Exponential Thermal Tensor Network Approach for Quantum Lattice Models

Chen et al., PRX **8**, 031082 (2018)
Chen et al., PRB **99**, 140404 (2019)
Li et al., PRB **100**, 045110 (2019)

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Outline

- XTRG (exponential thermal tensor network renormalization group)
  - Tensor network representation of thermal states for quasi-1D systems [in the spirit of 2D-DMRG, yet for finite T]
  - Entanglement in thermal states
  - Exponential energy scales and logarithmic β grid

Chen et al., PRX **8**, 031082 (2018)

- Application: 2D spin-half triangular Heisenberg model
  - Two temperature scales T_l and T_h
  - `Roton-like' excitations in intermediate regime $T_l \lesssim T \lesssim T_h$ with significant chiral component

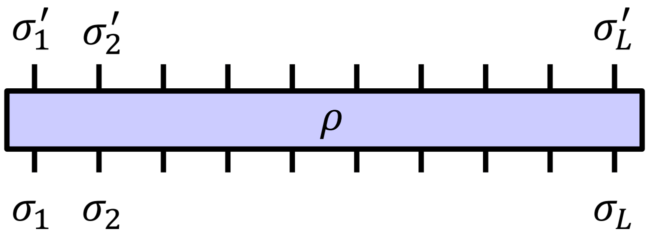
Chen et al., PRB **99**, 140404 (2019)

- Outlook: Application to DMFT?
- Summary

Tensor network representation of thermal density matrix

$$\hat{\rho}(\beta) \equiv e^{-\beta\hat{H}} = \sum_s e^{-\beta E_s}|s\rangle\langle s| = \sum_s \rho_{(\sigma_1\sigma_2\ldots\sigma_L),\,(\sigma_1'\sigma_2'\ldots\sigma_L')}|\sigma_1\sigma_2\ldots\sigma_L\rangle\langle\sigma_1'\sigma_2'\ldots\sigma_L'| \qquad (\ \sigma_i = 1,\ldots,d\ )$$

$\equiv$



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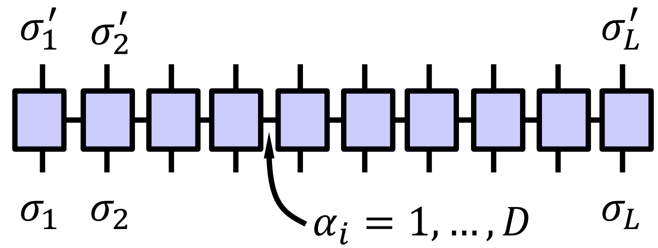
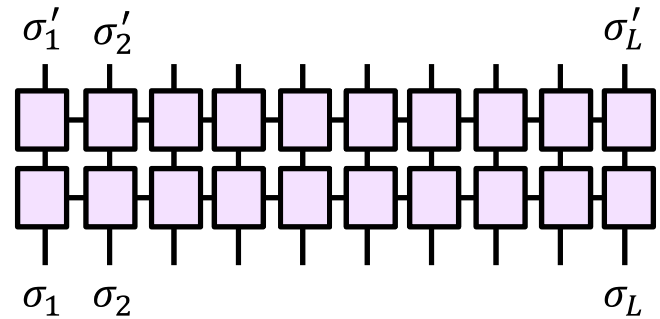


matrix product operator (MPO)

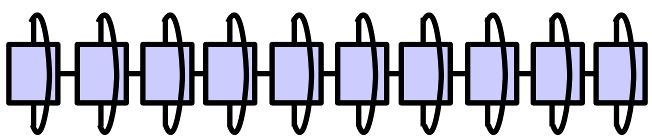
$$\hat{\rho}(\beta) = \left[e^{-\frac{\beta}{2}\hat{H}}\right]^2 = \rho\left(\tfrac{\beta}{2}\right) * \rho\left(\tfrac{\beta}{2}\right) =$$



$\equiv \hat{\Psi}^\dagger\hat{\Psi}$

always positive

$$Z = \mathrm{tr}[\hat{\rho}(\beta)] =$$



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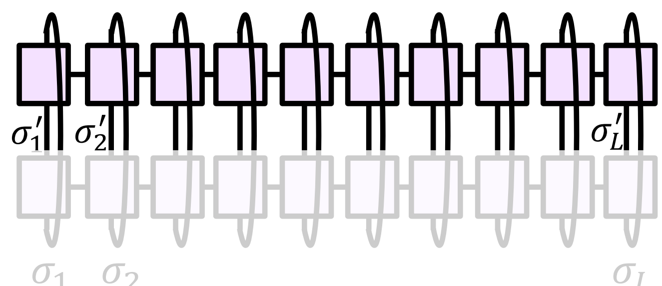


