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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Collaborators

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https://github.com/QMagen
Quantum Spin Liquid Candidates

Kitaev materials

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

Fu, et. al., Science 2015
Cu₃Zn(OH)₆FBr, CPL 2018

Y. Li, et. al., PRL 2015

YbMgGaO₄

AReCh₂: 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,

There are debates in these quantum materials …

How to decode the “DNA” of quantum magnets?

Spin Hamiltonian and interaction parameters
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**

- **Thermal data**

  - Forward
  - Inverse

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

- **Optimizer from Machine Learning**
Thermal Tensor Networks

- Linearized Tensor Renormalization Group (LTRG)

Directly in the thermodynamic limit

WL, S.-J. Ran, […], Gang Su, PRL 2011
Y.-L. Dong, […], WL, PRB 2017
Exponential Tensor Renormalization Group (XTRG)

- 2D Quantum Ising (up to 162-sites)
  - H. Li, [...], WL, PRB 2019

- Triangular-lattice Heisenberg
  - Rawl, et al., WL, PRX 2018

- Square-lattice Heisenberg
  - u_g^* ≈ -0.6694(4), m_s^* ≈ 0.30(1)

- 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.**
Automatic Gradient

computational graph \( x \to H \to Z \to O_\alpha \to \mathcal{L} \)

\[ \frac{\partial H}{\partial x} \xrightarrow{\text{many-body solver}} \frac{\partial Z}{\partial H} \xrightarrow{\text{O}_\alpha} \frac{\partial \mathcal{L}}{\partial \text{O}_\alpha} \xrightarrow{\text{loss}} \frac{\partial \mathcal{L}}{\partial x} \equiv \bar{x} \]

Define the loss:

\[ \mathcal{L}(x_i) = \sum_\alpha \frac{1}{N_\alpha} \lambda_\alpha \left( \frac{O_{\alpha}^{\text{exp}} - O_{\alpha}^{\text{sim}}}{O_{\alpha}^{\text{sim}}} \right)^2 \]

\[ \frac{\partial \mathcal{L}}{\partial x} = \frac{\partial \mathcal{L}}{\partial O_\alpha} \frac{\partial O_\alpha}{\partial Z} \frac{\partial Z}{\partial H} \frac{\partial H}{\partial x} \]

- Derivative of fitting loss over Hamiltonian parameters

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:

\[
\mathcal{GP} : X, D \rightarrow \mu, \sigma
\]

\[
D_n = ((x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n))
\]

\[
y_{n+1} \text{ to be estimated at } x_{n+1}
\]

\[
\mu_n(x_{n+1}) = k(x_{n+1})^T K^{-1} y,
\]

\[
\sigma_n^2(x_{n+1}) = k(x_{n+1}, x_{n+1}) - k(x_{n+1})^T K^{-1} k(x_{n+1}),
\]

\[
\alpha_{PI}(x; D_n) = \mathbb{P}[\mathcal{L}(x) \leq \tau] = \Phi \left( -\frac{\mu_n(x) - \tau}{\sigma_n(x)} \right),
\]

\[
\alpha_{EI}(x; D_n) = \mathbb{E}[\tau - \mathcal{L}(x)] = (\tau - \mu_n(x))*\Phi \left( \frac{\tau - \mu_n(x)}{\sigma_n(x)} \right) + \sigma_n(x) \phi \left( \frac{\tau - \mu_n(x)}{\sigma_n(x)} \right),
\]

\[
\alpha_{LCB}(x; D_n) = \mu_n(x) - k\sigma_n(x),
\]
Gradient-based vs. Bayesian optimization (animations)

Gradient-based

Bayesian
Artificial Experimental Data

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

High-temperature solver:

10-site ED

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

- Gaussian (white) noise introduced.
YES! Parameters Retrieved

Random Grid Search  auto-gradient  Bayesian

Probed Points  Probed Points  Probed Points

Godness of Fit

Iteration

Probed Points  Max Value

Probed Points  Max Value

Probed Points  Max Value

Iteration

Iteration

Iteration
Statistical box plot of 100 experiments

Bayesian optimization has the overall best performance.
High-Temperature Solver: \textit{Varying }\ T_{\text{cut}}

\[
J_{\chi}^2 + J_{\gamma}^2 + J_{\zeta}^2 = J_{\text{eff}}^2
\]

\(J_{\text{eff}}\) reveal the coupling strength!

