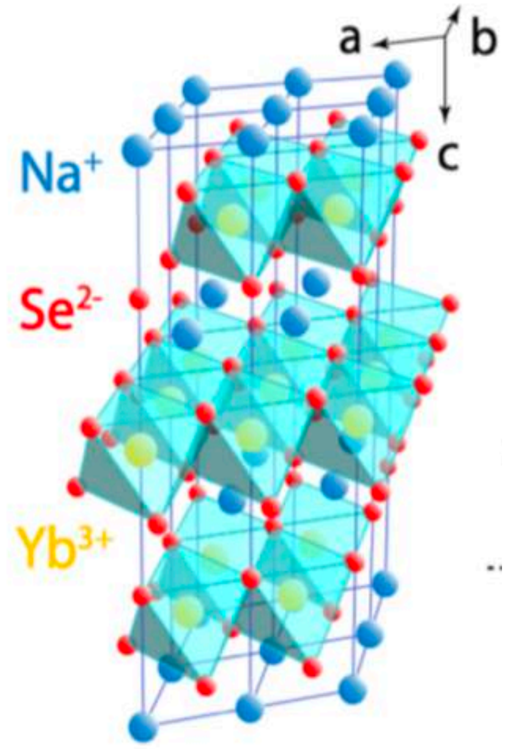


Y. Shen, *et. al.*, **Nature** 2016
Y. Li, *et. al.*, **PRL** 2015

There are debates in these quantum materials …

❑ **How to decode the *"DNA"* of quantum magnets?**

➢ **Spin Hamiltonian and interaction parameters**



$AReCh_2$: A family of frustrated magnets

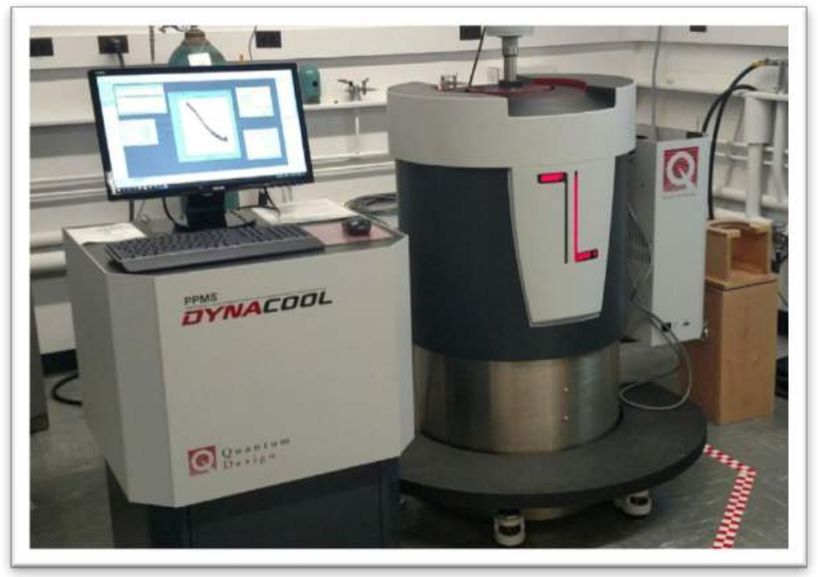
(A = alkali or monovalent ions, Re = rare earth, Ch = O, S, Se)

Liu, et. al, CPL 2018; Dai, et. al,

❑ Can we infer the many-body model from experiments?

And then determine the exotic quantum states therein …

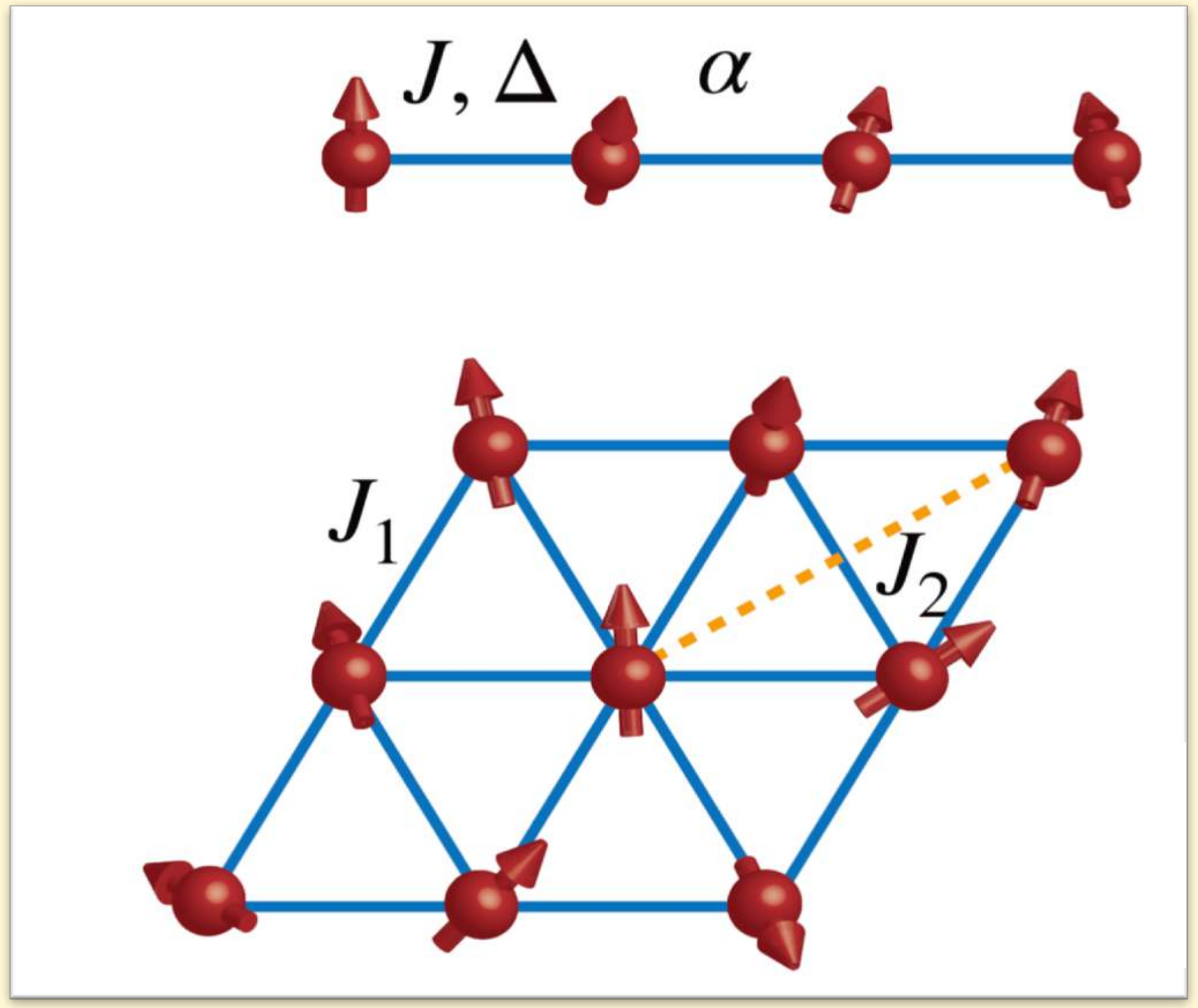
- **Dynamical** data are ***expensive*** to measure and ***difficult*** to compute/analysis via many-body approach



- What about **thermal** data *(easier to obtain and analysis)*?

❑ Solve the Inverse Many-body Problem with Thermal Data

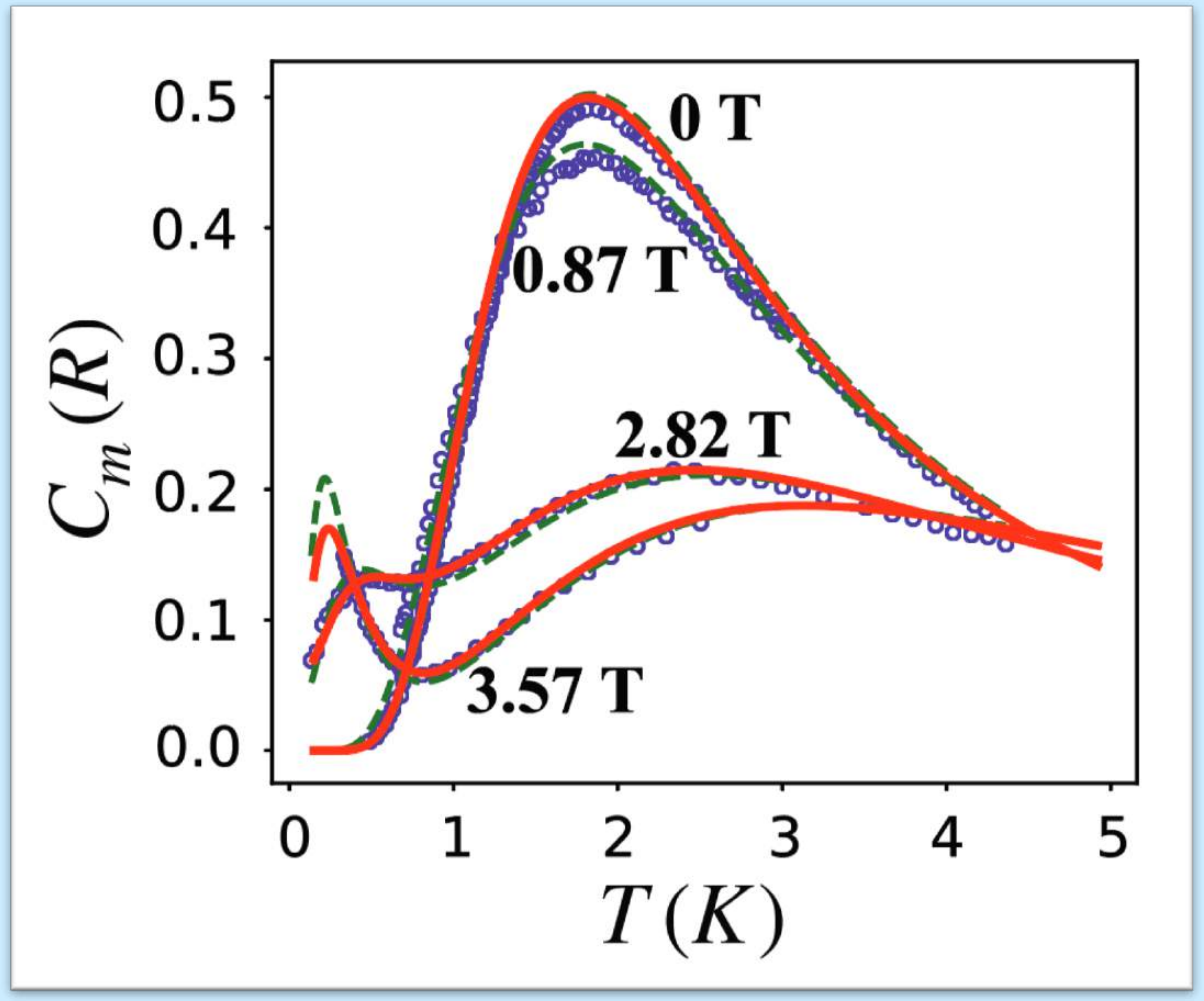
Lattice model



forward

inverse

Thermal data

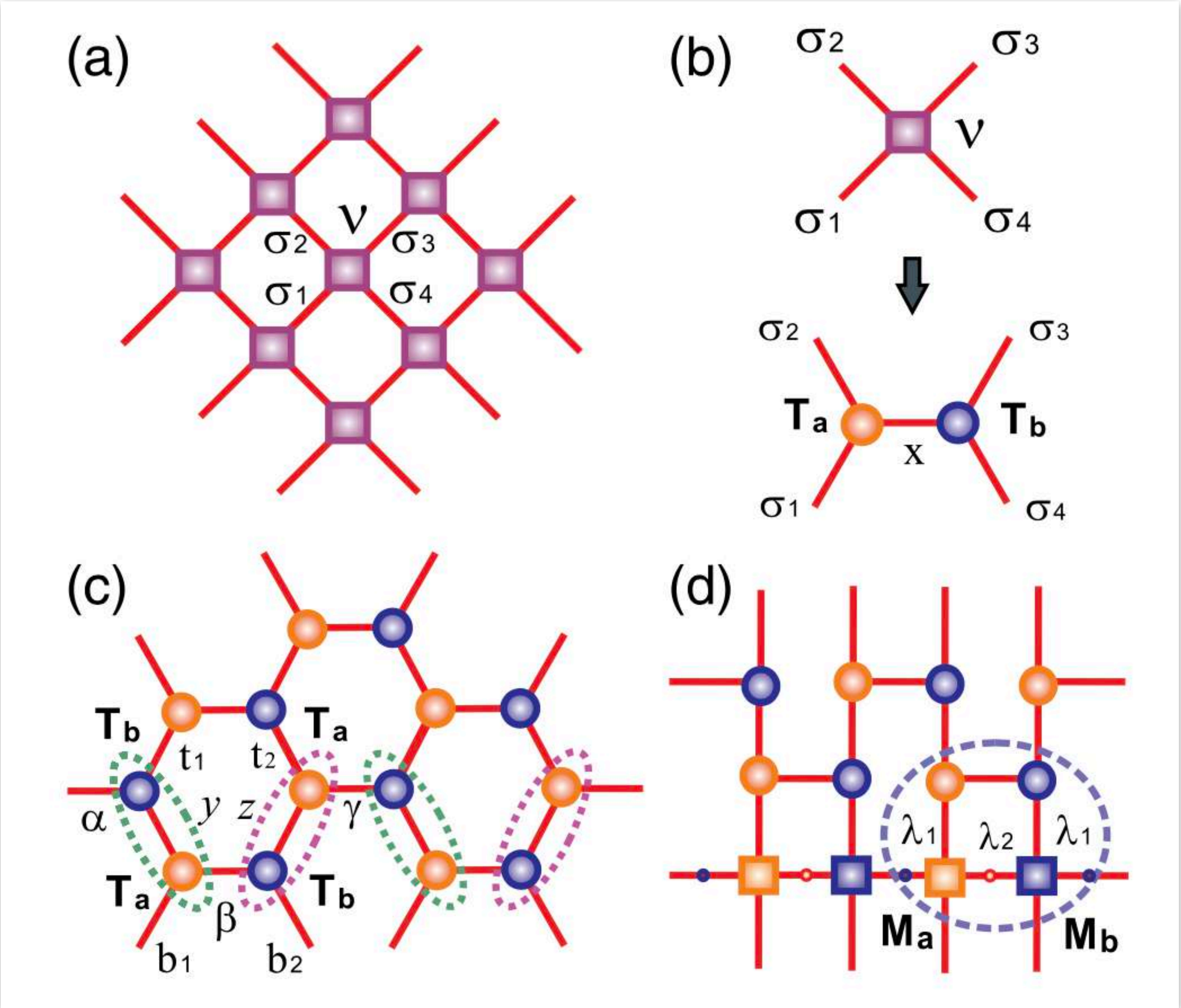


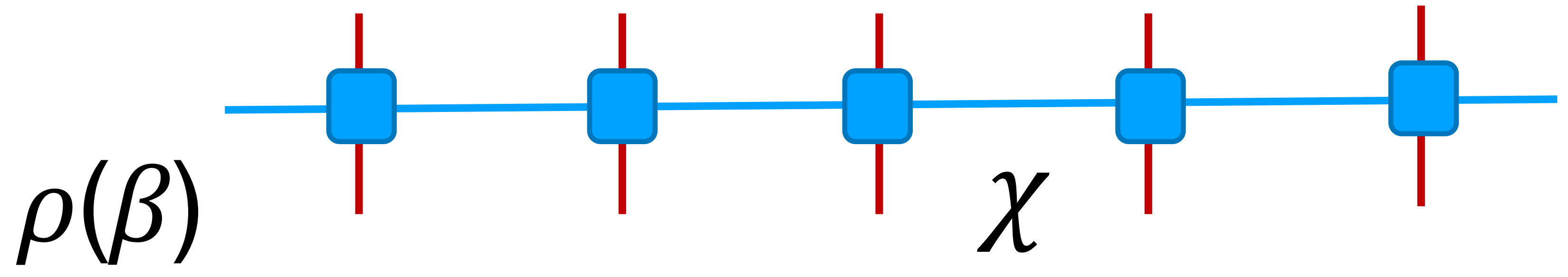
➢ ***Many-body Solver: Thermal Tensor Networks***