$\equiv \langle\Psi|\Psi\rangle$

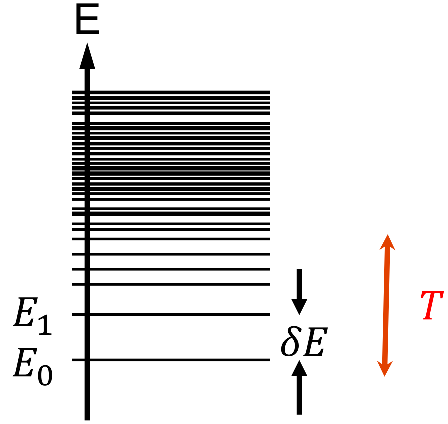
purification

$$\langle\hat{A}\rangle \equiv \frac{1}{Z}\mathrm{tr}[\hat{\rho}\hat{A}] \equiv \frac{1}{Z}\mathrm{tr}[\hat{\Psi}\hat{A}\hat{\Psi}^\dagger] \equiv \frac{1}{Z}\langle\Psi|\hat{A}|\Psi\rangle$$

Verstraete (2004)
Schollwoeck (review DMRG; 2010)
Thermofield approach (de Vega, Banuls; 2015; Schwarz et al, 2018)

Entanglement scaling in thermal states in 1D

- Many-body finite size spectrum



$$\rho(T) = \sum_s e^{-\beta E_s} |s\rangle\langle s|$$

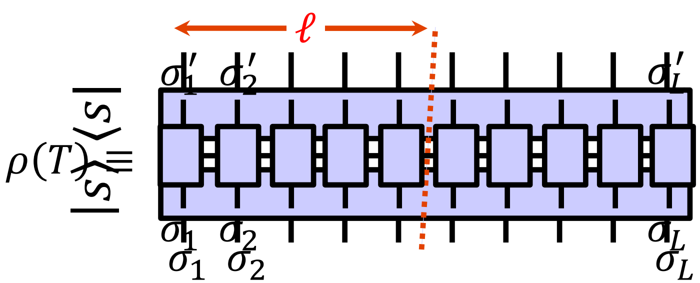
finite size level-spacing $\delta E \sim 1/L$

assuming critical systems,
or $\delta E \gg$ "gap" Δ

minimal requirement
for thermal simulations

$$\Rightarrow T \gtrsim \delta E \;\Rightarrow\; \beta \lesssim L$$

$$L \sim \beta$$



Calabrese (2004)

$$S(\ell) \sim \frac{c}{6}\log(\ell)$$

entropy of thermal state

$$\Rightarrow S(\ell) \sim \frac{c}{3}\log(\ell)$$

$$\Downarrow \;\; \ell \to \beta$$

$$S(\beta) \sim \frac{c}{3}\log(\beta)$$

More rigorous arguments based on conformal field theory (CFT)

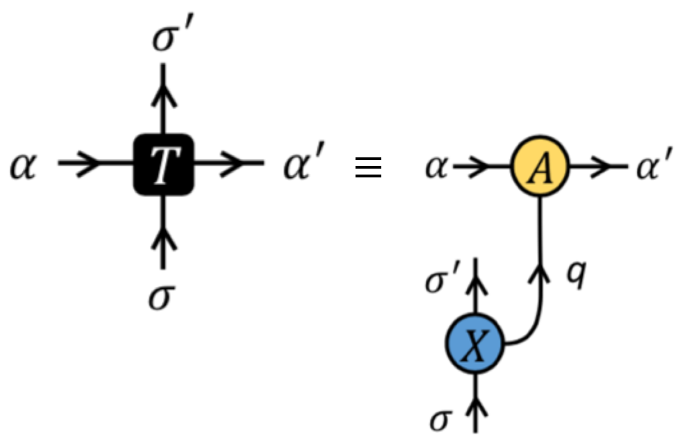
- J. Dubail [J. Phys. A: Math. Theor. **50** (2017) 234001]
- T. Barthel [arXiv:1708.09349 [quant-ph], 2017]

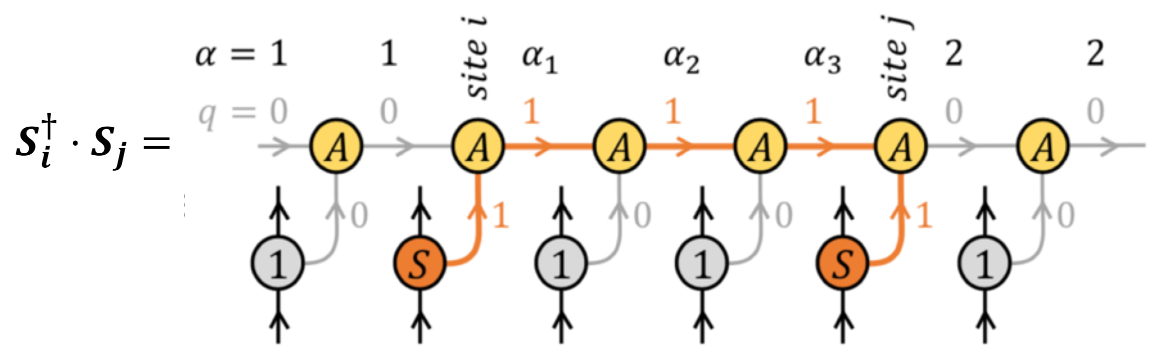
allows for efficient simulations of thermal states (comparable to simulation of pure states with periodic BC)