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

Ground truth: \(J_{xy} = 1, J_z = 1.5\)

\textit{fitting is robust}
High-Temperature Solver: including more thermal data

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

\[ J_{xy} = 1, J_z = 1.5 \]

\[ J_{xy} = 1 \] found!
Realistic Materials
Realistic materials: Spin-chain compound Copper Nitrate

HAFC with alternating couplings

\[ H = J \sum_{n=1}^{L/2} (S_{2n-1} S_{2n} + \alpha S_{2n} S_{2n+1}) - \sum_{m=1}^{L} \sum_{\nu=\{||,\perp\}} g_{\nu} B_{\nu} S_{m}^{\nu}, \]

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

Machine fitting (with LTRG): $J = 5.16$, $\alpha = 0.227$, $\Delta = 1.01$, $g = 2.23$ with $\mathcal{L} = 7.4 \times 10^{-4}$. 

Previous hand-tuned fitting: $J = 5.13$, $\alpha=0.23$, $\Delta=1$, $g=2.31$, with $\mathcal{L} =8.2\times 10^{-4}$.
Triangular-lattice Magnet
TmMgGaO$_4$
Thermodynamics and XTRG fittings to experimental results.

(a) $S_m$ (Rln2) vs $T$ (K)
- XTRG, $h=0$ kOe
- XTRG, $h=5$ kOe
- Ref. [32], $h=5$ kOe
- Ref. [32], $h=0$ kOe
- Ref. [33], $h=0$ kOe

(b) $C_m$ (J mol$^{-1}$ K$^{-1}$) vs $T$ (K)
- XTRG, $h=0$ kOe
- Ref. [32], $h=0$ kOe
- Ref. [33], $h=0$ kOe

(c) $\chi$ (cm$^3$ mol$^{-1}$) vs $T$ (K)
- XTRG, $h=1$ kOe
- XTRG, $h=10$ kOe
- Ref. [32], ZFC, $h=1$ kOe
- Ref. [32], FC, $h=1$ kOe
- Ref. [33], $h=10$ kOe

(d) $M$ ($\mu_B$ Tm$^{-1}$) vs $h$ (kOe)
- Ref. [32], T=2 K
- Ref. [32], T=1.9 K
- Ref. [33], T=2 K
- XTRG, T=1.9 K

- Two coupling strengths $J_1, J_2$
- Transverse field $\Delta$

[33] Li, et al., PRX 2020
Triangular-lattice quantum Ising model for TMGO

\[ H_{\text{TLI}} = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i^z S_j^z - \sum_i \left( \Delta S_i^x + h g_\parallel \mu_B S_i^z \right) \]

\[ J_1 = 0.99 \text{ meV}, \quad J_2 = 0.05 J_1, \quad \Delta = 0.54 J_1 \text{ and } g_J = 1.101 \]

2D quantum magnet realizing KT physics!

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 \( \text{TmMgGaO}_4 \)**

\[
H = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j' \rangle\rangle} S_i^z S_j^z - \Delta \sum_i S_i^x - g \mu_B B \sum_i S_i^z
\]
**Triangular-lattice Magnet TmMgGaO$_4$**

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

**ED**

\[ T_{\text{cut}} = 4 \text{ K} \]

**XTRG**

\[ T_{\text{cut}} = 1 \text{ K} \]

H. Li, […], WL, Nature Commun. 2020
Kitaev material $\alpha$-RuCl$_3$

- **Fitting Landscape**

- **Reproduce major exp. features**

\[ H = \sum_{(i,j)} [K S_i^\gamma S_j^\gamma + J S_i \cdot S_j + \Gamma S_i^\gamma S_j^\gamma + \Gamma' (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha + S_i^\gamma S_j^\gamma) + J' S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha + S_i^\gamma S_j^\gamma] \]
Outlook: The family of rare-earth triangular magnets

Rare-Earth Chalcogenides

\[ \text{AReCh}_2 \]

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

\[ \hat{H}_{\text{eff}} = \hat{H}_{\text{CEF}} + \hat{H}_{\text{spin-spin}} + \hat{H}_{\text{zeeman}} \]
\[ = \sum_i \sum_{m,n} B^n_m \hat{O}^n_m \]
\[ + \sum_{ij} [J_{zz} S_i^z S_j^z + J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+)] \]
\[ + J_{\pm} (\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij} S_i^- S_j^-) \]
\[ - \frac{i J_z}{2} (\gamma_{ij} S_i^+ S_j^- - \gamma_{ij} S_i^- S_j^+ + \langle i \leftrightarrow j \rangle) \]
\[ - \mu_0 \mu_B \sum_i [g_{xx} h x S_i^x + h_y S_i^y + g_c h_c S_i^z] \]

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

NaYbSe\textsubscript{2} analyzed, mean field
Open source package: QMagen

Matlab version: include ED, LTRG, and XTRG solvers

Python version

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!