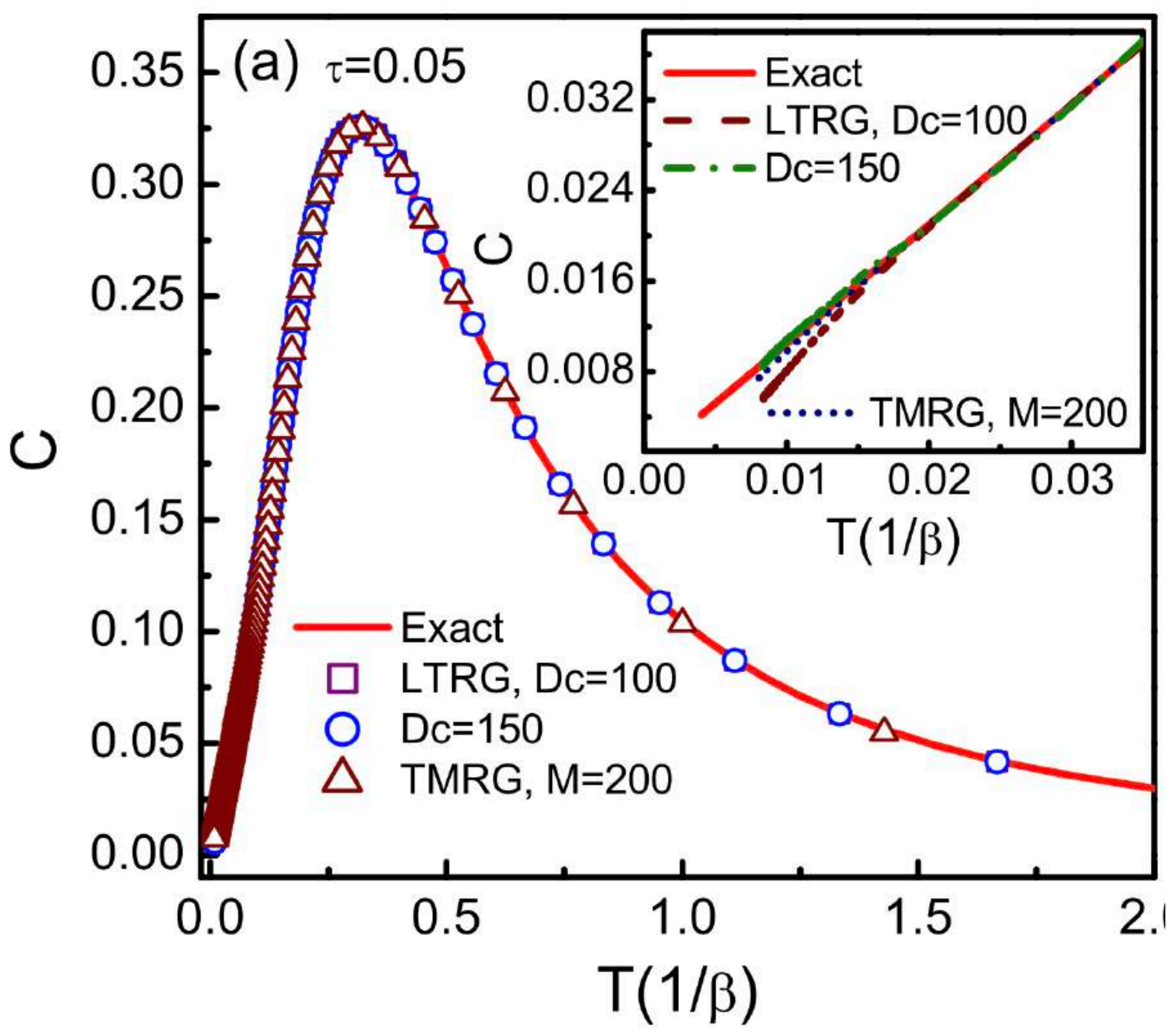
➢ ***Optimizer from Machine Learning***

Thermal Tensor Networks

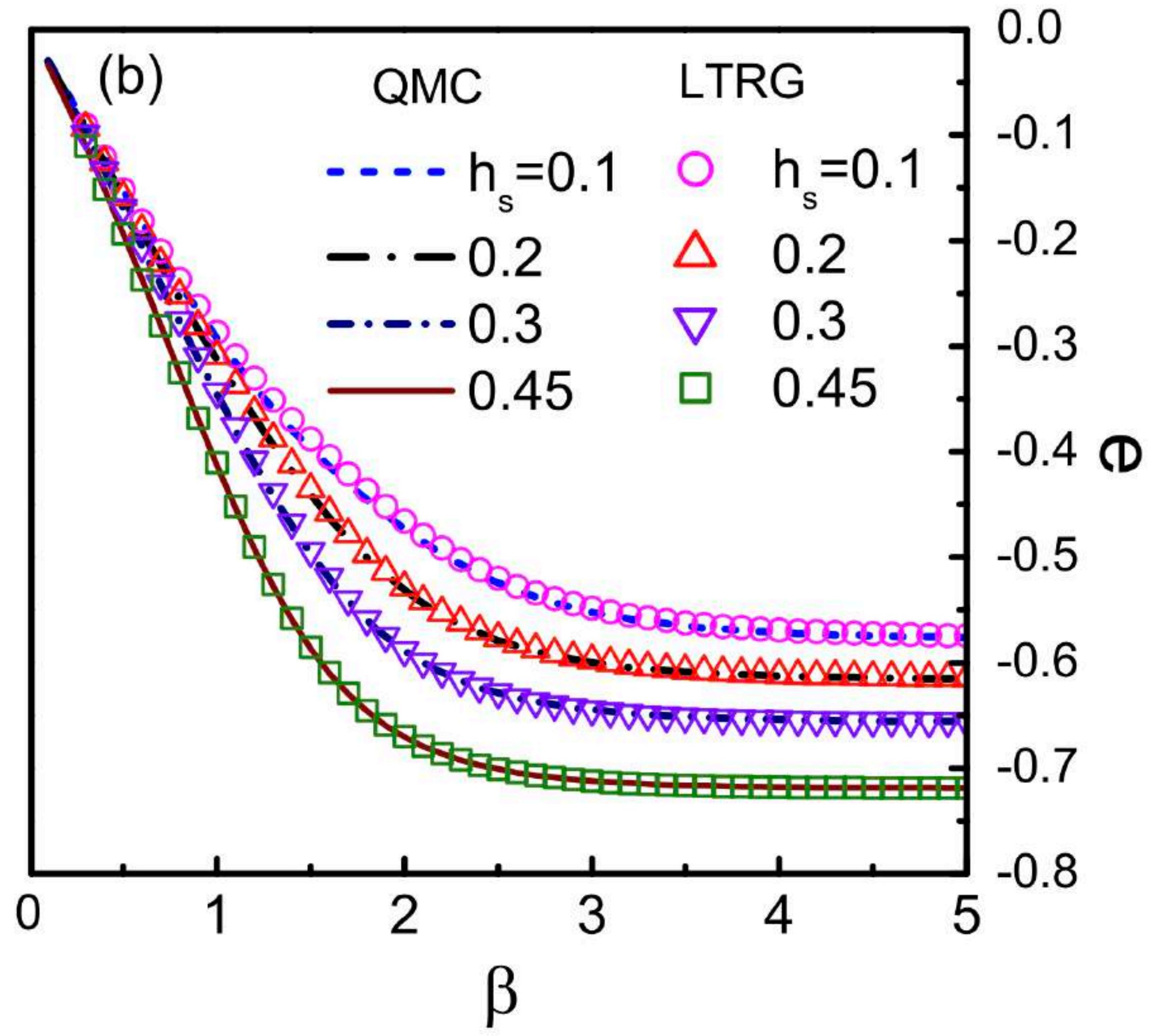
❑ Linearized Tensor Renormalization Group (LTRG)







Critical spin chain

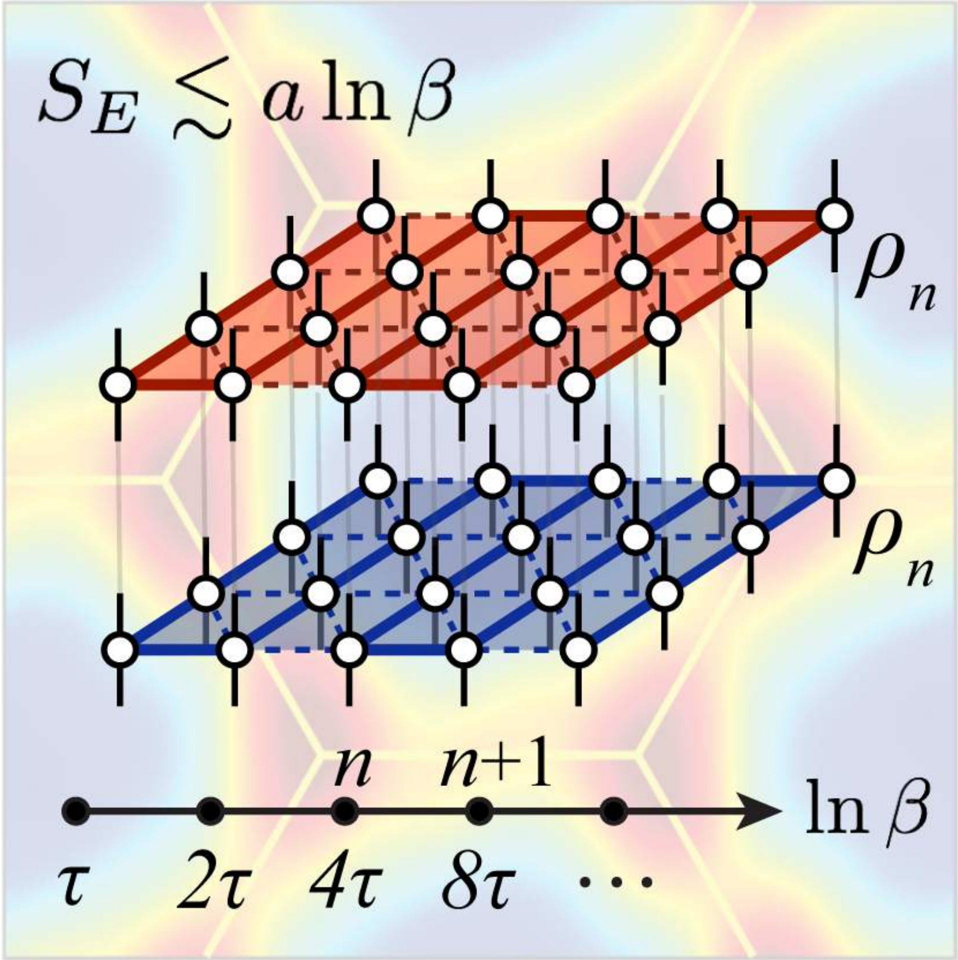


Honeycomb Heisenberg AF magnet

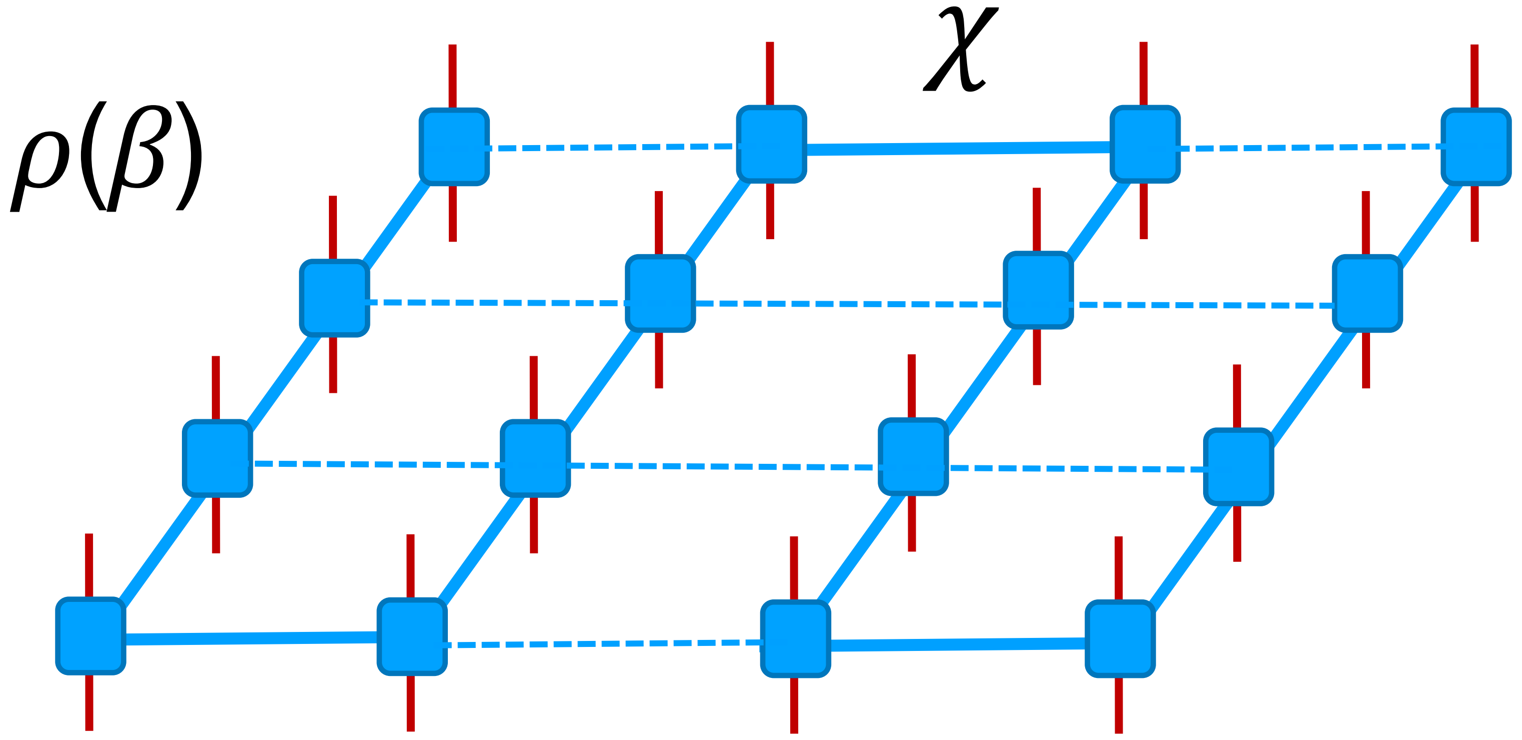
Directly in the thermodynamic limit

WL, S.-J. Ran, […], Gang Su, PRL 2011
Y.-L. Dong, […], WL, PRB 2017

❑ Exponential Tensor Renormalization Group (XTRG)

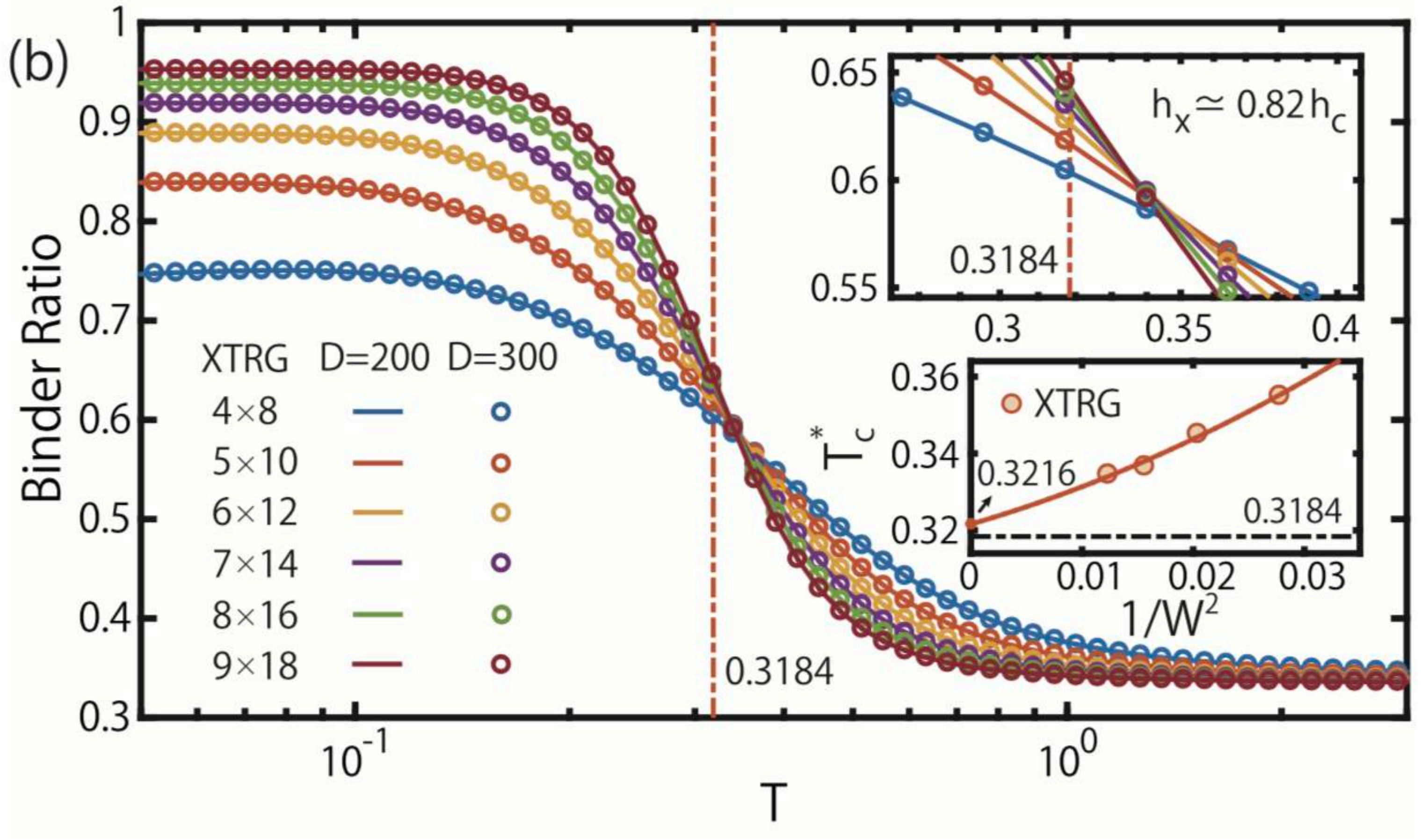


B.-B. Chen, […], WL, A. Weichselbaum, PRX 2018



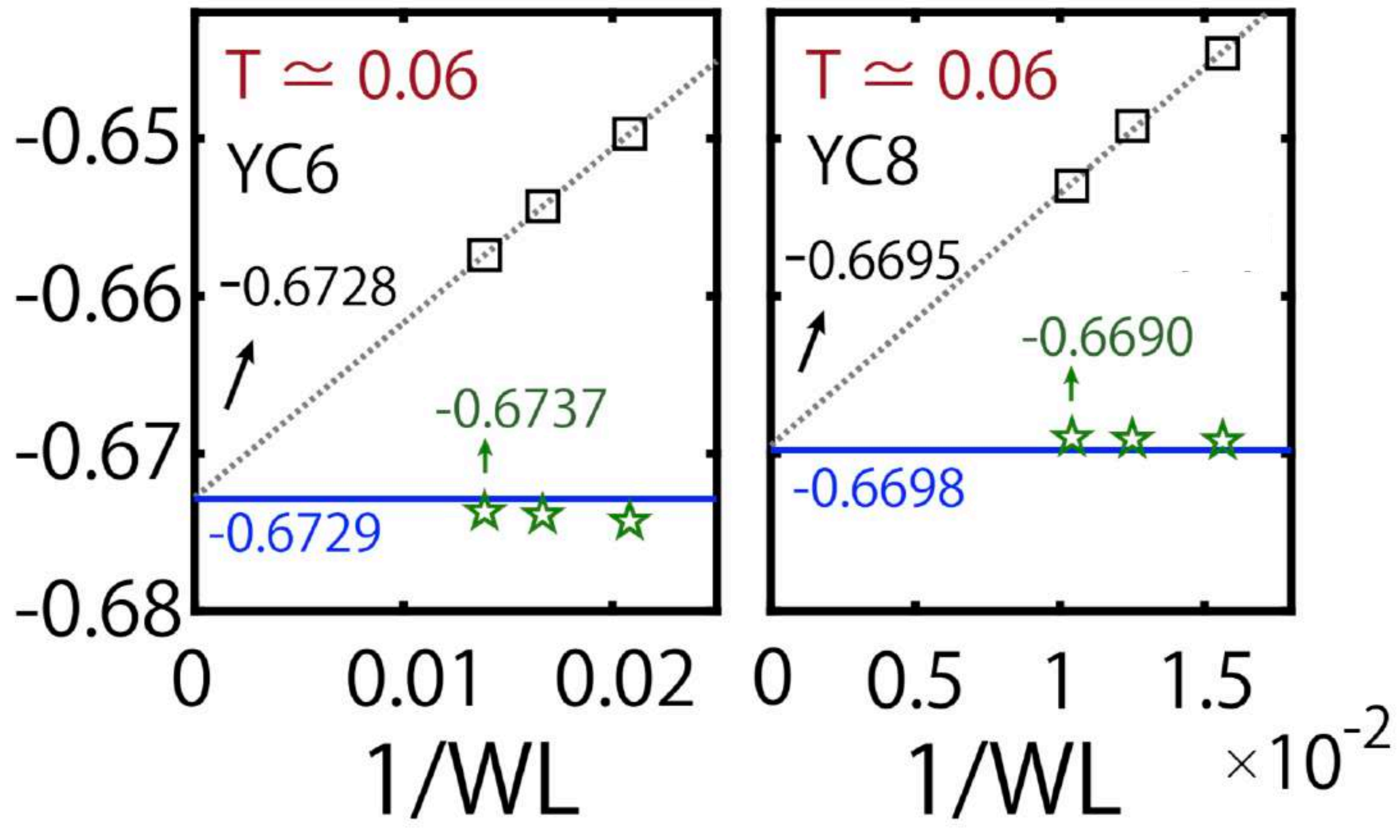
“*snake*” MPO

2D Quantum Ising (up to 162-sites)