Implication #1: Thermal correlation length

- $S(\beta) \lesssim \frac{c}{3}\log(\beta)$ independent of L for $L \to \infty$
  - ➪ finite correlation length $(\ell = \xi) \sim \beta$ in thermal state
    - ➪ can use finite system with open BC to simulate thermodynamic limit for $\mathrm{L} \geq \xi$
      - ➪ can exploit all abelian and non-abelian symmetries in an optimal way (in the absence of spontaneous symmetry breaking)

      - ➪ a natural generalization of 2D-DMRG to finite temperatures





e.g. spin-half site: $X \in \{1, \boldsymbol{S}\}$

QSpace tensor library - AW, Ann. Phys. (2012)
Chen et al., PRX **8**, 031082 (2018)

Implication #2: Exponential energy scales

- Weak bounded growth of block entropy of thermal state $S(\beta) \sim \frac{c}{3} \ln \beta$
  - suggests that *linear* imaginary time evolution schemes are non optimal
    e.g. Trotter: $\beta \to \beta + \tau$ with $\tau \ll \beta$

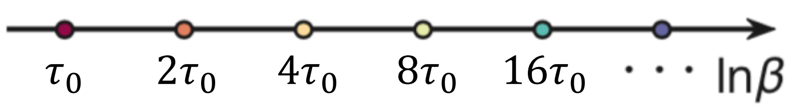
    $$e^{-H\tau} \simeq e^{-H_{even}\tau} e^{-H_{odd}\tau}$$

    small Trotter error enforces small constant τ for any β

- much more natural choice: $\beta \to \Lambda\beta \quad (\Lambda > 1) \quad \Rightarrow \quad \delta S \sim \text{const.}$
  need to make bold steps when increasing β to see a significant change
  in physical properties within a critical regime

simple choice: $\Lambda = 2$: $e^{-\beta H} * e^{-\beta H} = e^{-(2\beta)H}$

$$\hat{\rho}(\tau_0) \to \hat{\rho}(\tau_0) * \hat{\rho}(\tau_0) = \hat{\rho}(2\tau_0) \to \hat{\rho}(2\tau_0) * \hat{\rho}(2\tau_0) = \hat{\rho}(4\tau_0) \to \cdots$$



$\beta_n = \tau_0 2^n$

exponential thermal tensor renormalization group (XTRG)

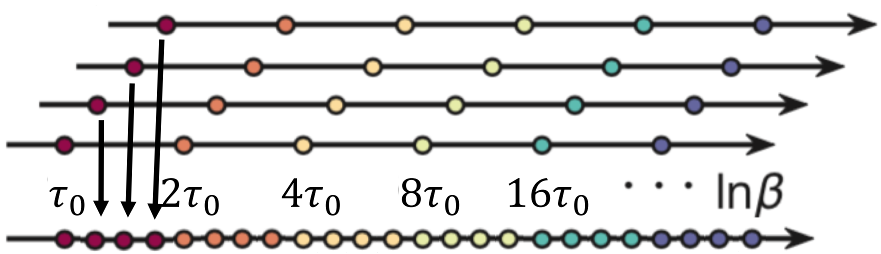
Chen et al., PRX **8**, 031082 (2018)

Benefits of logarithmic temperature grid

- Simple initialization of $\rho(\tau_0)$
  - can start with *exponentially* small τ_0 such that $\rho(\tau_0) = e^{-\tau_0 H} = 1 - \tau_0 H$
  - simply use the MPO of H $\Rightarrow$ up to minor tweak, *same* MPO for $\rho(\tau_0)$
- No Trotter error
  - simply applicable to longer range Hamiltonians
  - no swap gates to deal with Trotter steps
  - including (quasi-) 2D systems

Earlier Trotter based schemes, e.g.
Xie et al. (PRB 2012)
Czarnik et al. (PRB 2015)

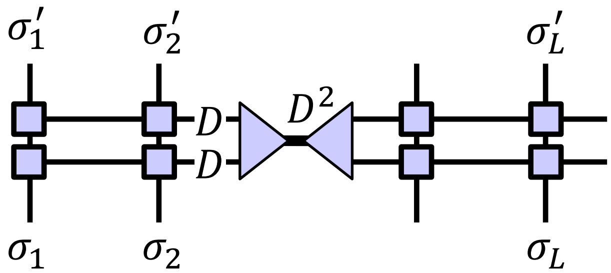
- Maximal speed to reach large β with minimal number of truncation steps
- Fine grained temperature resolution?
  - Yes! using temperature grids starting from shifted $\tau_0 \to \tau_0 2^z$ with $z \in [0,1[$