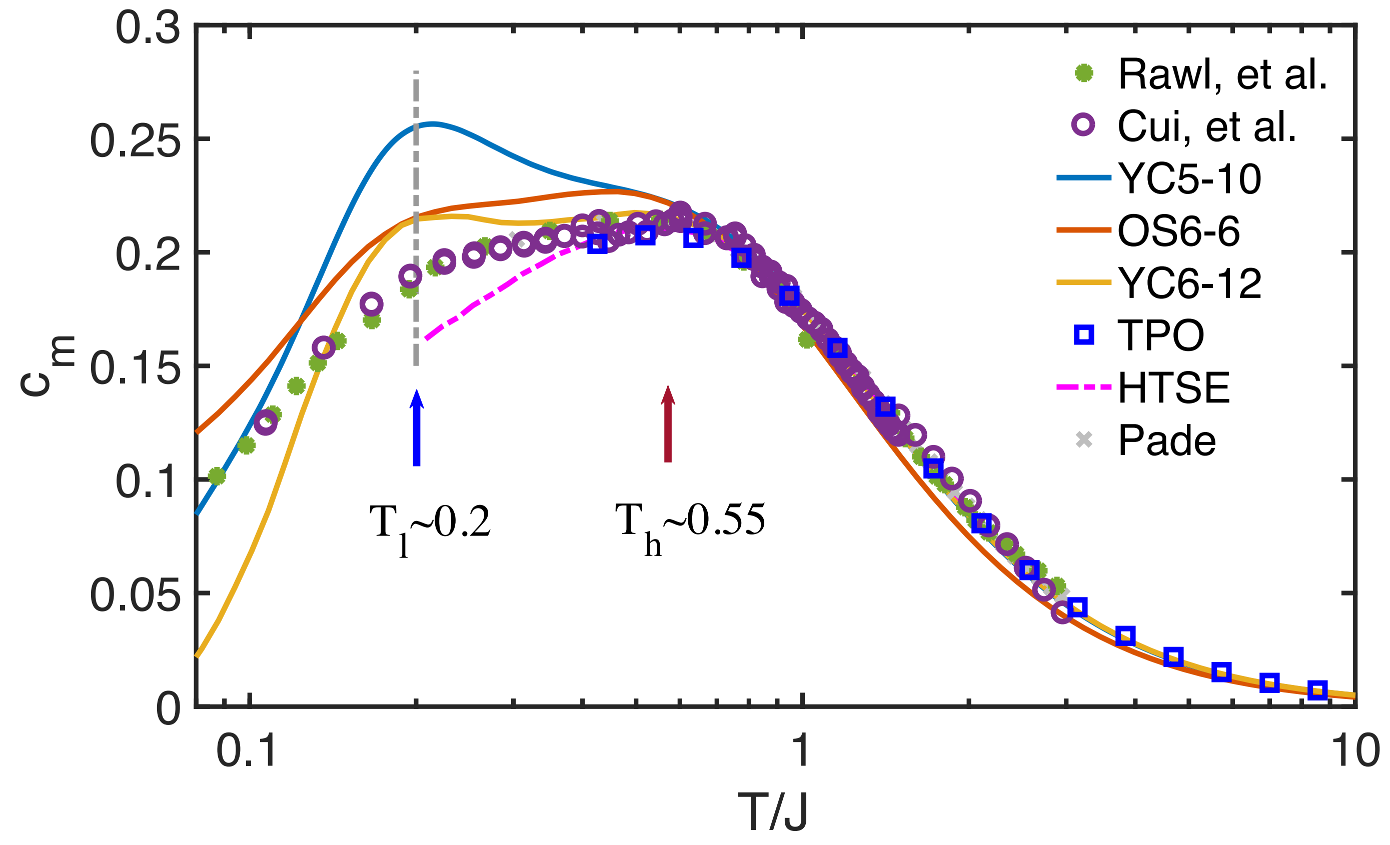
H. Li, […], WL, PRB 2019

Square-lattice Heisenberg



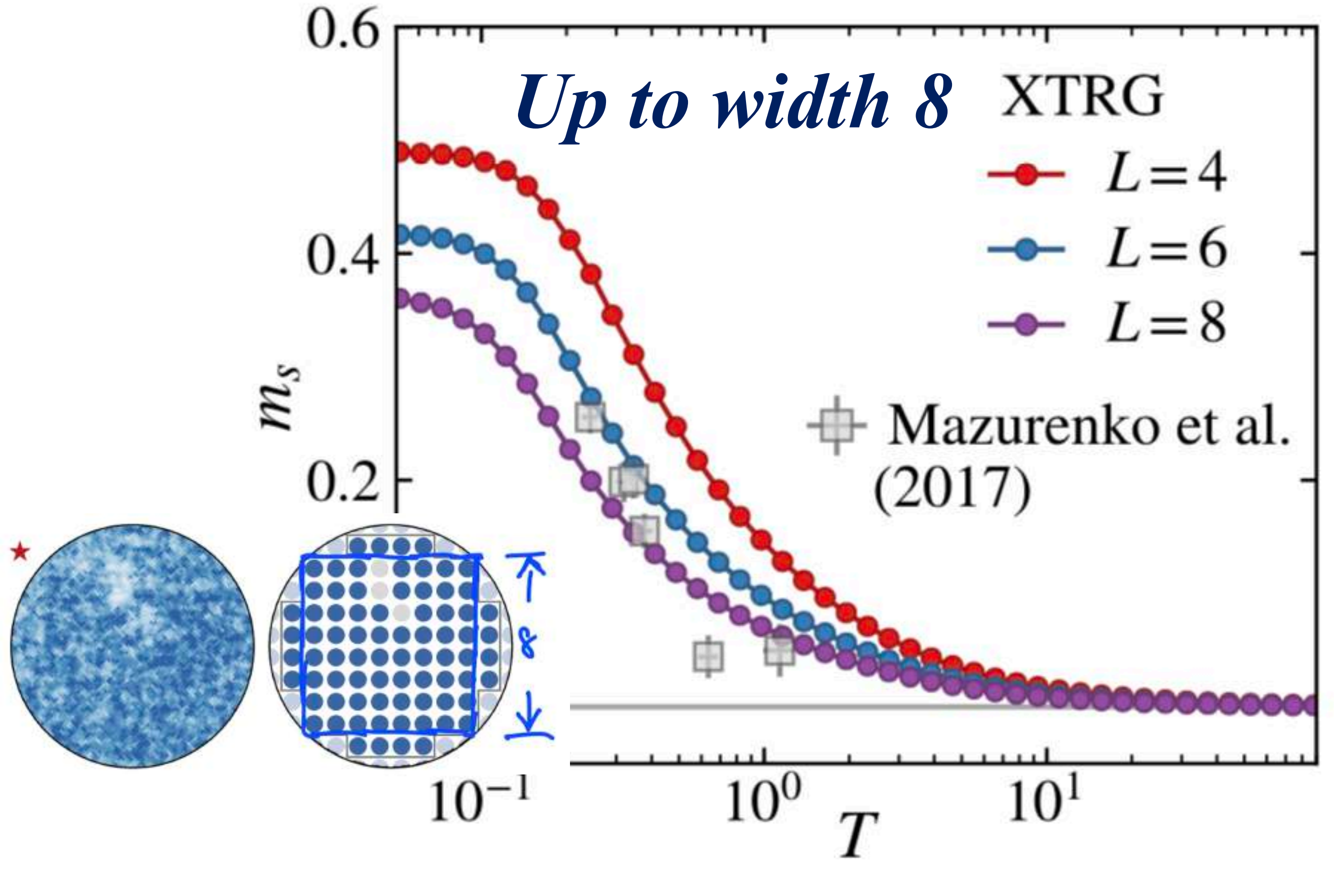
$u_g^* \simeq -0.6694(4)$, $m_s^* \simeq 0.30(1)$

Triangular-lattice Heisenberg



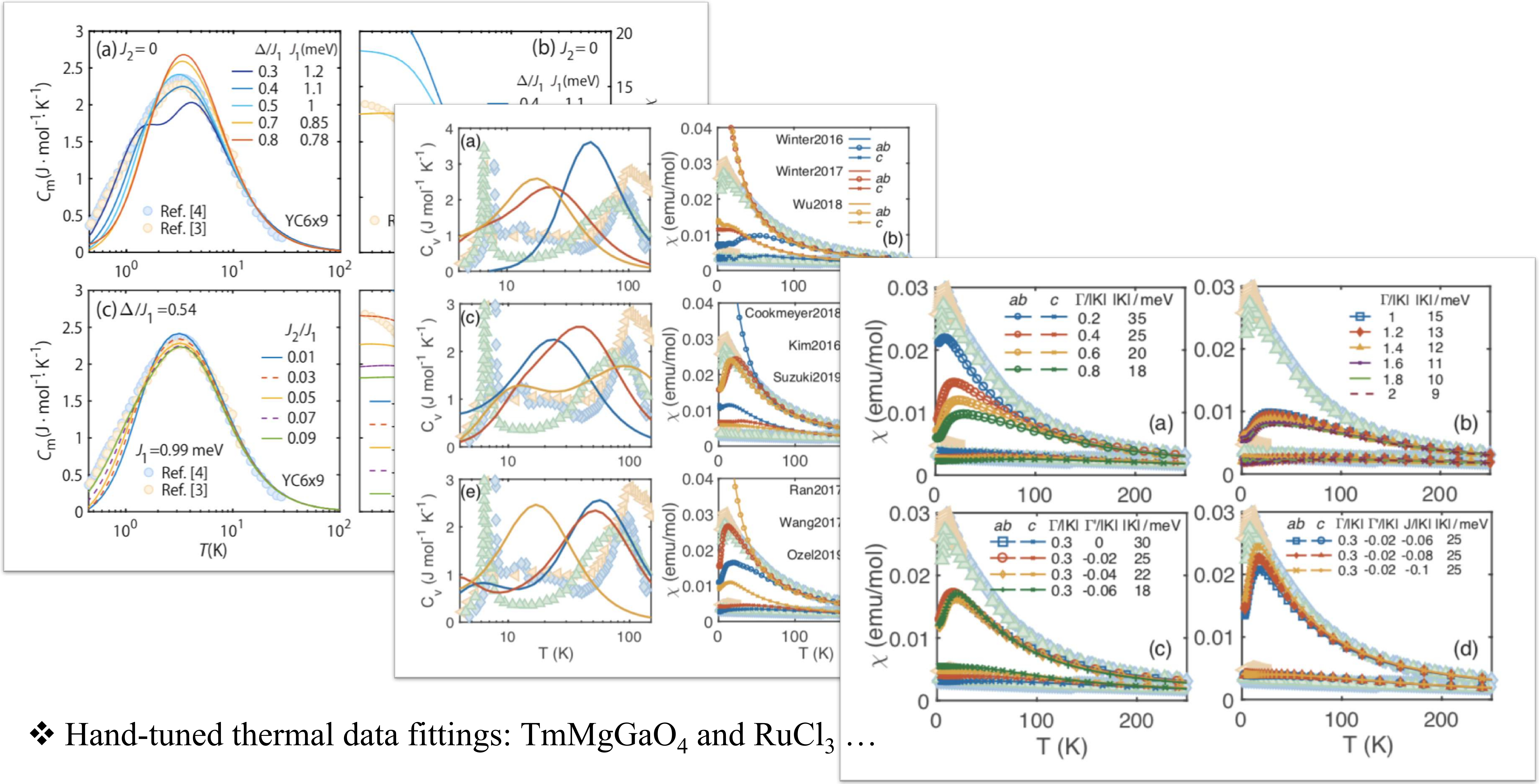
L. Chen, […], WL, PRB (Rapid) 2019

2D Fermi-Hubbard



B.-B. Chen, […], WL, PRB (Lett.) 2021

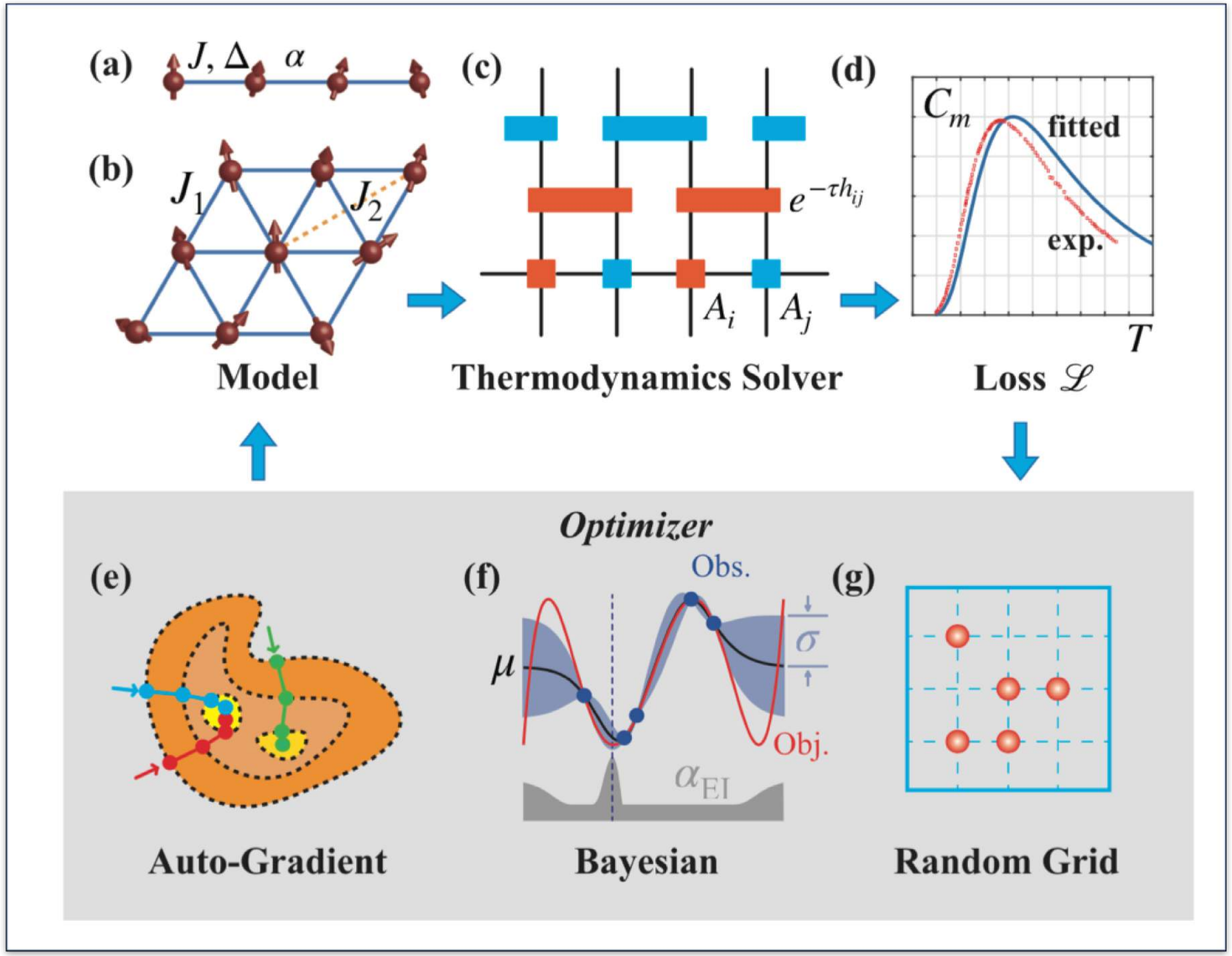
❑ Fitting the thermodynamics: very laborious if hand-tuned …



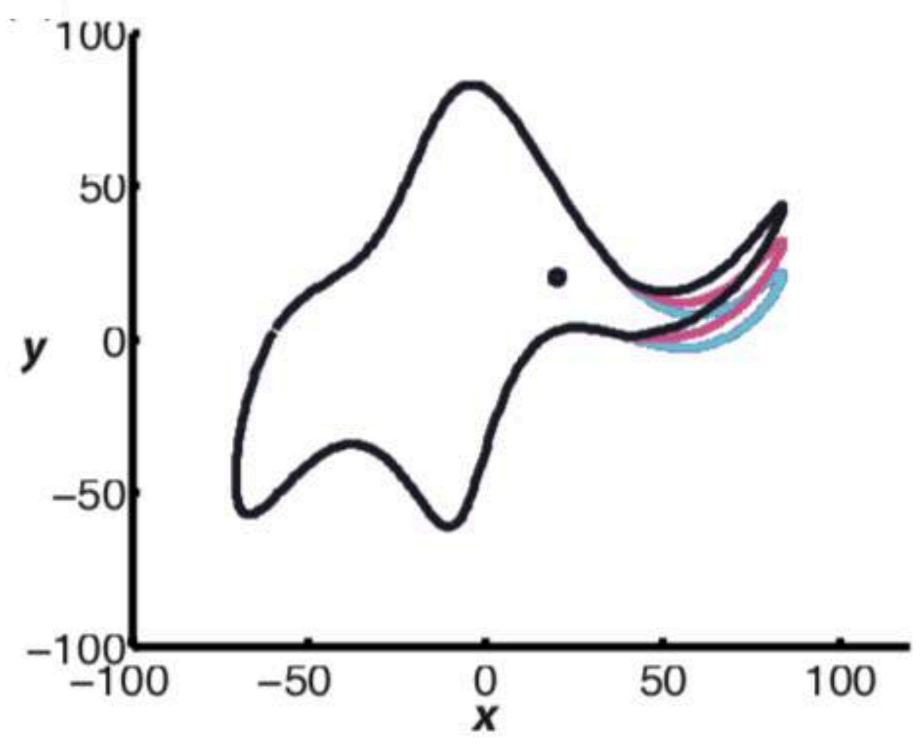
❖ Hand-tuned thermal data fittings: $TmMgGaO_4$ and $RuCl_3$ …

Parameter Optimizer

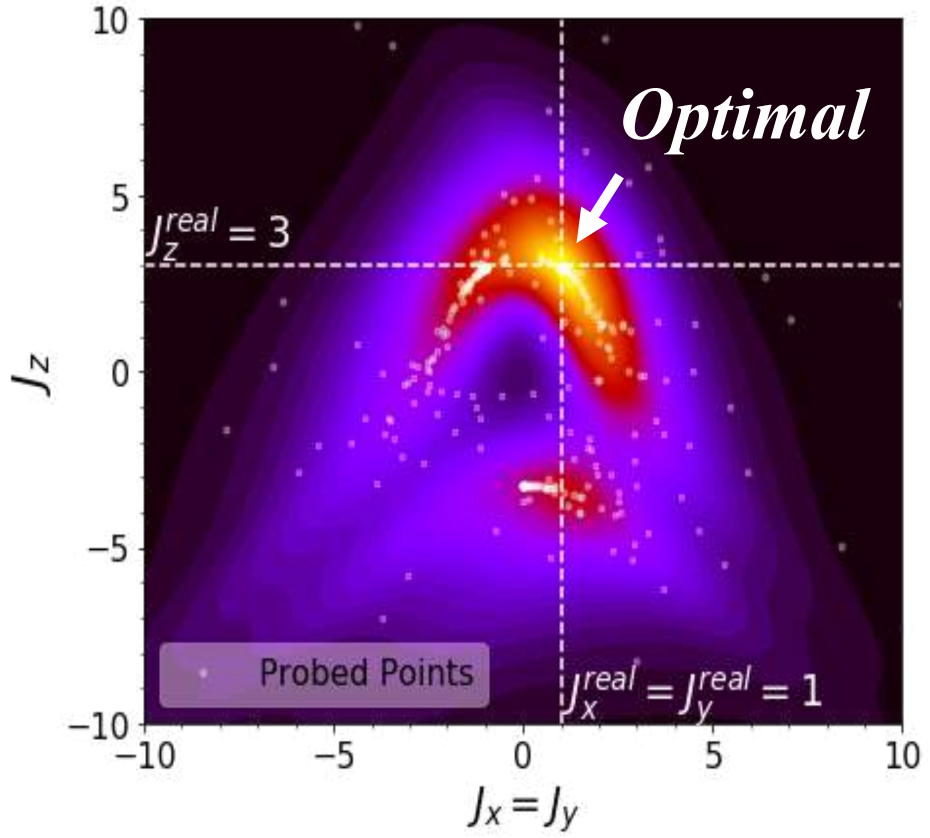
❑ An automatic parameter searching approach



- ➢ ***Automatic*** **and** ***efficient!***
- ➢ ***Systematic*** **and human bias** ***reduced*****.**



Fermi's elephant



Global optimization

❑ Automatic Gradient

$$\text{computational graph } \mathbf{x} \to H \to Z \to O_\alpha \to \mathcal{L}$$

$$\overrightarrow{\text{many-body solver}}$$

$$\underbrace{\mathbf{x} \underset{\frac{\partial H}{\partial \mathbf{x}}}{\rightleftarrows} H \underset{\frac{\partial Z}{\partial H}}{\rightleftarrows} Z \underset{\frac{\partial O_\alpha}{\partial Z}}{\rightleftarrows} O_\alpha \underset{\frac{\partial \mathcal{L}}{\partial O_\alpha}}{\rightleftarrows}}_{\overline{\mathbf{x}} \equiv \frac{\partial \mathcal{L}}{\partial \mathbf{x}}} \mathcal{L},$$

Define the loss:

$$\mathcal{L}(\mathbf{x}_i) = \sum_\alpha \frac{1}{N_\alpha} \lambda_\alpha \left(\frac{O_\alpha^{\text{exp}} - O_\alpha^{\text{sim}}}{O_\alpha^{\text{sim}}} \right)^2.$$

- ***Derivative of fitting loss over Hamiltonian parameters***

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}} = \frac{\partial \mathcal{L}}{\partial O_\alpha} \frac{\partial O_\alpha}{\partial Z} \frac{\partial Z}{\partial H} \frac{\partial H}{\partial \mathbf{x}}.$$

PyTorch

H.-J. Liao, et. al., PRX 2019

B.-B. Chen, […], Wei Li, and Z.Y. Xie, PRB(R) 2020

❑ Bayesian Optimization

Gaussian Process & Acquisition function

- **Fitting Loss Function $\mathcal{L}$:** ***least square***
- **Gaussian Process:** ***high-dimensional optimization problem***
- **Acquisition function:** ***balance exploitation and exploration***

Suppose:

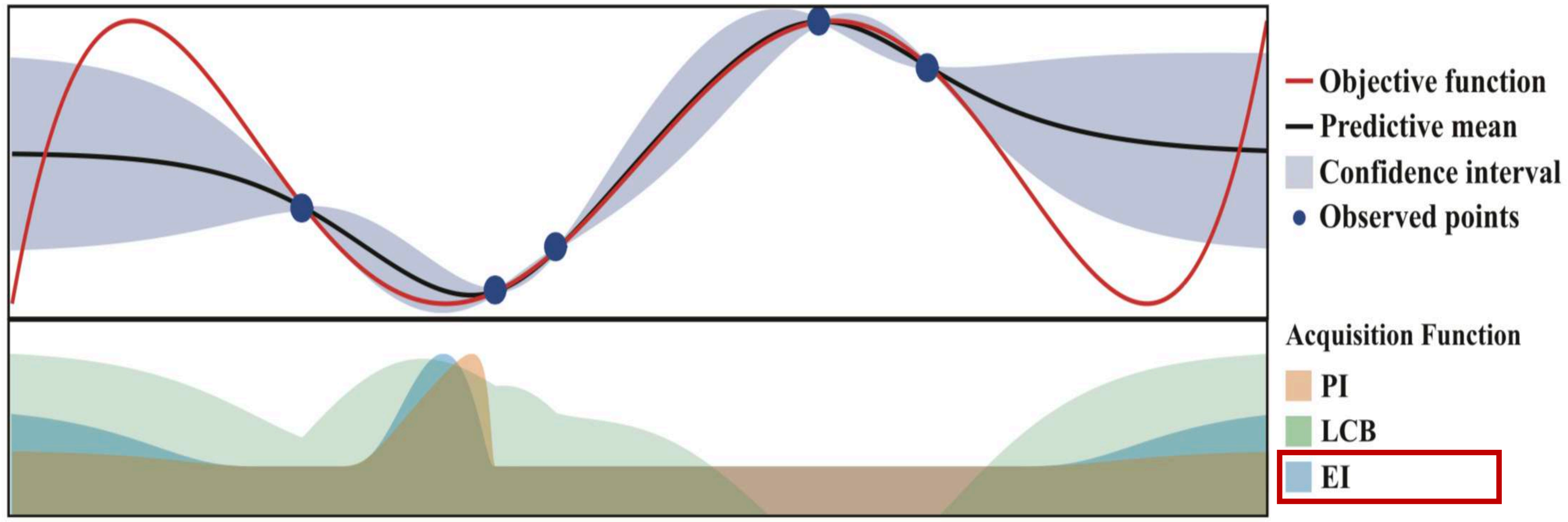
$$\mathcal{GP} : \mathcal{X}, \mathcal{D} \longrightarrow \mu, \sigma$$

$$\mathcal{D}_n = ((\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), ..., (\mathbf{x}_n, y_n))$$

y_{n+1} to be estimated at $\mathbf{x}_{n+1}$

$$y_{n+1} \sim \mathcal{N}(\mu_n, \sigma_n^2)$$

$$\mu_n(\mathbf{x}_{n+1}) = \mathbf{k}(\mathbf{x}_{n+1})^\top \mathbf{K}^{-1} \mathbf{y},$$
$$\sigma_n^2(\mathbf{x}_{n+1}) = k(\mathbf{x}_{n+1}, \mathbf{x}_{n+1}) - \mathbf{k}(\mathbf{x}_{n+1})^\top \mathbf{K}^{-1} \mathbf{k}(\mathbf{x}_{n+1}),$$



$$\alpha_{\mathrm{PI}}(\mathbf{x}; \mathcal{D}_n) = \mathbb{P}[\mathcal{L}(\mathbf{x}) \le \tau] = \Phi\left(-\frac{\mu_n(\mathbf{x}) - \tau}{\sigma_n(\mathbf{x})}\right),$$

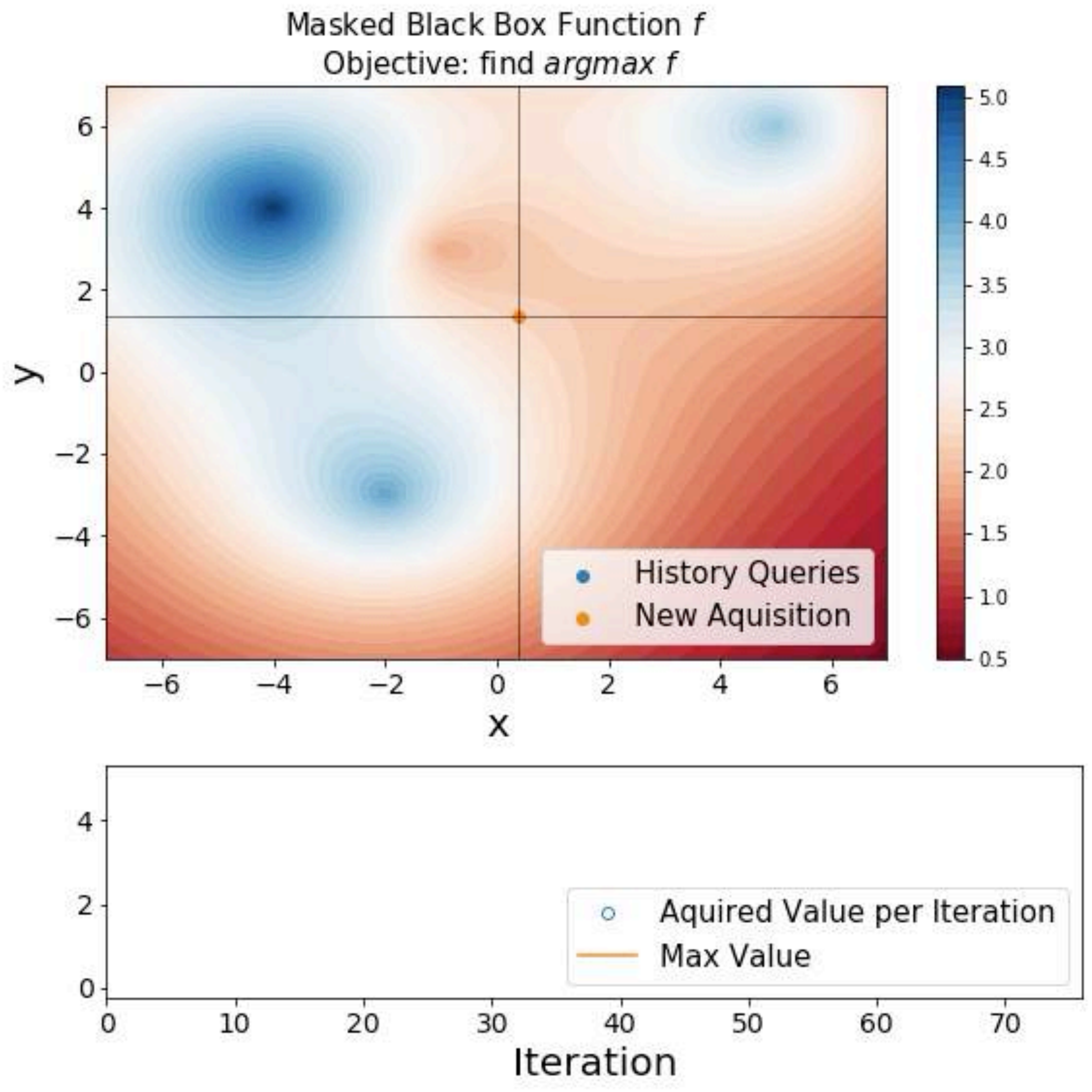
$$\alpha_{\mathrm{EI}}(\mathbf{x}; \mathcal{D}_n) = \mathbb{E}[\tau - \mathcal{L}(\mathbf{x})] = (\tau - \mu_n(\mathbf{x}))\Phi\left(\frac{\tau - \mu_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right) + \sigma_n(\mathbf{x})\phi\left(\frac{\tau - \mu_n(\mathbf{x})}{\sigma_n(\mathbf{x})}\right),$$

$$\alpha_{\mathrm{LCB}}(\mathbf{x}; \mathcal{D}_n) = \mu_n(\mathbf{x}) - \kappa\sigma_n(\mathbf{x}),$$

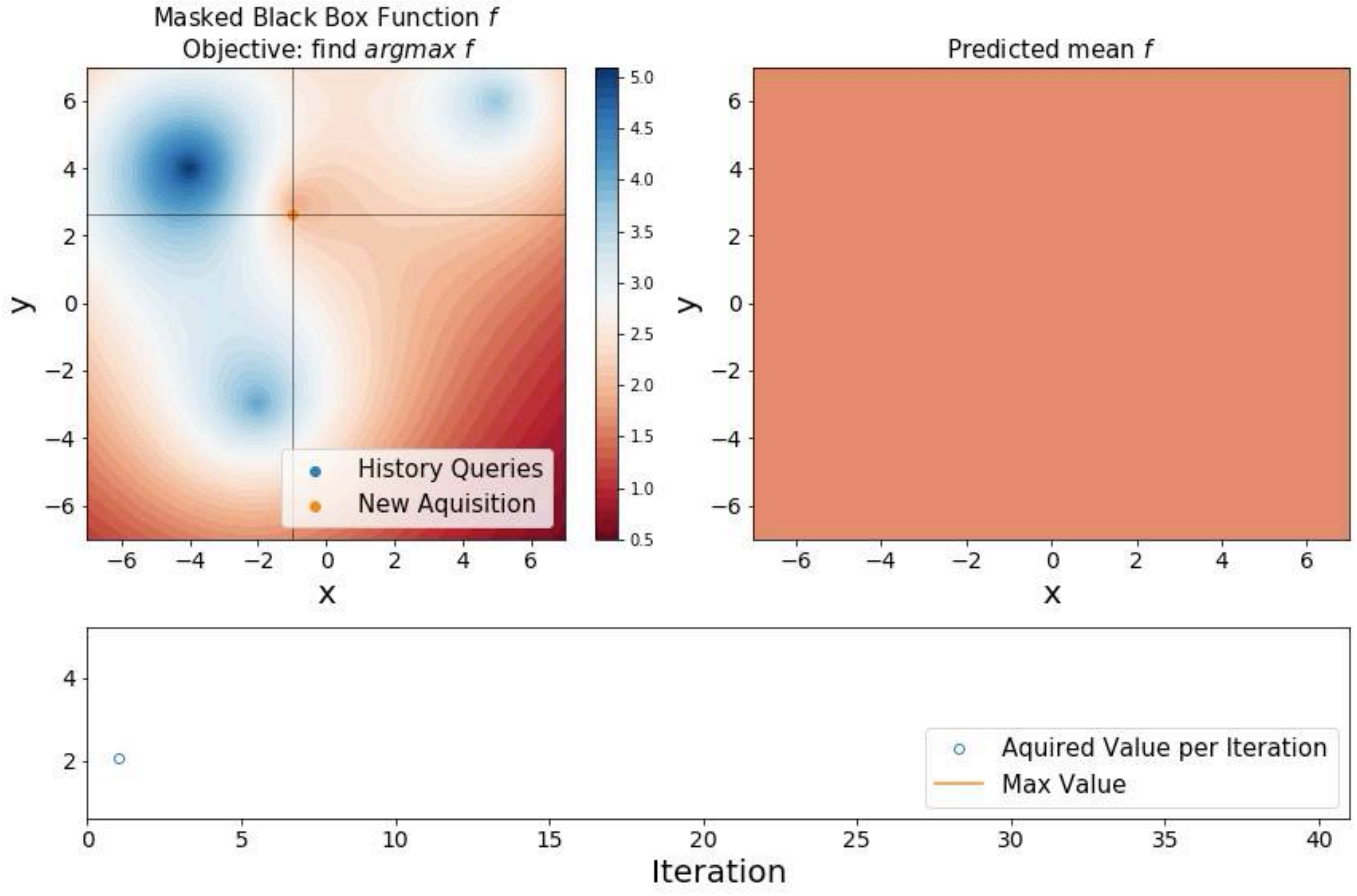
❑ **Gradient-based vs. Bayesian** optimization

(animations)

Gradient-based

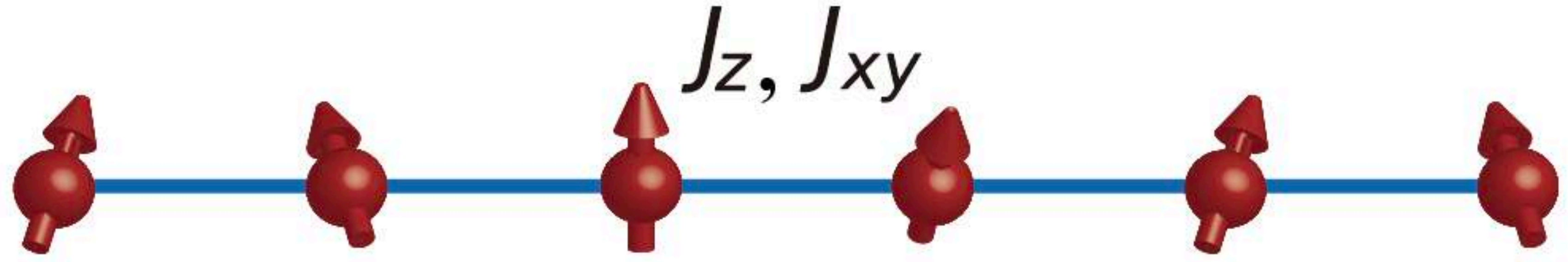


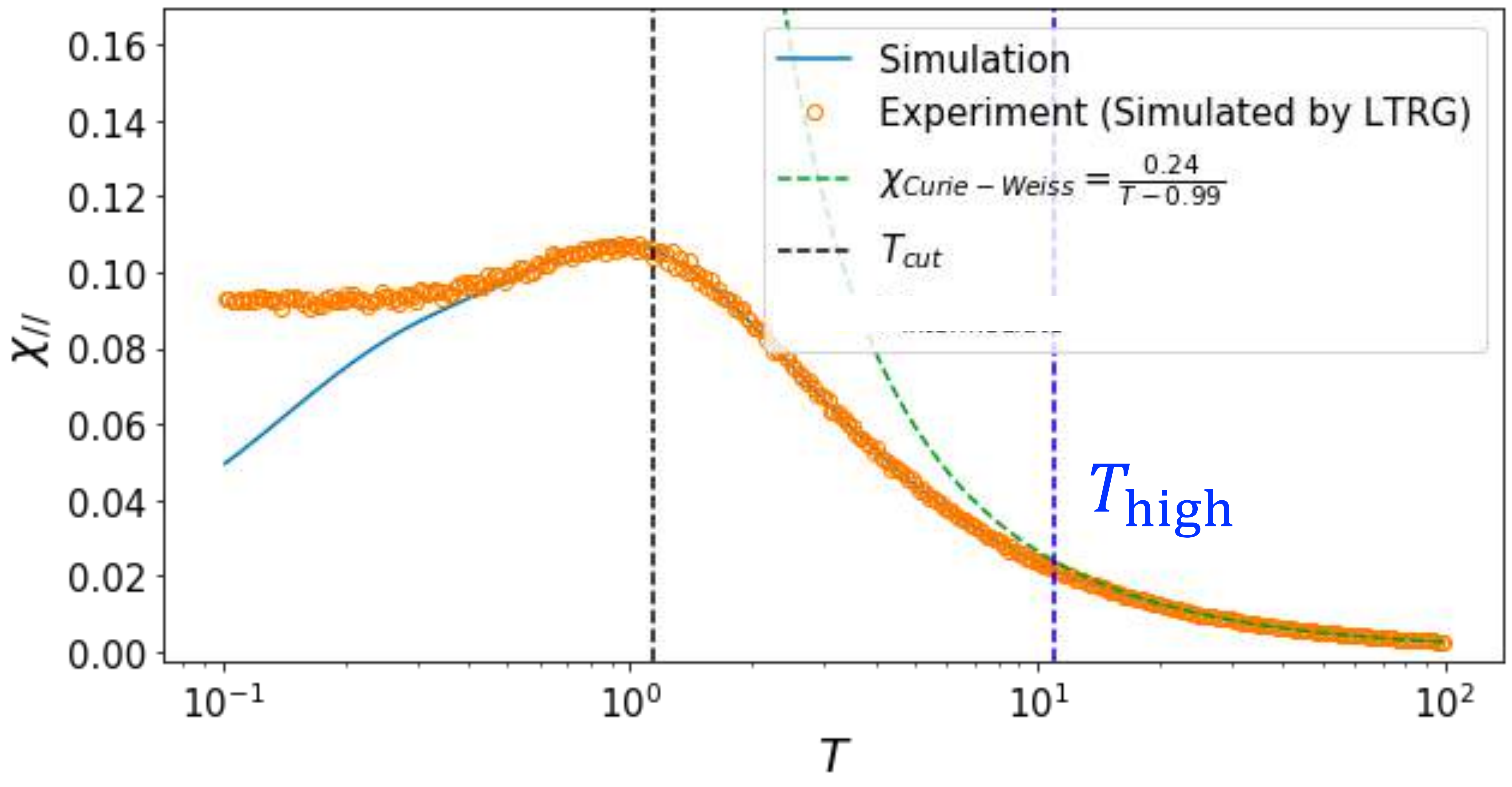
Bayesian



❑ Artificial Experimental Data

❖ **Generated by LTRG, XXZ HAFC model with two parameters J_{xy} and J_z**





➢ **Gaussian (white) noise introduced.**

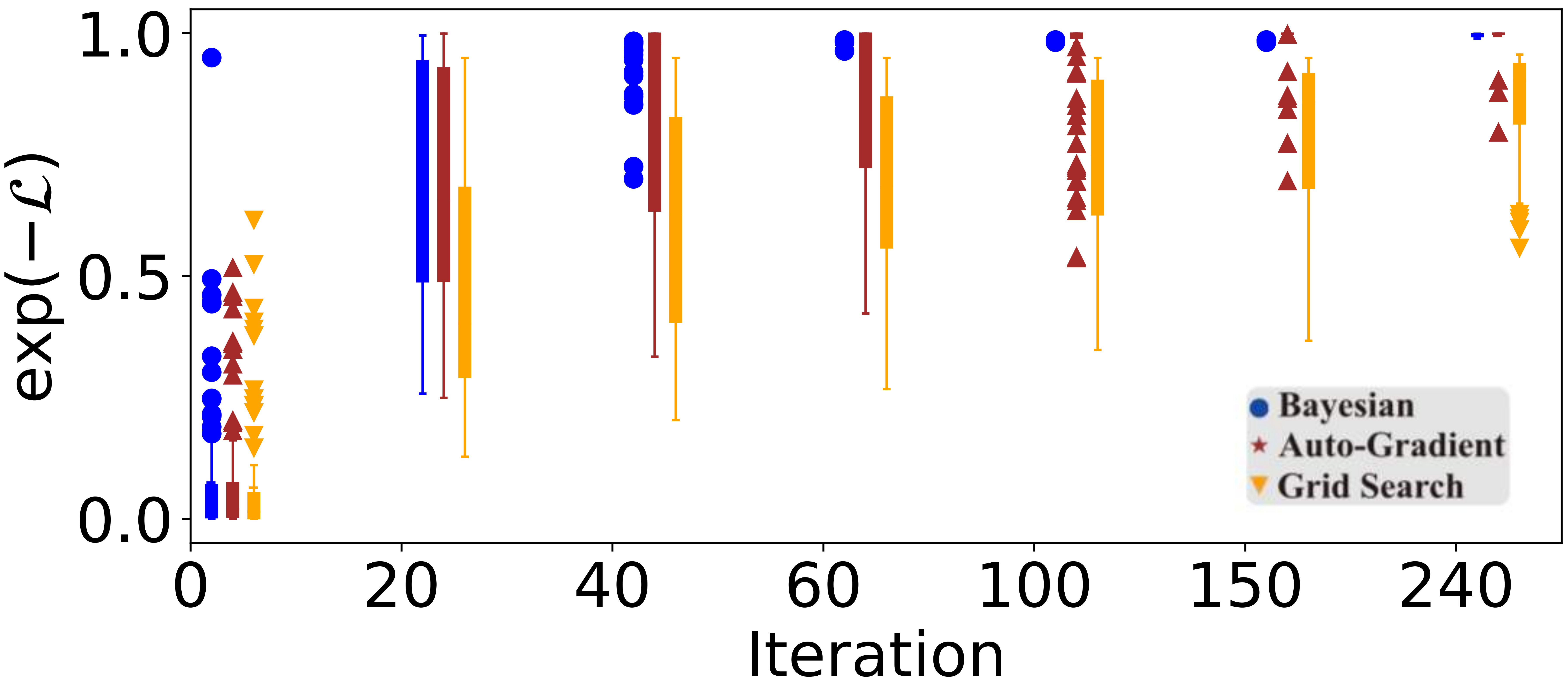
❑ **High-temperature solver:**

10-site ED

➢ **Only $T > T_{cut}$ data are included in the fitting.**

❑ YES! Parameters Retrieved

Statistical box plot of 100 experiments



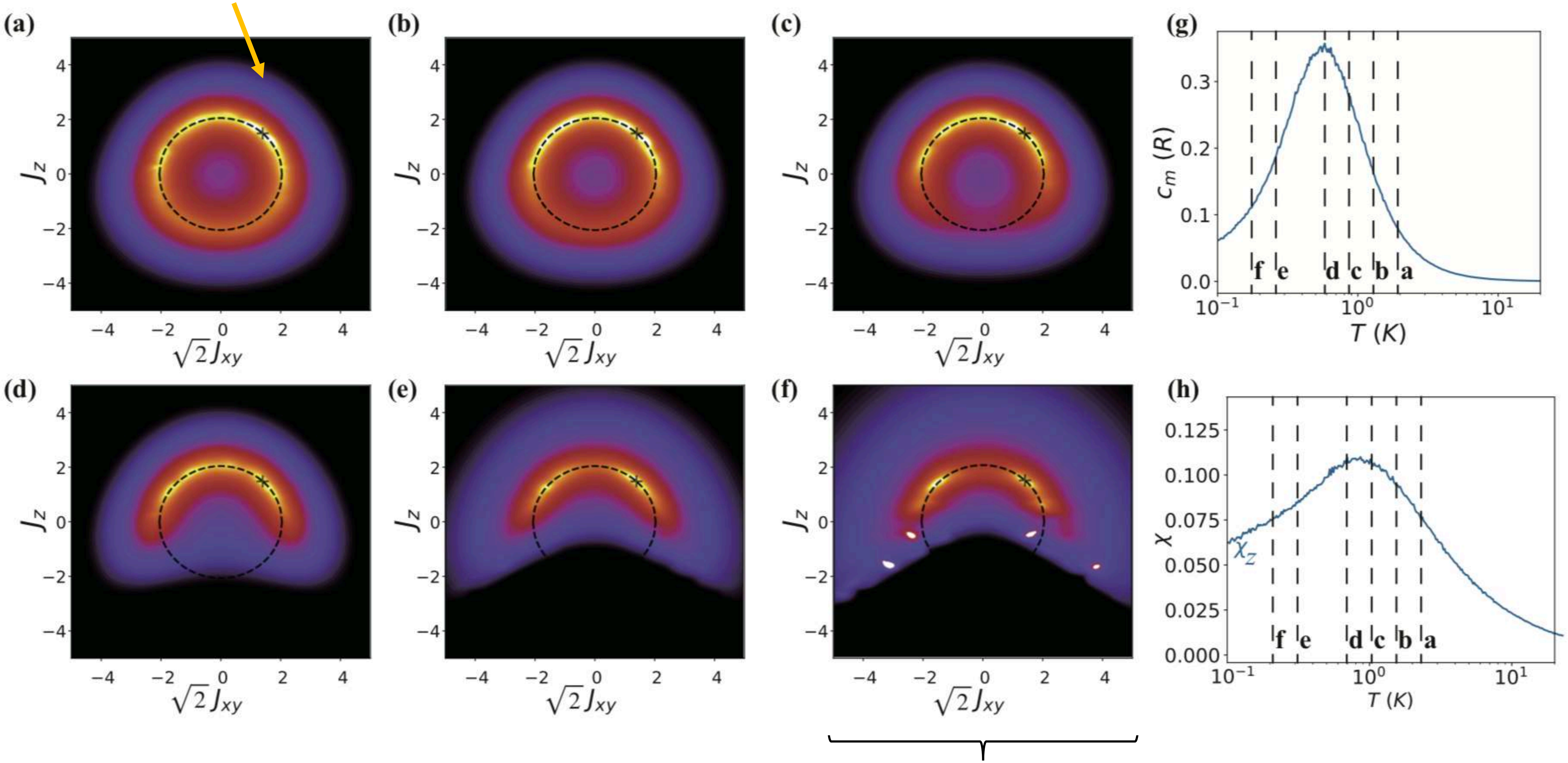
Bayesian optimization has the overall best performance.