  - simply combine interleaved data sets
  - trivially parallelizable

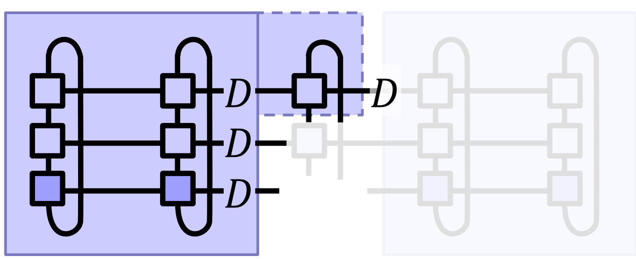
Numerical cost of XTRG

- Naively



SVD → $O(D^6)$

- Variationally: $\left\|\rho_\beta * \rho_\beta - \tilde{\rho}_{2\beta}\right\|^2 \rightarrow min$



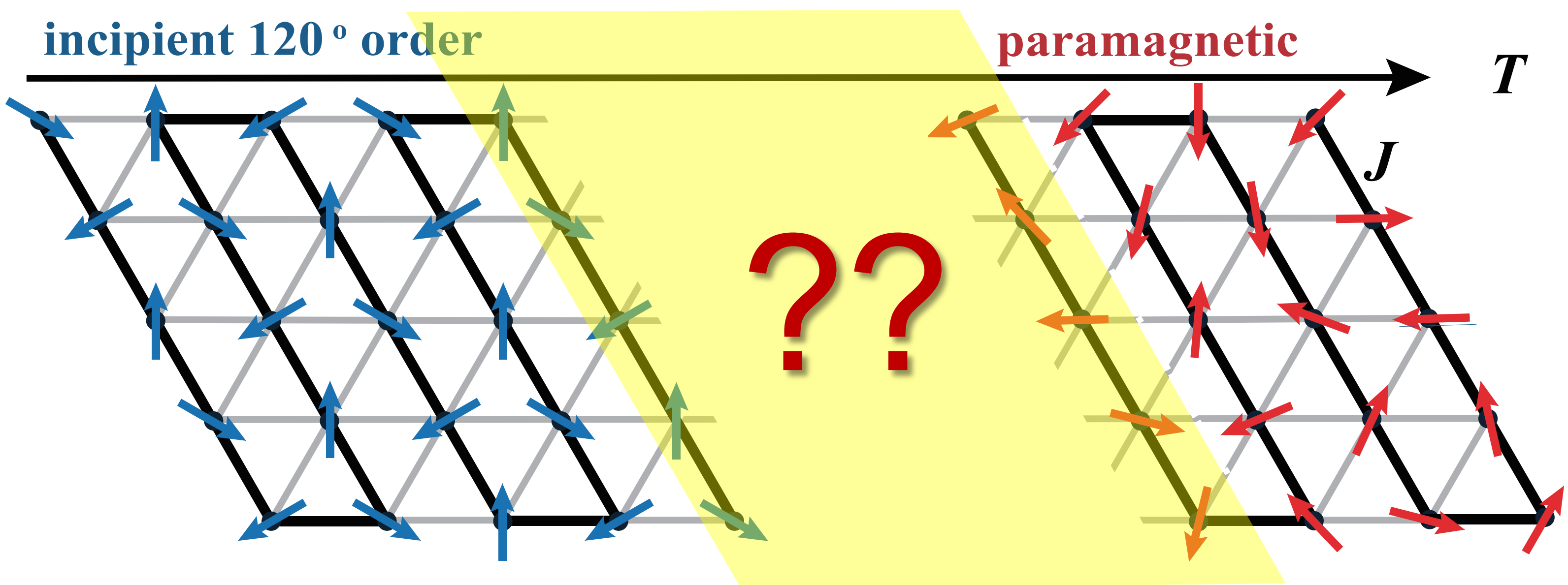
overlap → $O(D^4) \xrightarrow{\times \sim 100} O((D^*)^4)$

- Computational gain by using symmetries: D states → D^* multiplets
  e.g. SU(2) spin-half Heisenberg: $D^* \simeq D/4$

Application: 2D triangular Heisenberg model (S=1/2)

Chen et al.,
PRB **99** (2019)