❑ High-Temperature Solver: *Varying T_{cut}*

$J_x^2 + J_y^2 + J_z^2 = J_{\text{eff}}^2$

J_{eff} reveal the coupling strength!

$J_{xy} = \pm 1$ exactly the same spectra

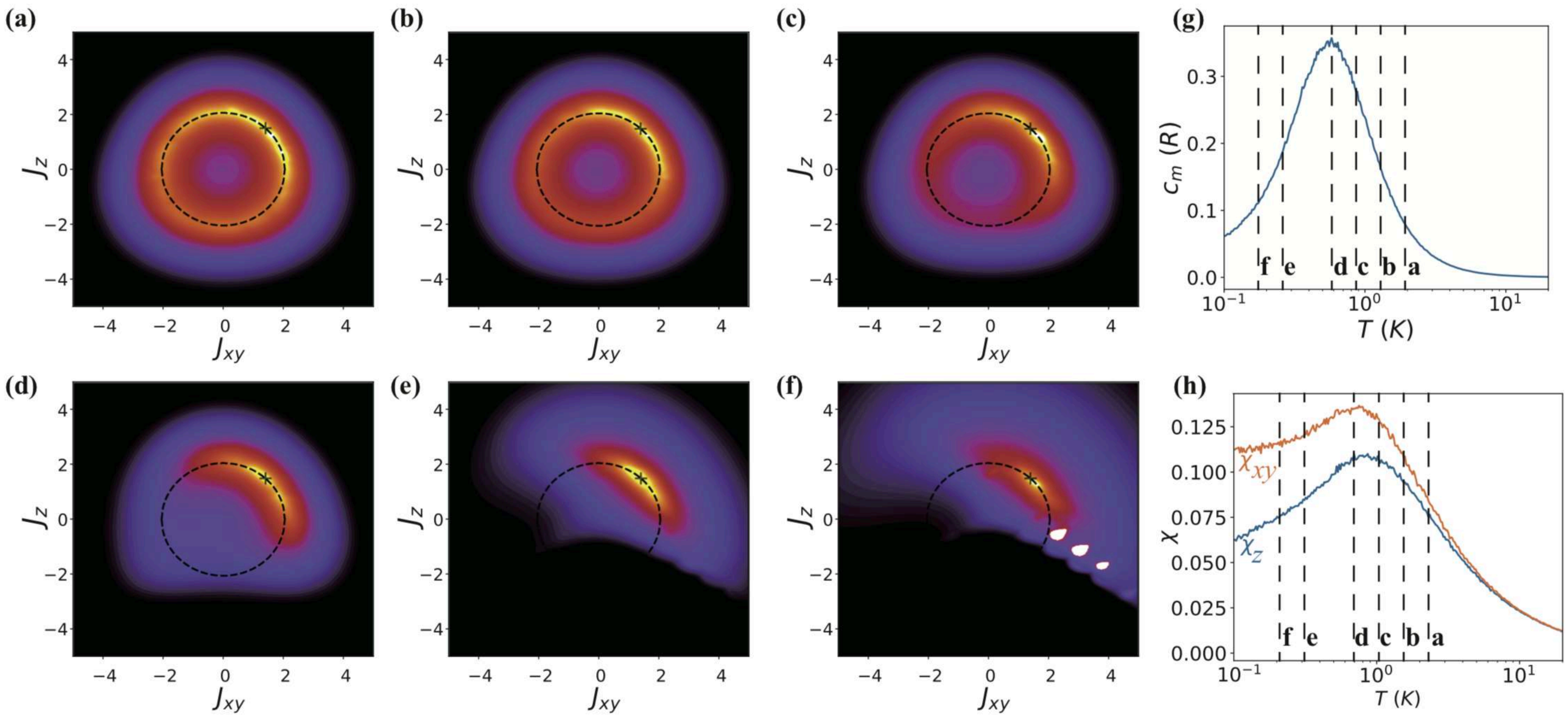


Ground truth: $J_{xy} = 1$, $J_z = 1.5$

fitting is robust

❑ High-Temperature Solver: including more thermal data

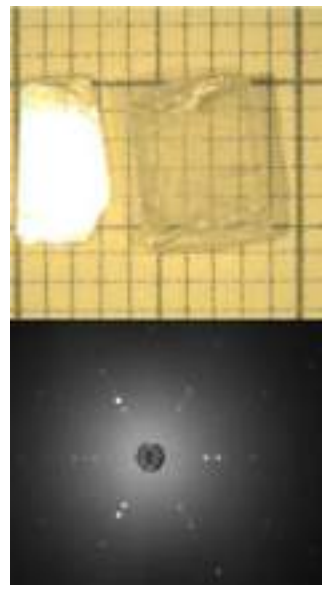
✓ Add more data ***transverse susceptibility*** **can help improve the resolution**



Ground truth: $J_{xy} = 1$, $J_z = 1.5$

$J_{xy} = 1$ **found!**

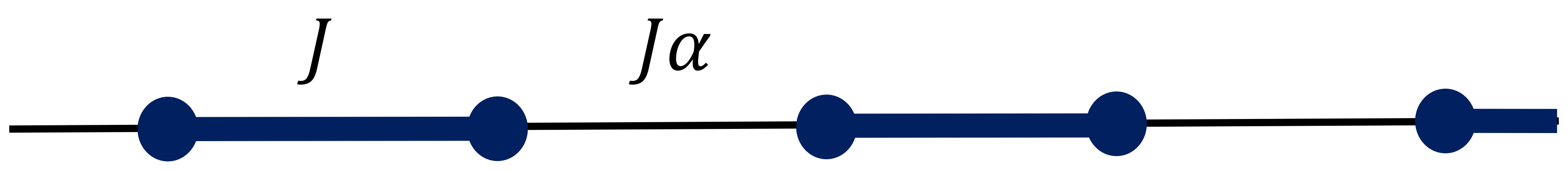
Realistic Materials

❑ Realistic materials: Spin-chain compound Copper Nitrate

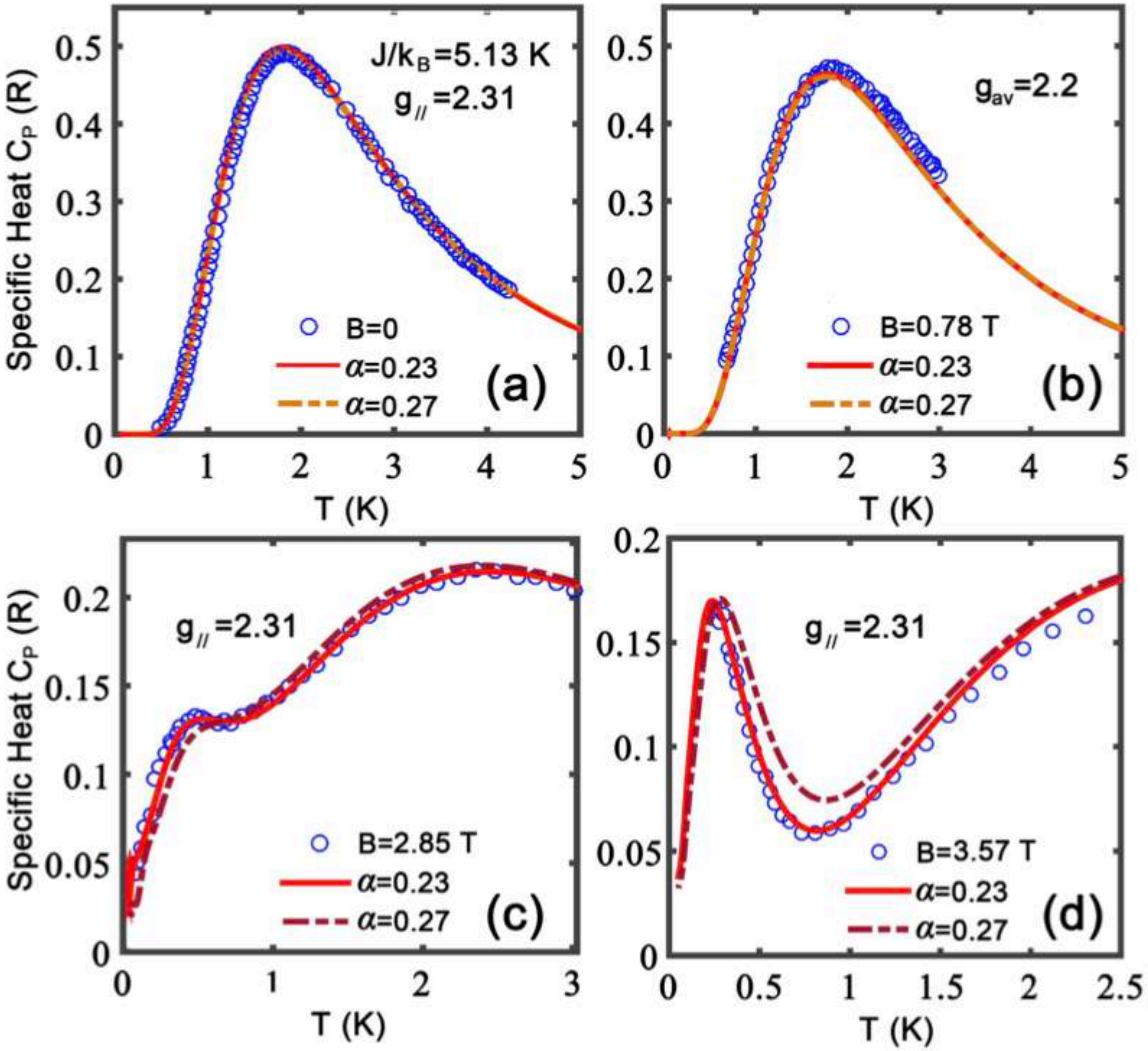
➢ HAFC with alternating couplings

$$H = J\sum_{n=1}^{L/2}(\vec{S}_{2n-1}\vec{S}_{2n} + \alpha\,\vec{S}_{2n}\vec{S}_{2n+1}) - \sum_{m=1}^{L}\sum_{\nu=\{\parallel,\perp\}} g_\nu B_\nu S^z_m,$$



❖ **4 parameters $J, \alpha, g_{//}, g_\perp$**

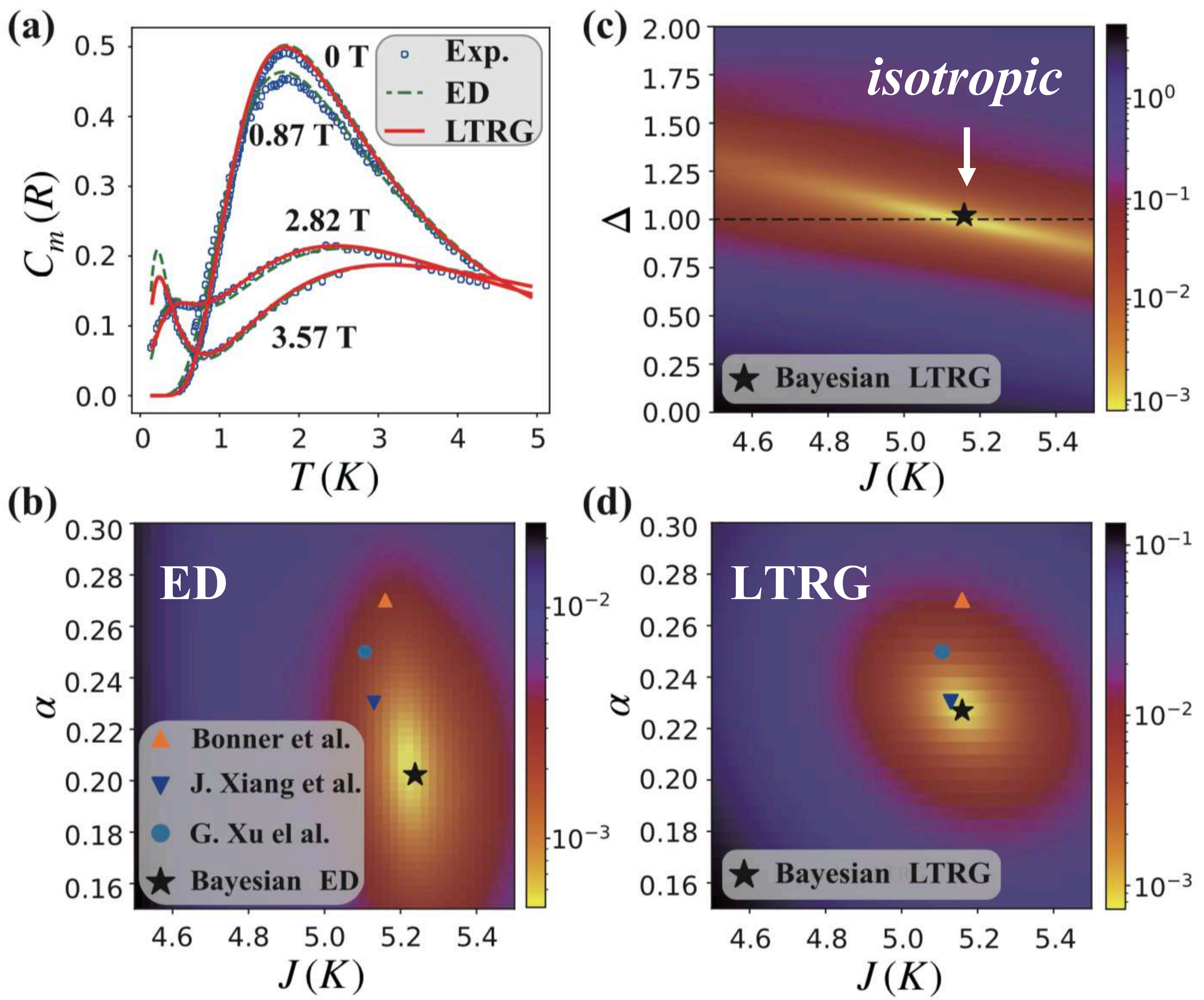
✓ $J = 5.13, \alpha = 0.27$, Bonner et al. 1983
✓ $J = 5.14, \alpha = 0.23$, J. Xiang et al. 2017



What about automatic parameter searching?

❑ Spin-chain material Copper Nitrate

- **Finite-size (10-site) solver: *ED, already works***
- **Infinite-size solver: *LTRG,* resolution improved**



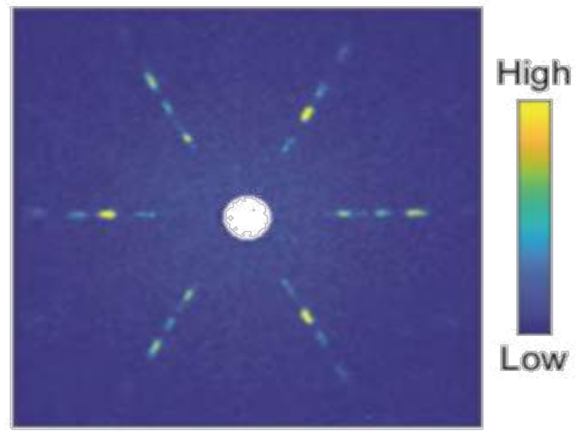
XXZ anisotropy

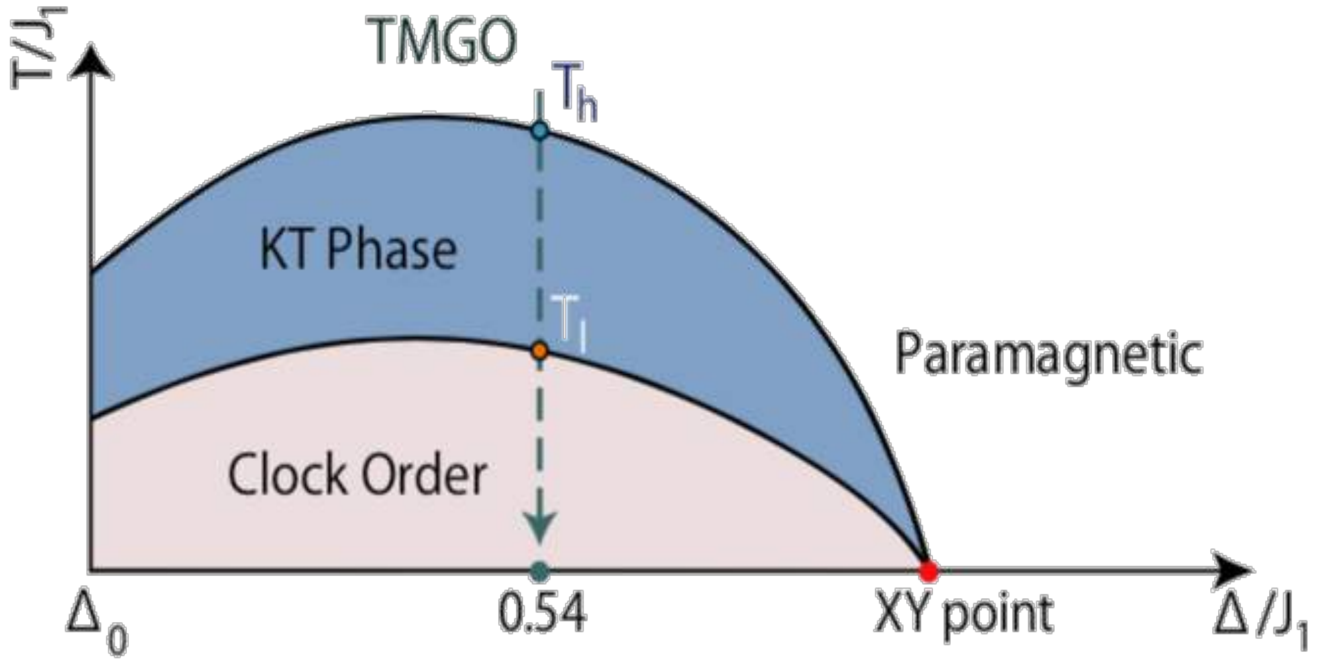
$$H = J \sum_{n=1}^{L/2} [(S^x_{2n-1} S^x_{2n} + S^y_{2n-1} S^y_{2n} + \boxed{\Delta S^z_{2n-1} S^z_{2n}}) + \alpha (S^x_{2n} S^x_{2n+1} + S^y_{2n} S^y_{2n+1} + \boxed{\Delta S^z_{2n} S^z_{2n+1}})] - g\mu_B B \sum_{i=1}^{L} S^z_i.$$