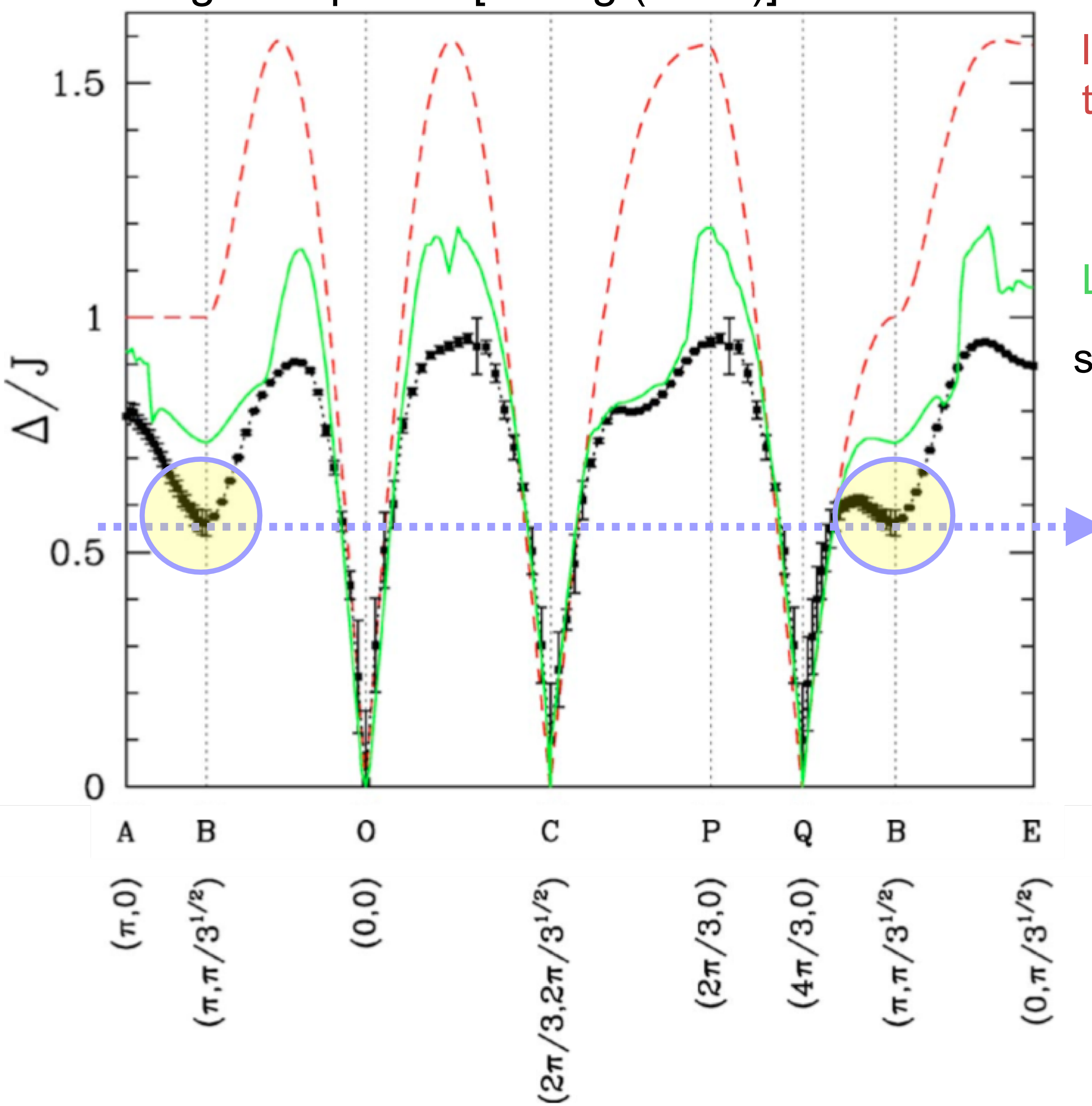
- What is known (theory)
  - 120° magnetically ordered state at T=0: $M_0 = 0.205(15)$, [White et al. (2007)]
  - paramagnetic at large T
  - problem [Kulagin et al (2013) using `sign-blessed' BDQMC]:
    data extrapolates to disordered, i.e., *non*-magnetic state for $T \to 0$!?

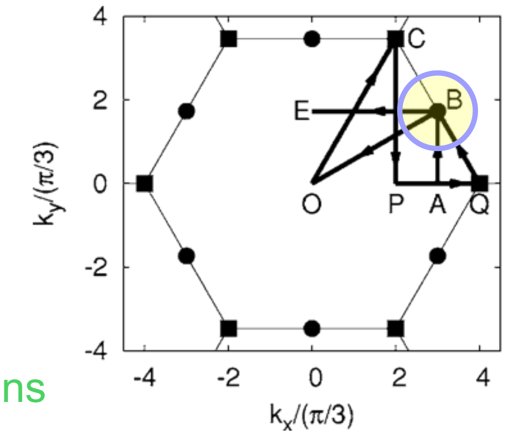


Roton-like excitations in the TLH

Zheng et al., PRB (2006)
Starykh et al., PRB(R) (2006)

Magnon spectra [Zheng (2006)]





linear spine wave theory (LSWT)

LSWT + 1/S corrections

series expansion

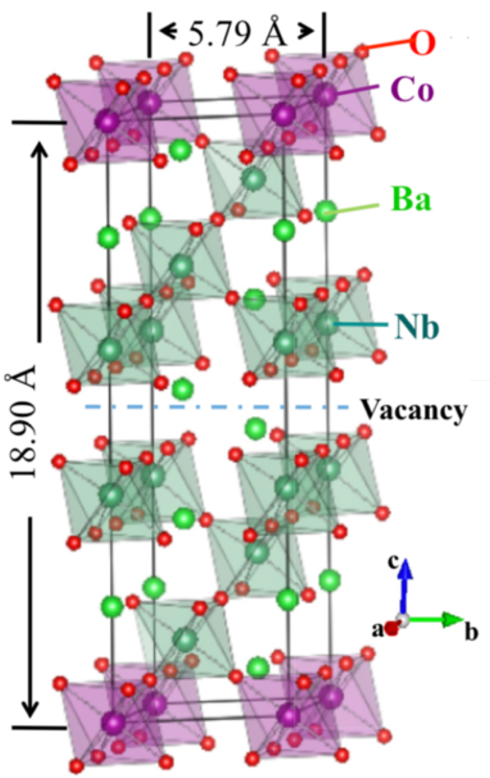
effective \`massive' quasiparticles at finite energy with $\Delta \simeq 0.55$