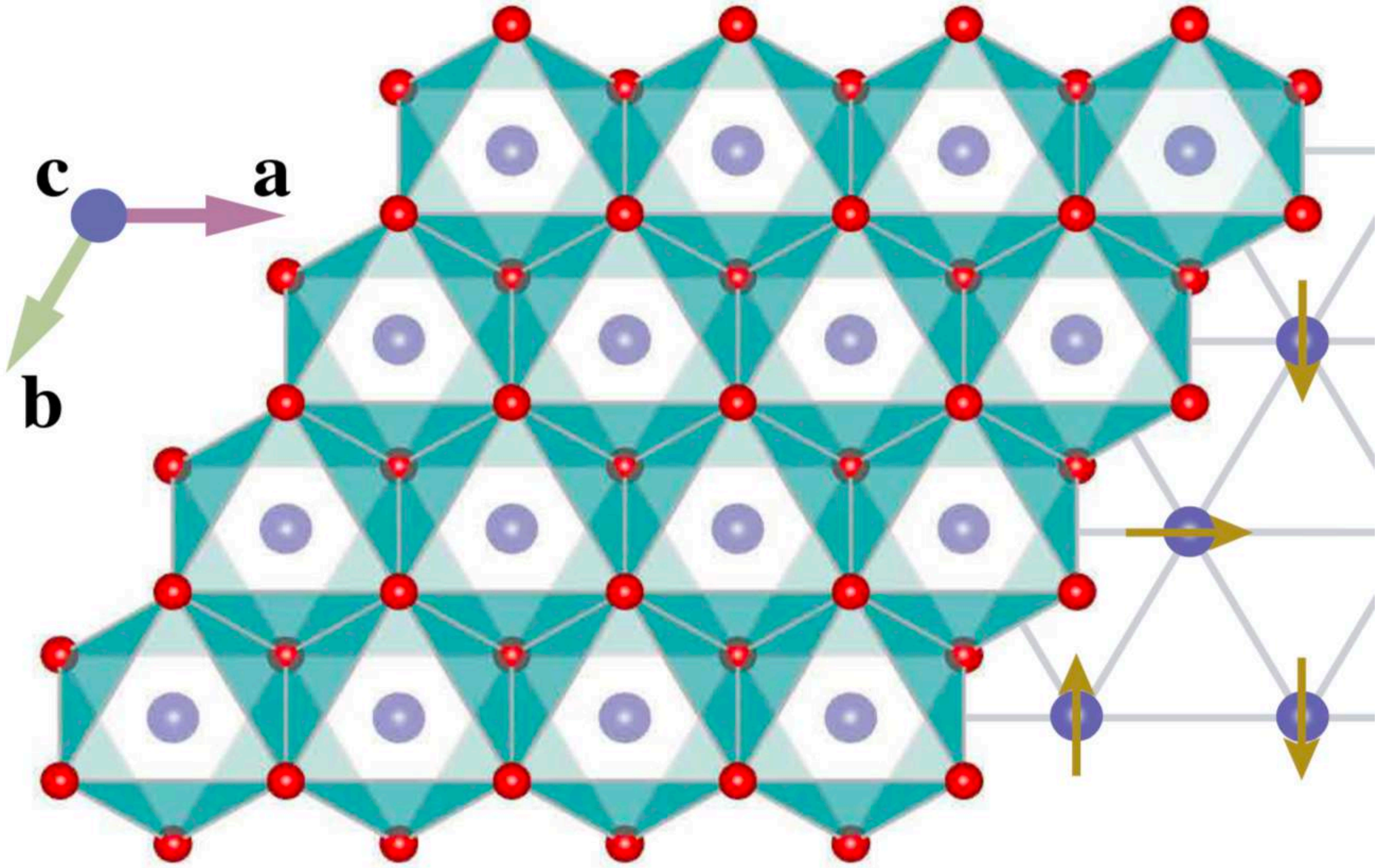
- Machine fitting (with LTRG): ***J* = 5.16, α = 0.227, Δ = 1.01, *g* = 2.23** with $\mathcal{L}$ = 7.4 × 10^{-4}.

- Previous hand-tuned fitting: ***J* = 5.13, α=0.23, Δ=1, *g*=2.31**, with $\mathcal{L}$ =8.2×10^{-4}

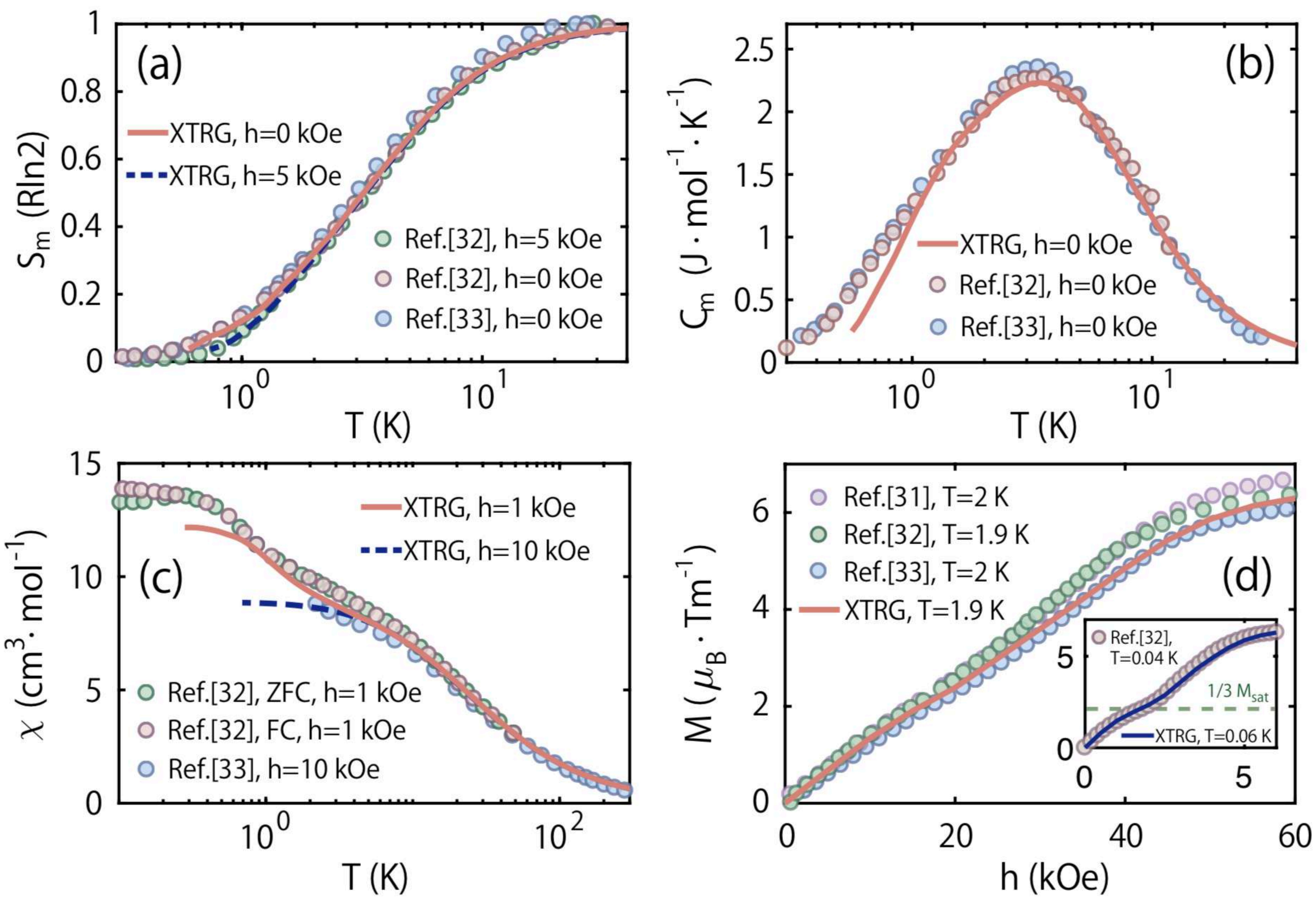
Triangular-lattice Magnet $TmMgGaO_4$







Thermodynamics and XTRG fittings to experimental results.



✓ Two coupling strengths J_1, J_2

✓ Transverse field Δ

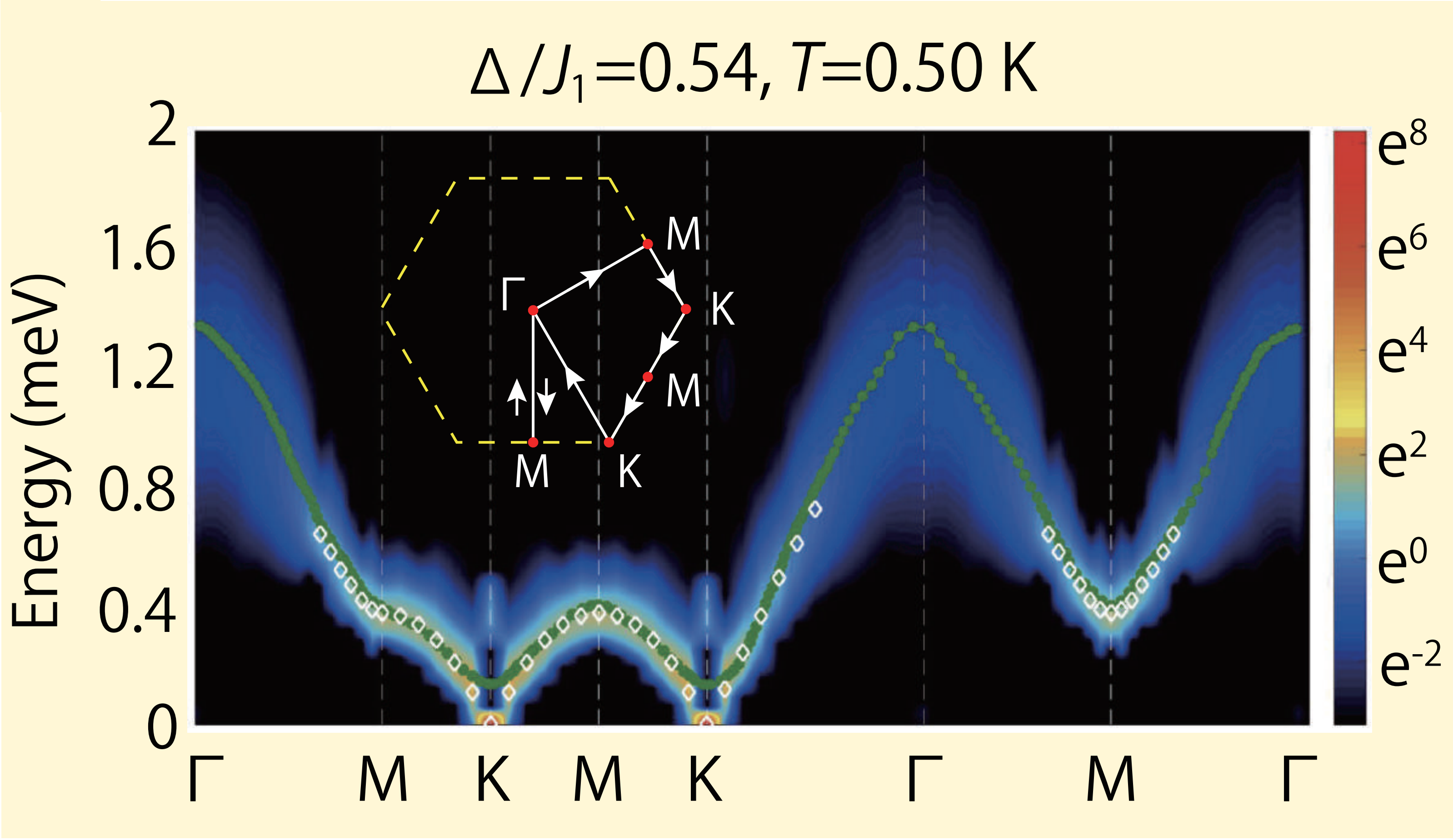
[31] Cevallos, et al., Mater. Res. Bull. 2018
[32] Shen, et al., Nature Commun. 2019
[33] Li, et al., PRX 2020

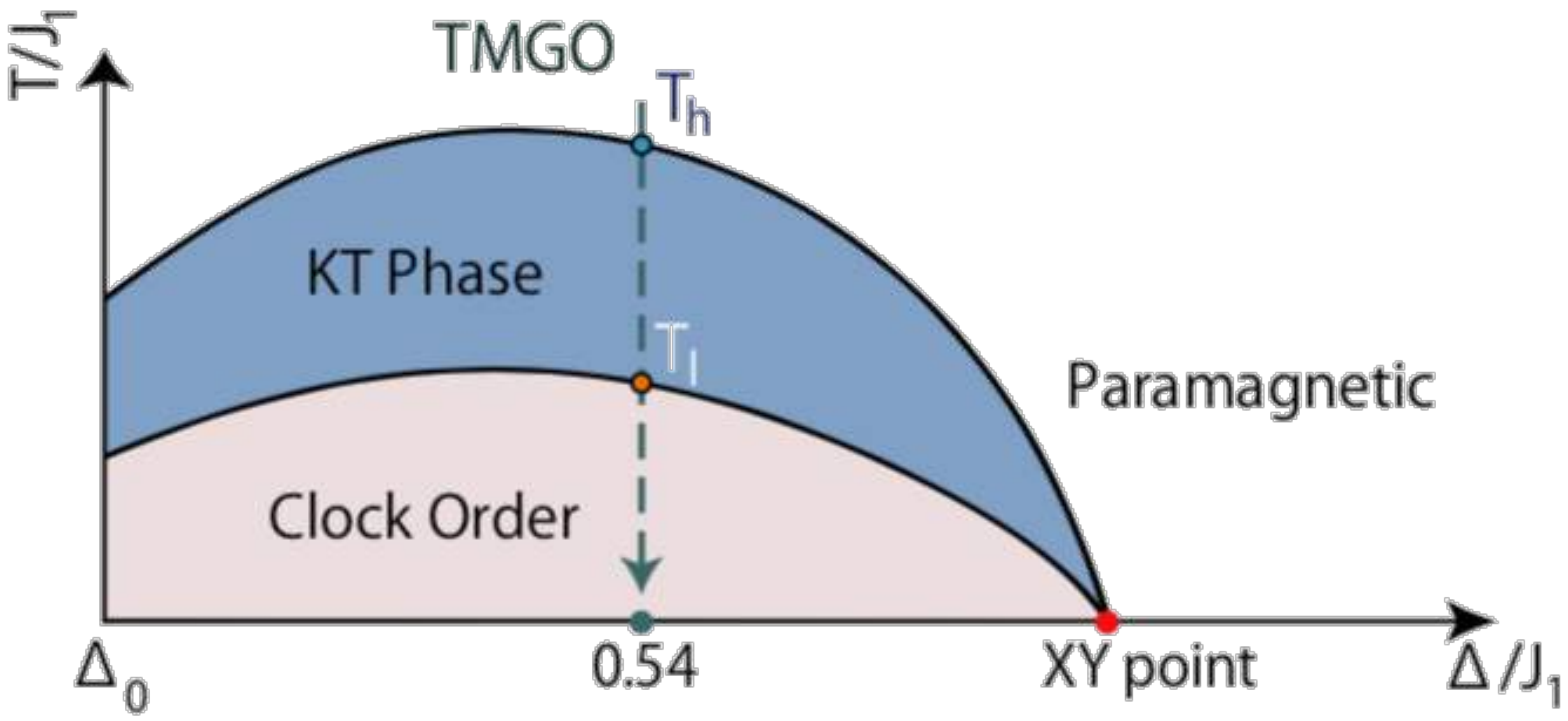
❑ Triangular-lattice quantum Ising model for TMGO

$$H_{\mathrm{TLI}} = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i^z S_j^z - \sum_i (\Delta S_i^x + h\, g_{\|} \mu_B\, S_i^z)$$

$J_1 = 0.99$ meV, $J_2 = 0.05 J_1$, $\Delta = 0.54 J_1$ and $g_J = 1.101$

➢ 2D quantum magnet realizing KT physics!

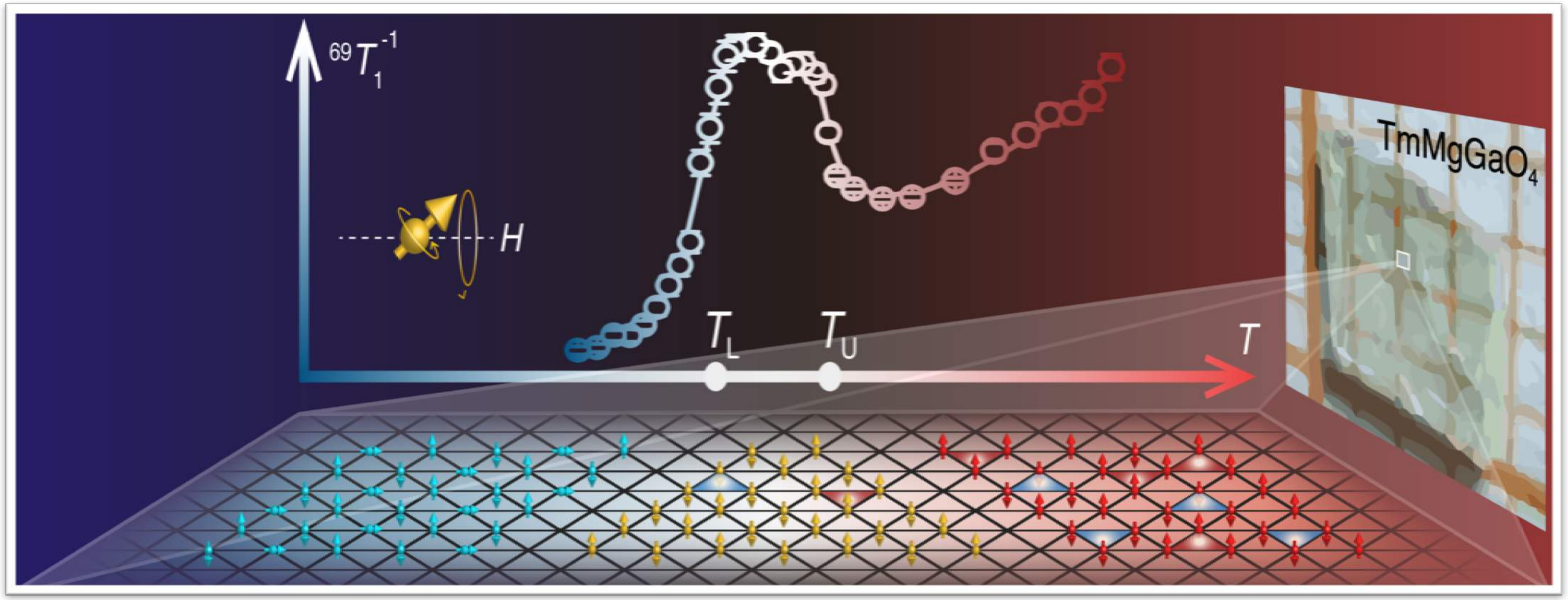




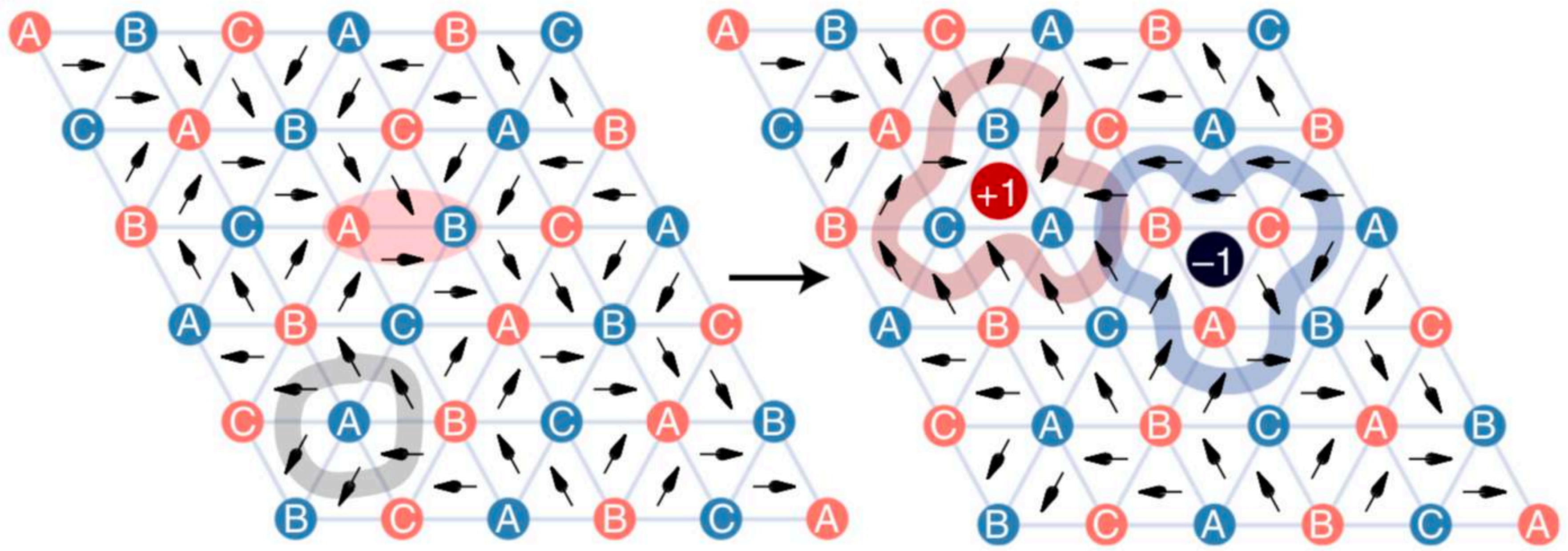
S. Isakov and R. Moessner, PRB (2003)

Y.-C. Wang, Y. Qi, S. Chen, and Z. Y. Meng PRB (2017)

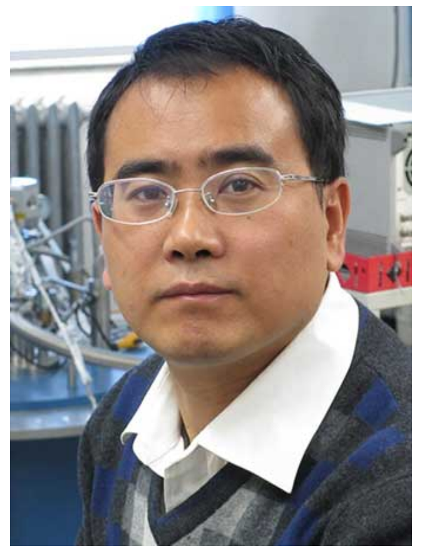
❑Evidence of the Kosterlitz-Thouless Phase in TMGO



- NMR shows a **quasi-plateau** at intermediate temperature, floating KT phase.



Collaborators:

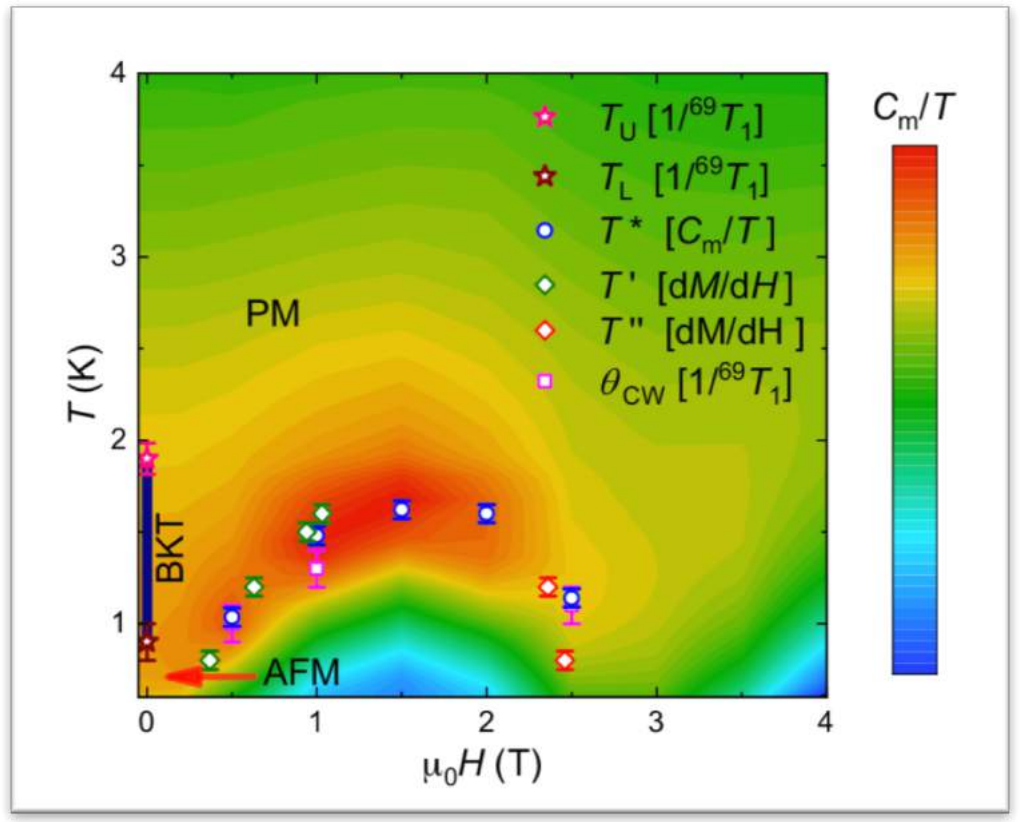


于伟强（人大）

温锦生（南大）

孟子杨（港大）

戚扬（复旦）



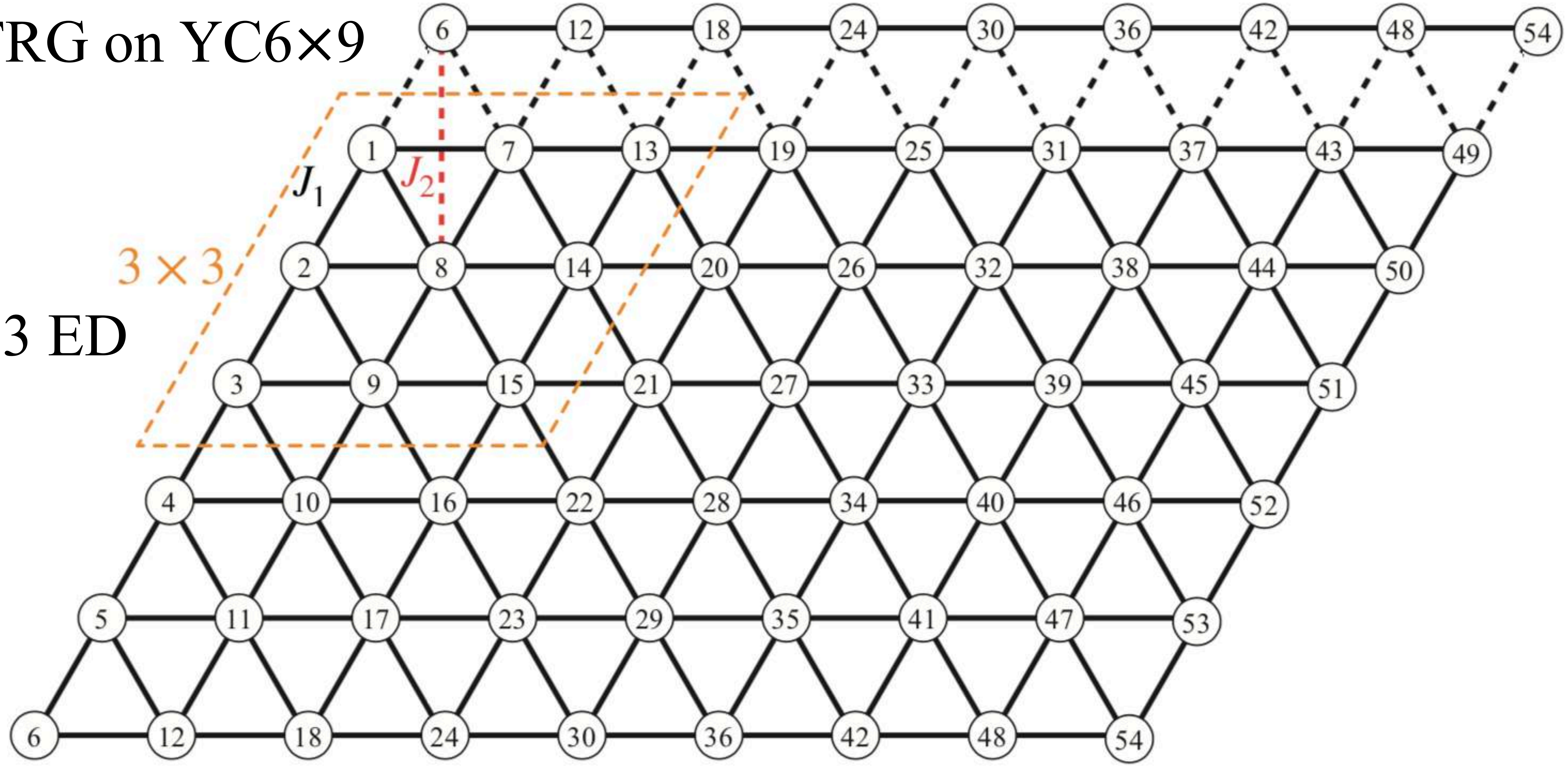
Nat. Commun. 11, 5631 (2020)

❑ Triangular-lattice Magnet $TmMgGaO_4$

$$H = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j' \rangle\rangle} S_i^z S_{j'}^z - \Delta \sum_i S_i^x - g\mu_B B \sum_i S_i^z$$

XTRG on YC6×9

3×3 ED



4 params $\boldsymbol{\Delta, J_1, J_2, g_{\mathrm{eff}}}$

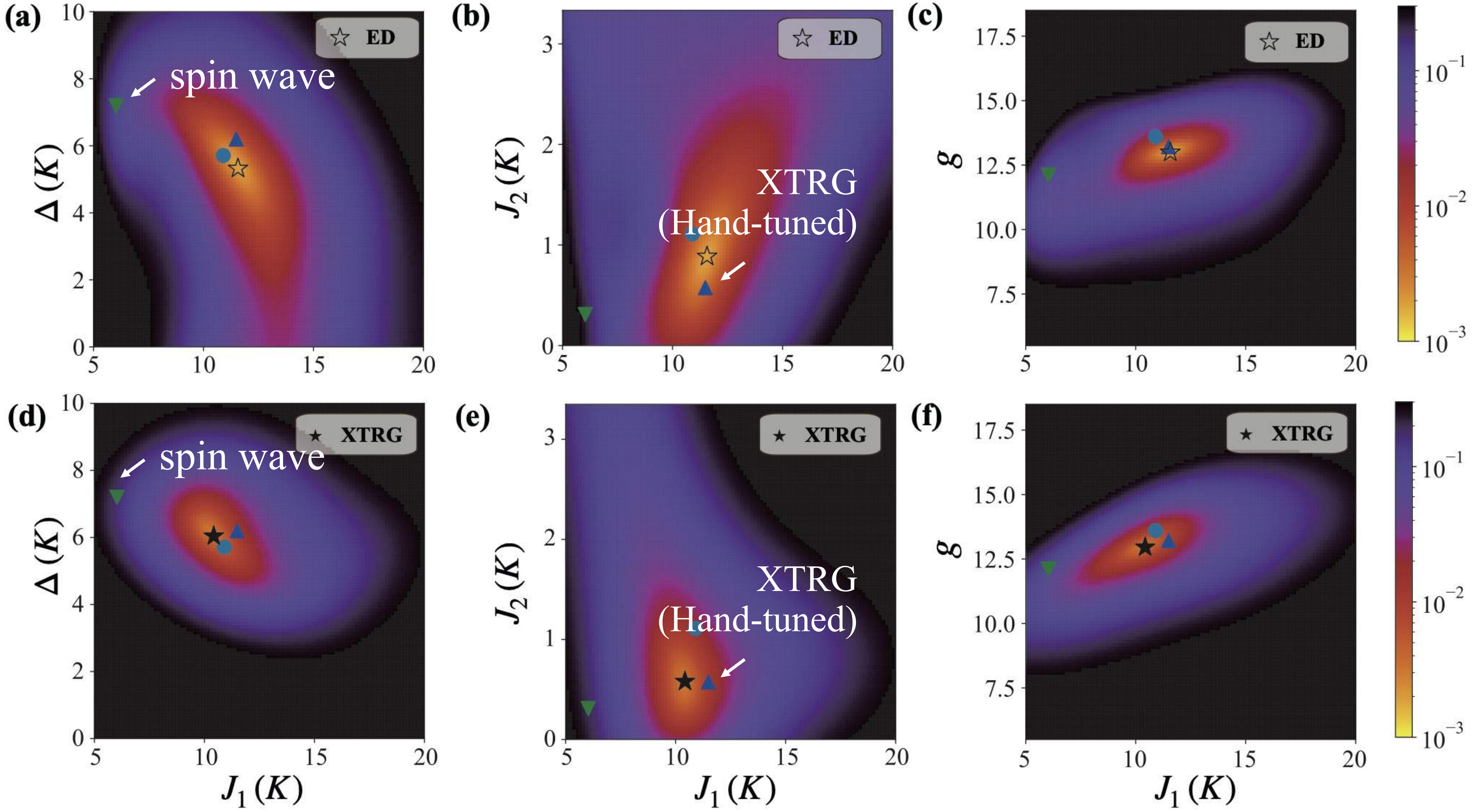
$\langle ij \rangle$ NN pair of sites

$\langle\langle ij \rangle\rangle$ NNN pair of sites

❑ Triangular-lattice Magnet $TmMgGaO_4$

ED
T_{cut}=4 K

XTRG
T_{cut}=1 K



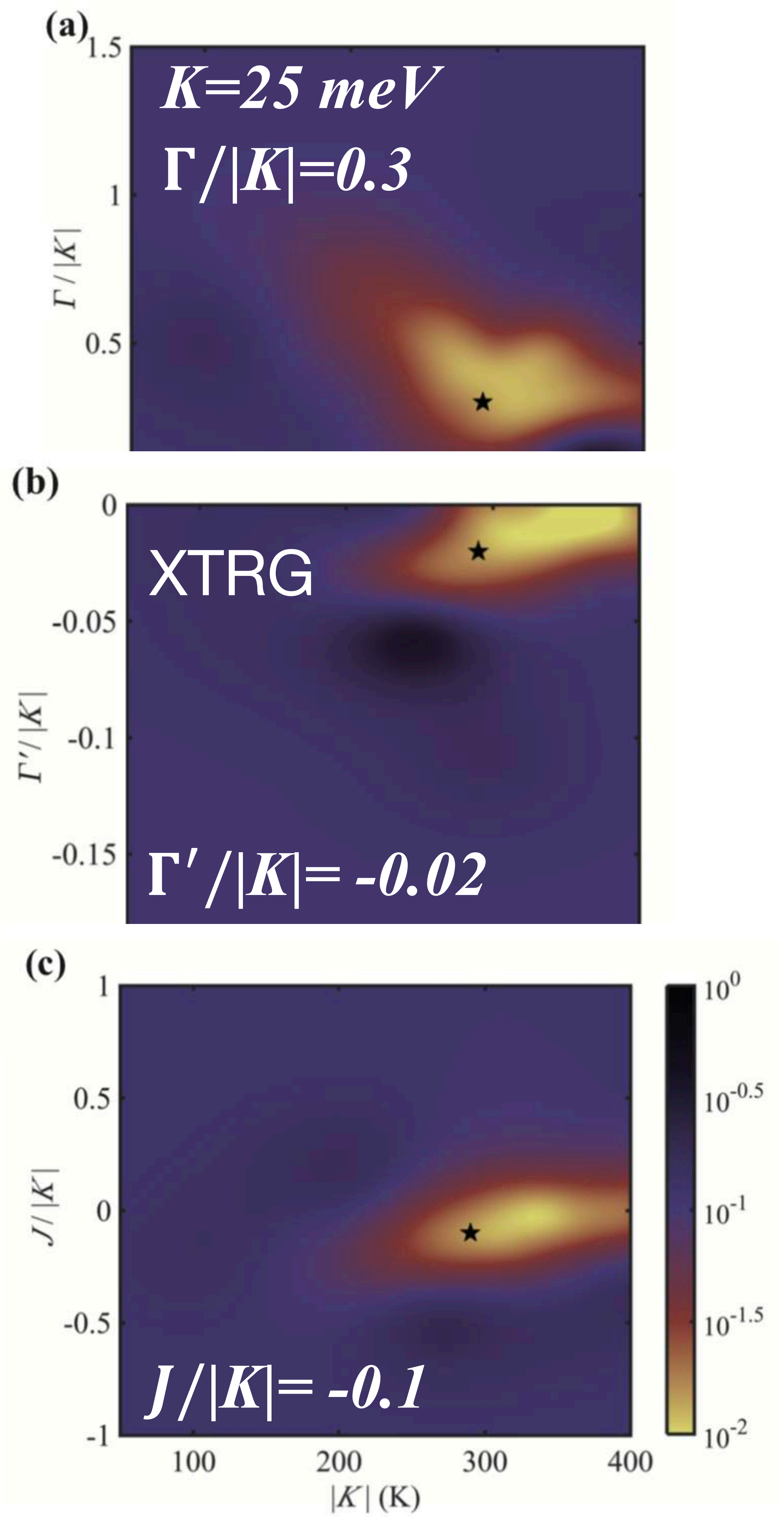
$$H = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j' \rangle\rangle} S_i^z S_{j'}^z - \Delta \sum_i S_i^x - g\mu_B B \sum_i S_i^z$$