Zheng (2006): *We have called this feature a "roton" in analogy with similar minima that occur in the excitation spectra of super-fluid ^{4}He and the fractional quantum Hall effect.*

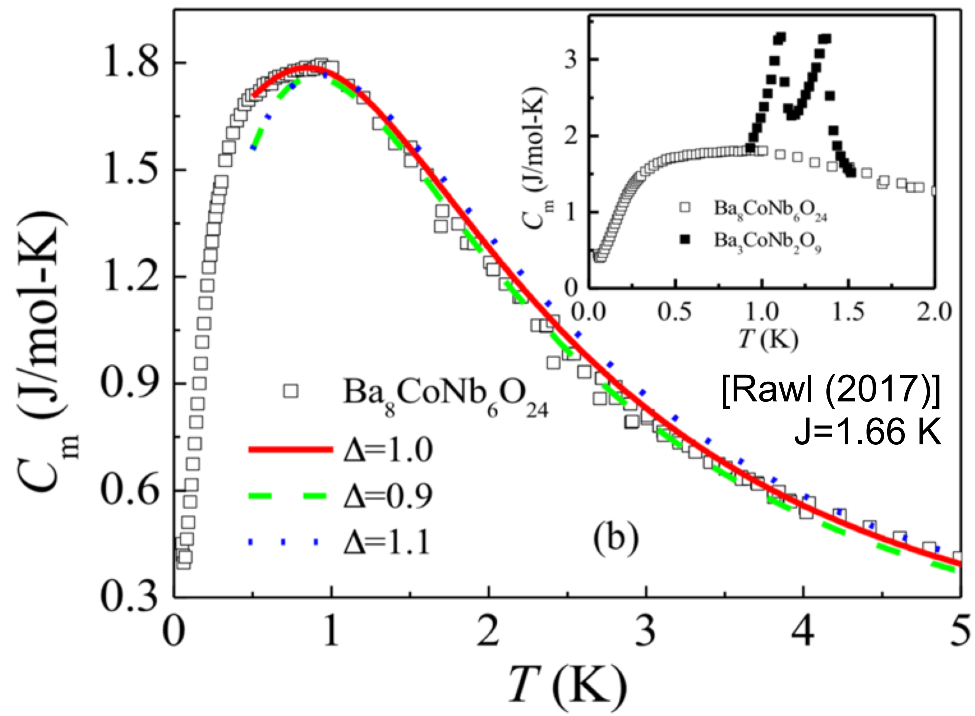
Experimental progress

- $Ba_8CoNb_6O_{24}$ - close to ideal 2D triangular Heisenberg material!
  - Perovskite, first synthesized by Mallinson et al. (Angew. Chem. Int. Ed., 2005)
  - *equilateral effective spin-1/2 Co2+ triangular layers separated by six nonmagnetic layers.*
  - [Rawl et al., 2017] *A spin-1/2 triangular Heisenberg antiferromagnet in the 2D limit*
  - [Cui et al., 2018] *Mermin-Wagner physics, (H,T) phase diagram, and candidate quantum spin-liquid phase in the spin-1/2 triangular antiferromagnet $Ba_8CoNb_6O_{24}$*

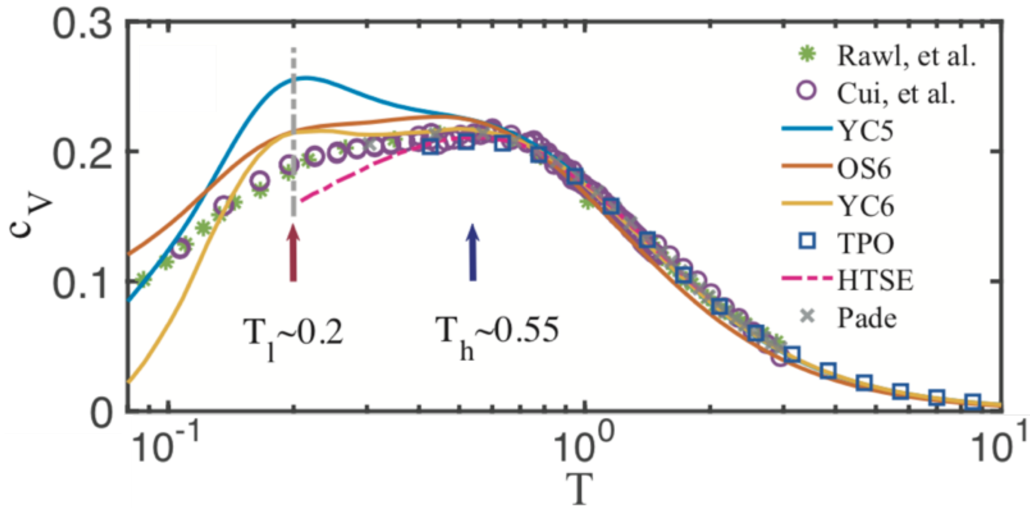
$Ba_3CoNb_2O_9$: 7.23Å
(2 non-magnetic layers)