H. Li, […], WL, Nature Commun. 2020
Y. Li, et al, PRX 2020; Y. Shen, et al, Nature Commun. 2019

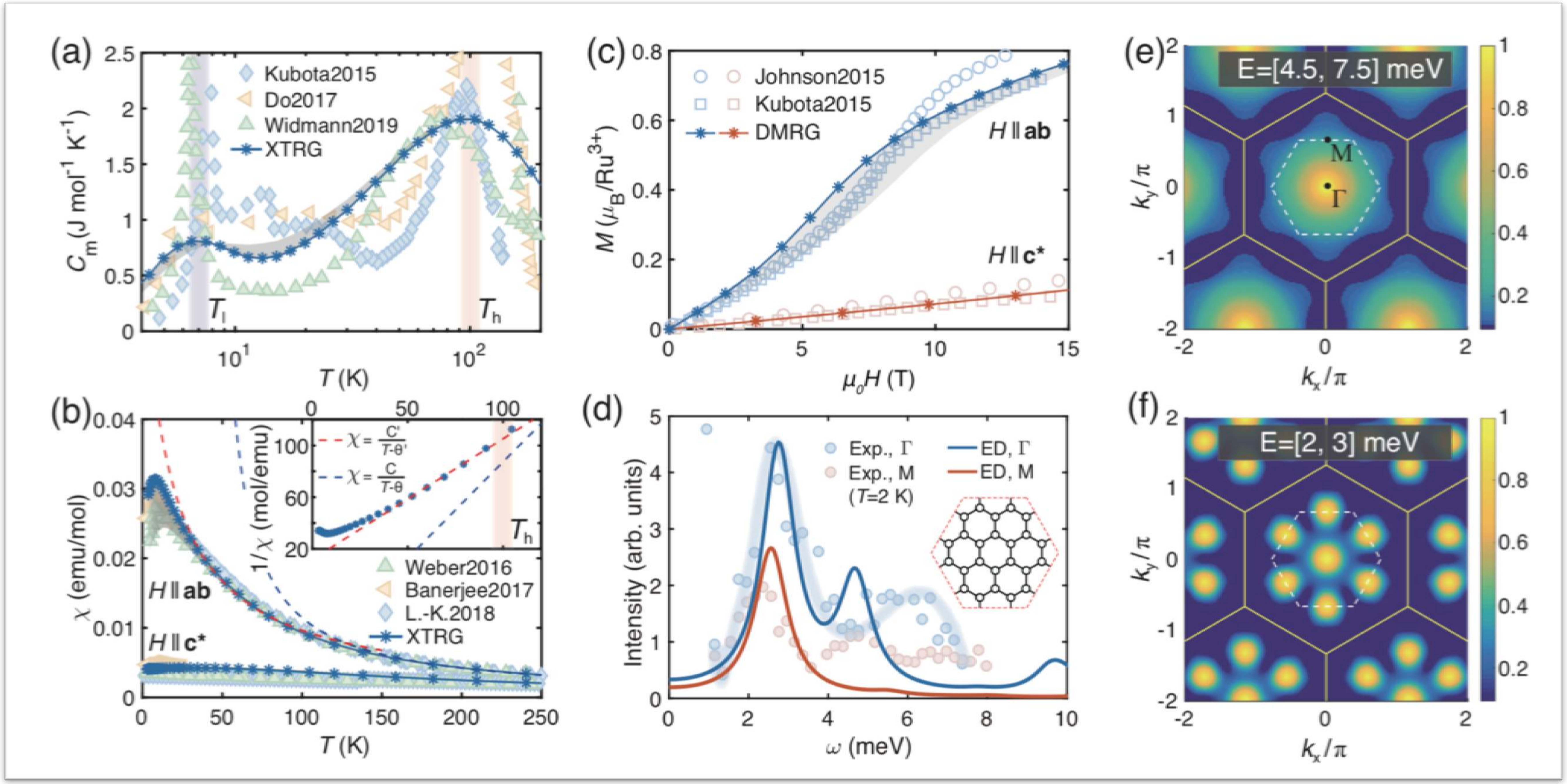
❑ Kitaev material α-$RuCl_3$

H. Li, […], WL, in process

❖ **Fitting Landscape**



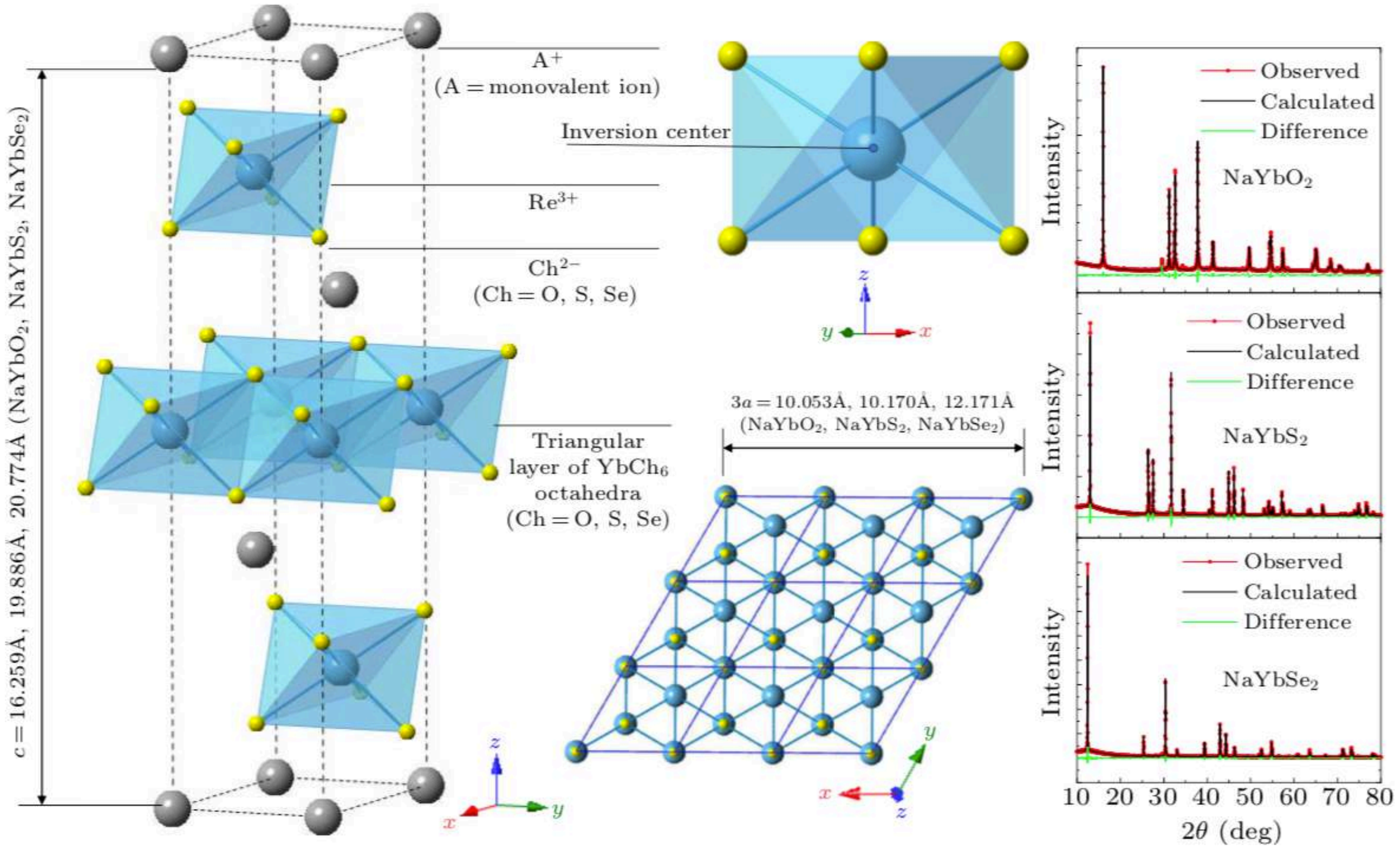
❖ **Reproduce major exp. features**



$$H = \sum_{\langle i,j\rangle_\gamma} [K S_i^\gamma S_j^\gamma + J \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) + \Gamma'(S_i^\gamma S_j^\alpha + S_i^\alpha S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\beta S_j^\gamma)]$$

❑ Outlook: The family of rare-earth triangular magnets

➢ Rare-Earth Chalcogenides



W. Liu, et. al., Chin. Phys. Lett. 2019

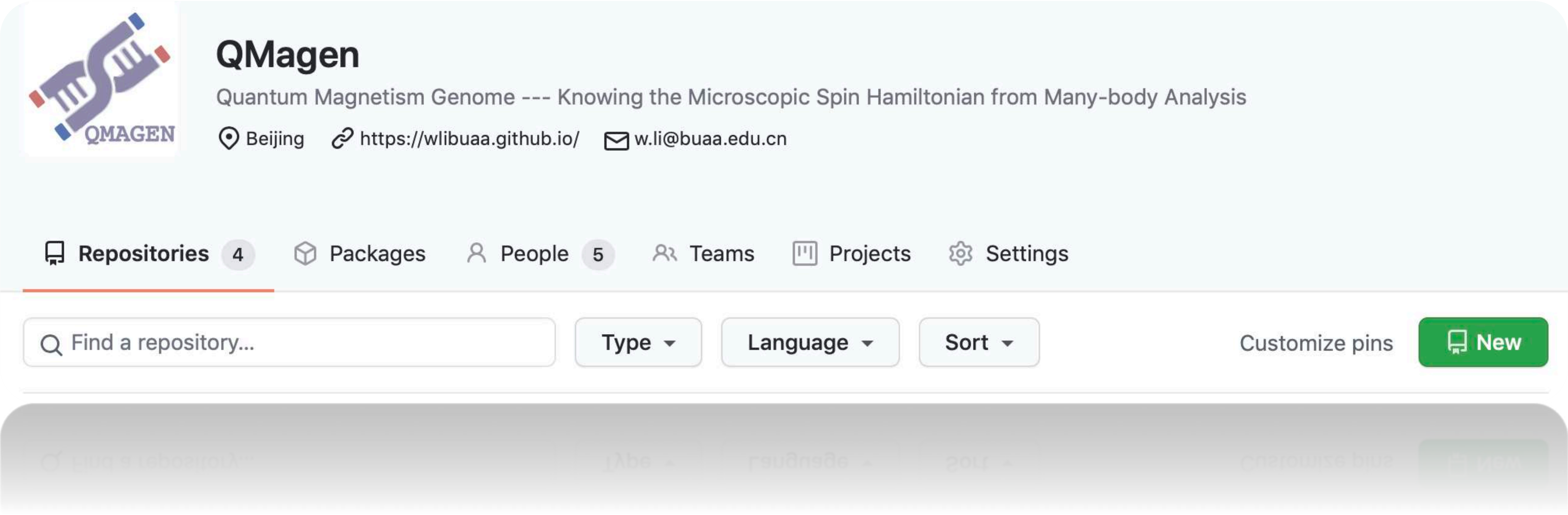
$ARe Ch_2$

[A=alkali or monovalent metal, RE=rare earth, Ch=O, S, Se, Te]

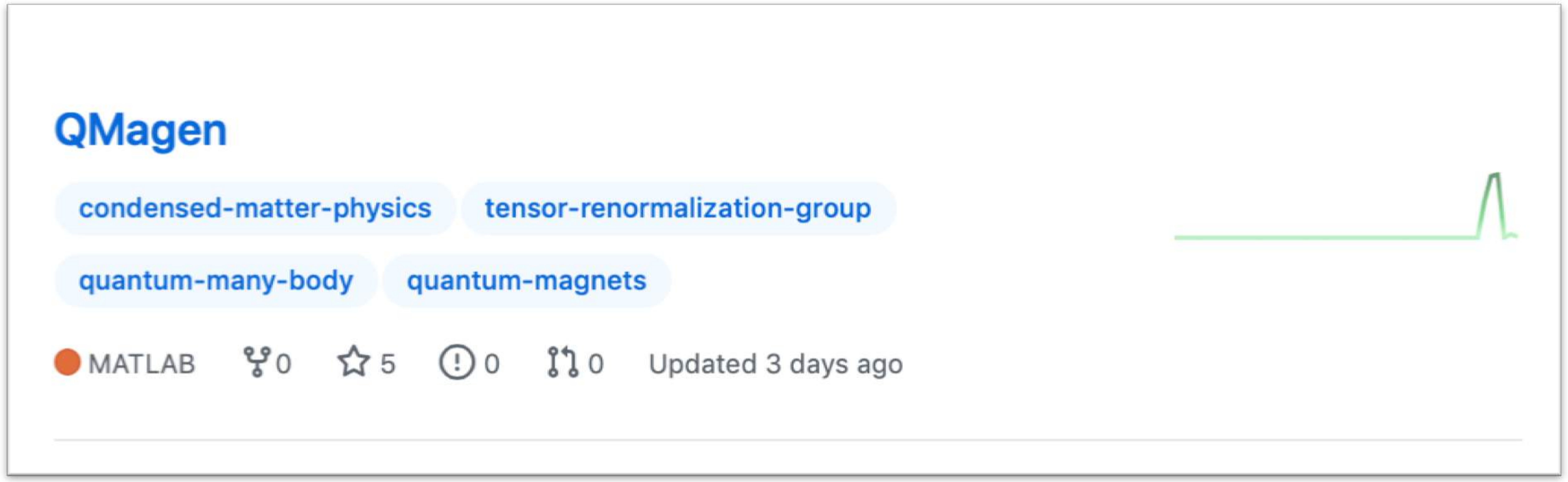
$$
\begin{aligned}
\hat{H}_{eff} &= \hat{H}_{CEF} + \hat{H}_{spin-spin} + \hat{H}_{zeeman} \\
&= \sum_i \sum_{m,n} B_m^n \hat{O}_m^n \\
&\quad + \sum_{\langle ij \rangle} [J_{zz} S_i^z S_j^z + J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+) \\
&\quad + J_{\pm\pm}(\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-) \\
&\quad - \frac{i J_{z\pm}}{2}(\gamma_{ij} S_i^+ S_j^z - \gamma_{ij}^* S_i^- S_j^z + \langle i \longleftrightarrow j \rangle)] \\
&\quad - \mu_0 \mu_B \sum_i [g_{ab}(h_x S_i^x + h_y S_i^y) + g_c h_c S_i^z]
\end{aligned}
$$

Z. Zhang arXiv:2011.06274 (2020)
$NaYbSe_2$ analyzed, mean field

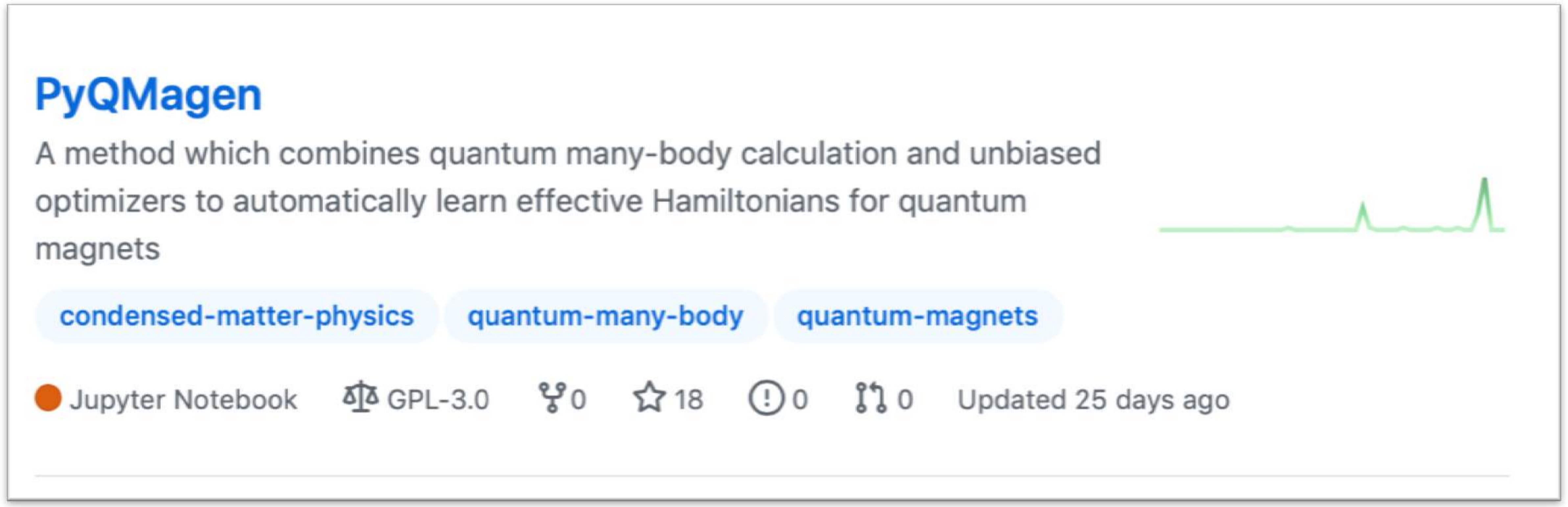
❑ Open source package: QMagen



Matlab version: include ED, LTRG, and XTRG solvers



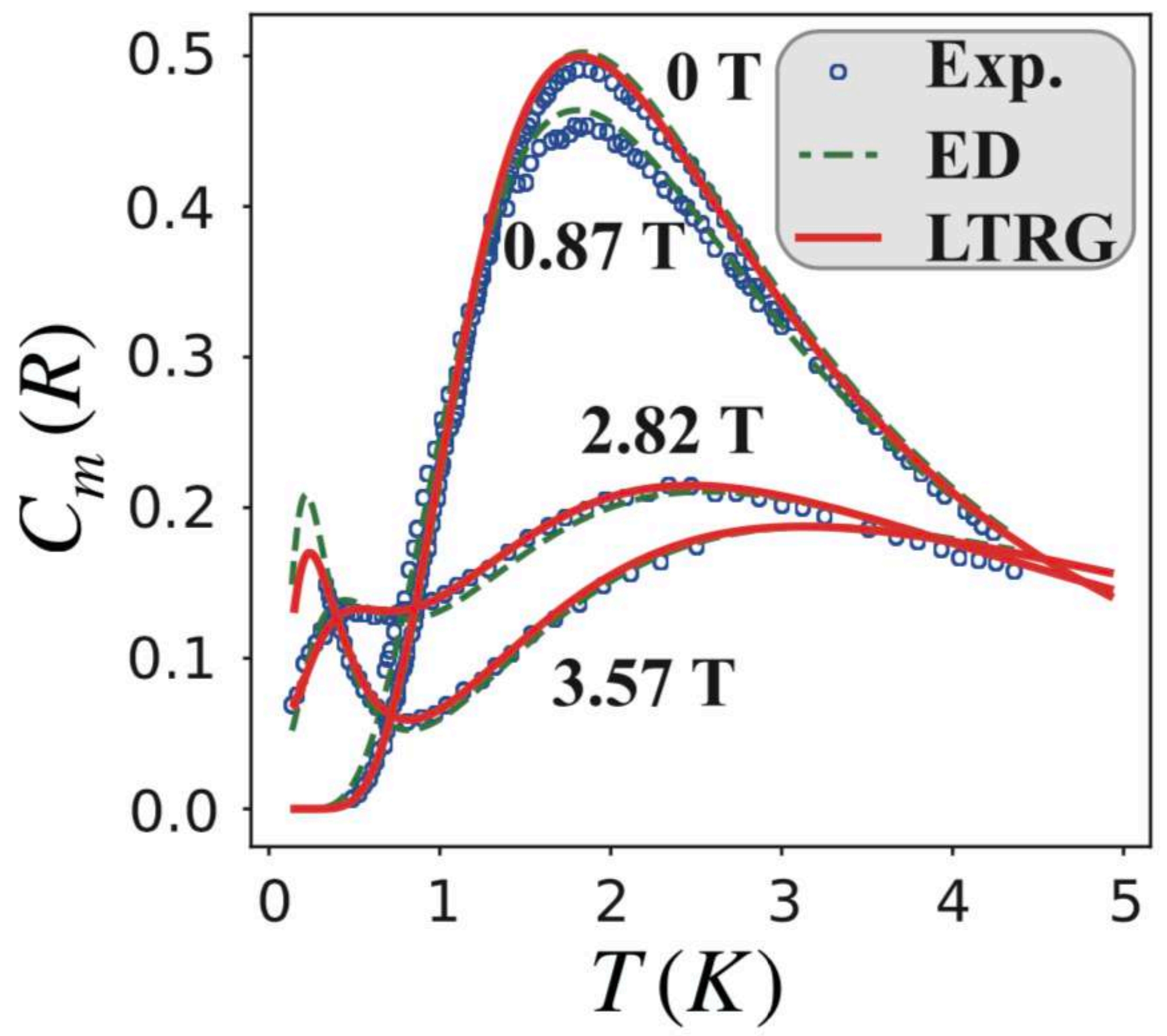
Python version

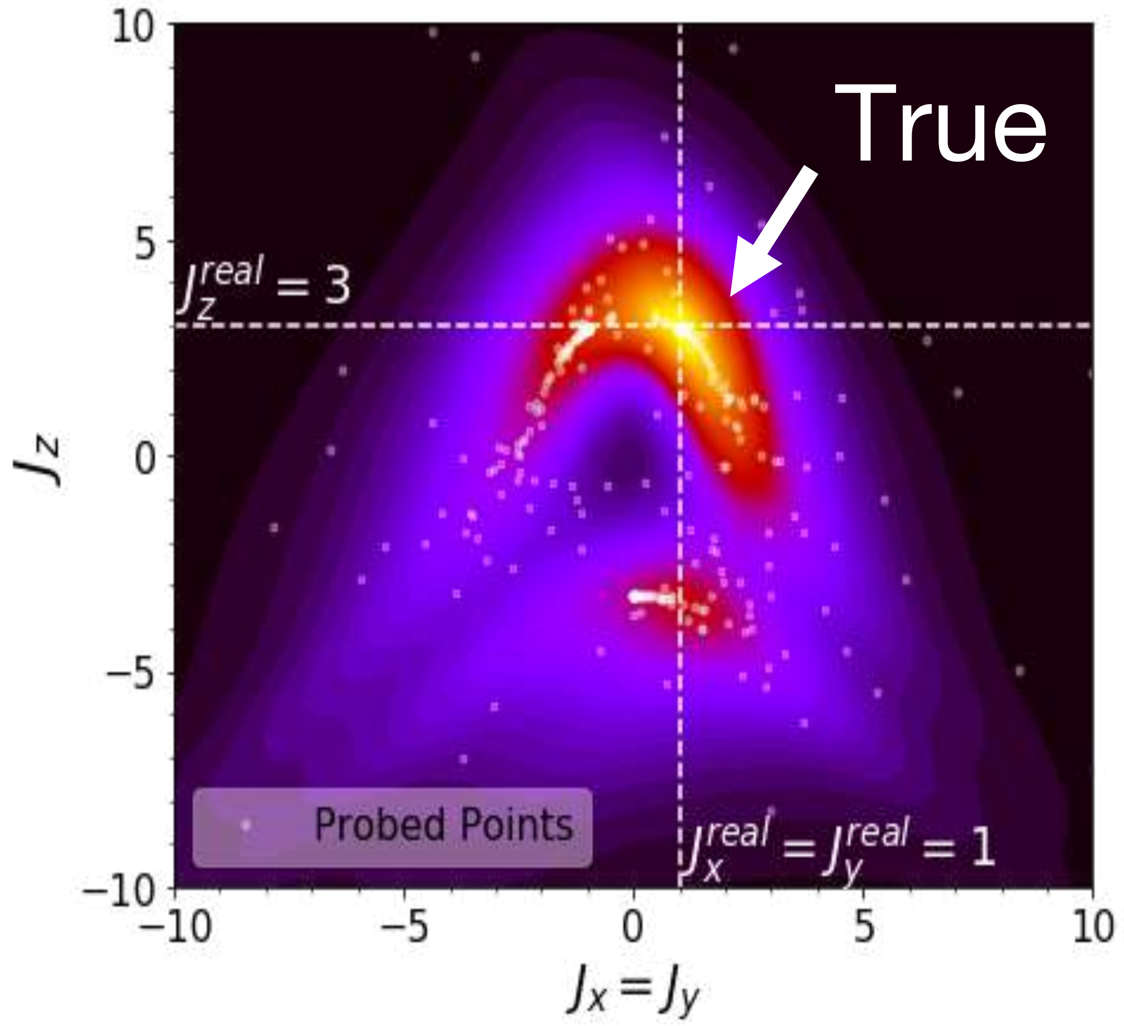


S. Yu, Y. Gao, WL, arXiv:2011.12282 (2020)

Summary

- **Tensor network solvers** + **efficient optimizers** can be used to solve the **inverse many-body problem**
- ***QMagen***: *uniform framework for the many-body analysis of thermal data, and search for spin liquids*





Thank you for your attention!

S. Yu, Y. Gao, WL,
arXiv:2011.12282 (2020)