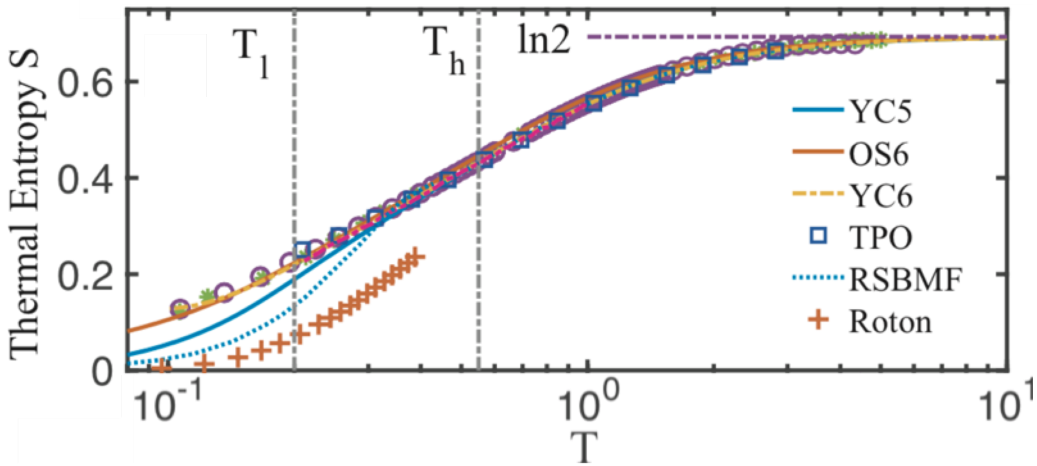


magnetic contribution to specific heat
(by ref. to non-magnetic compound $Ba_8ZnTa_6O_{24}$)



XTRG data





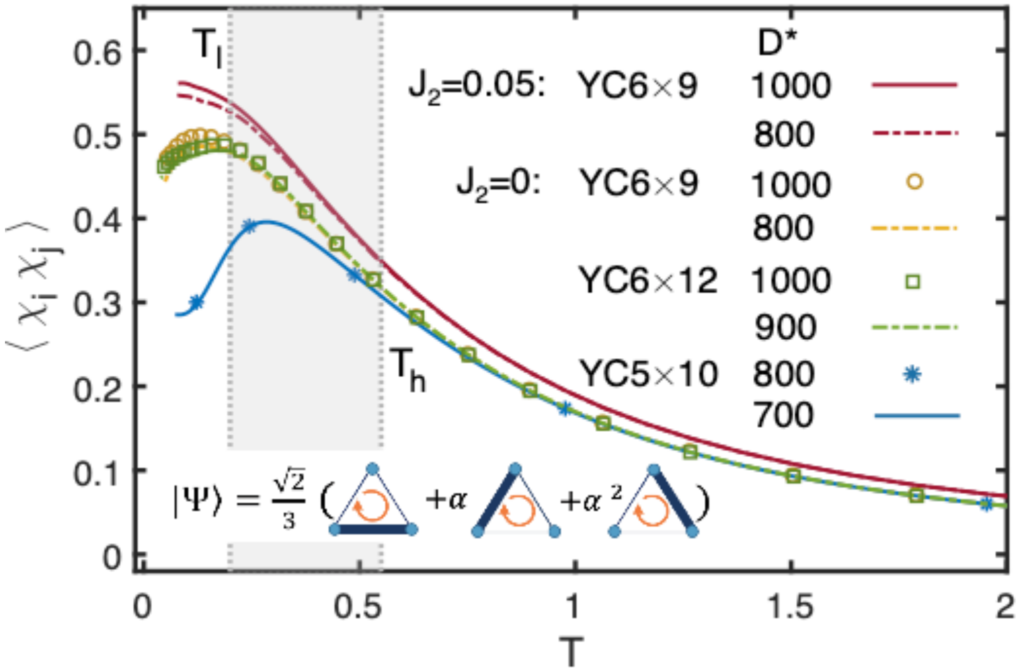
For sufficiently large system sizes

- consistently, two energy scales $T_l \simeq 0.2$ and $T_h \simeq 0.55$
- in agreement with experiment ("thermodynamic limit")

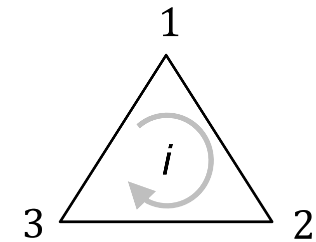
- `roton' contribution only relevant for $T \gtrsim T_l$
- strongly enhanced thermal entropy for $T \lesssim T_l$ due to frustration

TPO . . . tensor product operator method (complimentary to XTRG)
RSBMF . reconstructed Schwinger boson mean field [Mezio et al, NJP (2012)]
Roton . . roton contribution only [Zheng et al, PRB (2006)]
HTSE . . high temperature series expansion (Elstner et al, PRL (1993)]
Pade . . a particular way to deal with the low-T divergence of the partition function in HTSE [Rawl (2017)]

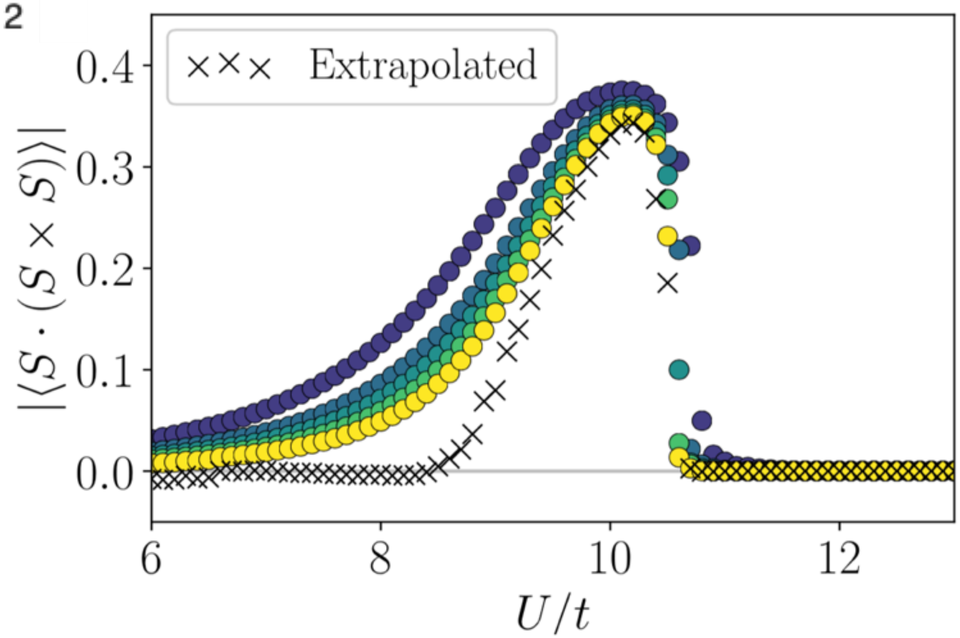
Significant chiral component in intermediate regime



$\chi = \langle S_1 \cdot (S_2 \times S_3) \rangle$



For comparison:
triangular lattice Hubbard model at T=0
[Szasz et al., condmat (2018)]



- significant chiral component in intermediate regime!
- chiral contribution cutoff only at $T \lesssim T_l$

Outlook: Application to DMFT?

- Computing Matsubara Greens function

$$G(i\omega_n) = \int_0^\beta d\tau \, e^{i\omega_n \tau} G(\tau)$$

with $G(\tau) = \langle \hat{c}(\tau)\hat{c}^\dagger \rangle_T = \frac{1}{Z}\mathrm{tr}\big(\underbrace{e^{-(\beta-\tau)\hat{H}}}_{=\hat{\rho}(\beta-\tau)} \; \hat{c} \; \underbrace{e^{-\tau\hat{H}}}_{=\hat{\rho}(\tau)} \; \hat{c}^\dagger\big)$ $\rightarrow \frac{1}{Z}\mathrm{tr}(\hat{\rho}_n \hat{c} \hat{\rho}_{n'} \hat{c}^\dagger)$

  - compute in parallel on fine-grained z-interleaved grid $\beta_n = \tau_0 2^{z+n}$ with $z \in [0,1[$
  - interpolate for integral in $G(i\omega_n)$
  - exact, well-controlled, no sign problem
  - wide flexibility in tensor-network setup
  - larger temperatures always accessible, also for multi-orbital setups

  - Q. comparison of efficiency / lowest accessible T with QMC?

Summary

- **XTRG** [Chen et al., PRX 2018]
  - an extremely simple, yet efficient and accurate tensor-network approach to thermal states: $\rho \to \rho * \rho$ resulting in $\beta \to 2\beta$
  - motivated by entanglement scaling $S \sim \frac{c}{3} \log \beta$
  - no Trotterization whatsoever ⇨ no Trotter error, no swap gates, etc.
  - simply applicable to longer-range interactions (quasi-2D), truncation permitting
  - clean exploitation of all symmetries in the Hamiltonian
- **Application: Triangular lattice Heisenberg model** [Chen et al., PRB 2019]
  - Unified picture to describe crossover from high to low temperature with 2 crossover scales T_l and T_h
  - incipient 120° order for $T \lesssim T_l$
  - intermediate temperature regime dominated by roton-like excitations with significant chiral component

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