Algorithms for frustrated spin models

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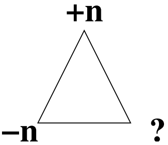
Antiferromagnetism in Mott insulators:

- Antiferromagnetic exchange interactions of magnetic ions in insulators:
  $E = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad J > 0$
- When is J>0, large? Difficult (quauntum chemistry) question, with thumb-rule answer: Goodenough-Kanamori-Anderson rules
  J.B. Goodenough, *Magnetism and the Chemical Bond (1963)*
  (exceptions known, *e.g.* Oles *et. al.* 2006)
- Sometimes possible to "measure" J: Inelastic neutron scattering in high field.
  e.g. $Yb_2Ti_2O_7$ Ross *et al.* PRX 2011

Triangles on my mind: Frustration and spin liquid behaviour

- Triangles $\rightarrow$ *frustrated* antiferromagnetism



  Competing interactions frustrate Neel order

- ‘Quenching’ of exchange allows new physics to take center-stage: Spin liquids
- Macroscopic degeneracy of *classical* minimum energy configurations.
- At intermediate $T_f < T < JS^2$, spin correlations reflect this macroscopic degeneracy:
  No Bragg peaks in structure factor $\rightarrow$ correlated liquid state

Frustration and entropic interactions

- Frustrated magnets: Large degeneracy of minimum energy configurations
- At $T \ll J$: system samples minimally frustrated subspace
  (Or falls out of equilibrium...)
- Fluctuations generate entropic interactions

Order by disorder:

- Low temperature physics dominated by entropic interactions
- Characteristic signatures in structure factor
- More dramatic cases: Order-by-thermal/quantum disorder

Sign problem in Quantum Monte Carlo

- $Z = \sum_{\mathcal{C}} W(\mathcal{C})$
- In classical stat. mech.
  $W \propto \exp(-E/k_B T) > 0$
- For quantum systems $Z = \mathrm{Tr}(e^{-H/k_B T})$
  Berry phase effects: W need not be positive
  $\rightarrow$ Exponentially deteriorating error bars

Sign problem and frustration

- Hamiltonian written as sum over links: $H = \sum_l H_l$
- $Z = \mathrm{Tr}[\exp(-H/T)] = \sum_{\alpha_0} \langle \alpha_0 | \exp(-H/T) | \alpha_0 \rangle$
- High-temp expansion:
  $Z = \sum_{n=0}^{\infty} \frac{1}{n! T^n} \sum_{\mathcal{S}_n} \langle \alpha_0 | (-H_n) | \alpha_{n-1} \rangle \langle \alpha_{n-1} | (-H_{n-1}) | \alpha_{n-2} \rangle \ldots \langle \alpha_1 | (-H_1) | \alpha_0 \rangle$
  Stochastic series expansion (SSE): Sample sum over *operator-strings* $\mathcal{S}_n$ of length n with weight above. (Sandvik 1991)
- Every $J > 0 \rightarrow$ minus sign

Periodicity, closed-loops and the overall sign

- Overall sign insensitive to $|\alpha\rangle \to e^{i\gamma(\alpha)}|\alpha\rangle$
  no quick fix...
- Diagonal matrix elements can always be shifted to make sign positive
- Off-diagonal “hops” control sign
- Constrained by periodicity in τ and lattice structure

(Sign) Problems and "Solutions"...

- Notorious problems:
  $H = \sum_{\langle rr' \rangle} \vec{S}_r \cdot \vec{S}_{r'}$ on Kagome, triangular lattices
  $d = 2$ square lattice Hubbard model away from half-filling
- Some "solutions":
  1. Looking under the (Ising) streetlamp: Frustrated exchange couplings only involving one component of spins
  2. Clever change of simulation basis...?
  3. Finessing the problem: Effective field theory/Hamiltonian description of low-energy physics can be numerically tractable
  4. Identifying symmetries that cancel -ve signs in pairs

Very difficult even if sign-free!

- Quantum and thermal fluctuations determine nature of low temperature phase & excitations
- Computational scheme needs to be ergodic within macroscopically degenerate minimally frustrated subspace
- Also needs to capture thermal fluctuations out of minimally frustrated subspace

Ideas that help: Clusters, worms, and loops.

- Cluster constructions (Wolff, Swendsen & Wang) identify and update large regions that "want to" move together (Accurately capture the physics of large correlation lengths associated with ferromagnetic criticality)
- Worm constructions (Evertz & Wiese; Prokofev & Svistunov) identify a one-dimensional cascade of moves that take system out of physical (constrained) configuration space (When worm closes on itself, system returns to physical subspace, but with large changes in configuration)
- Dual (loop) representations Bond-variables often more convenient (Hitchcock, Sorensen, Alet . . .)

Issues

- Key challenge for clusters and worms:
  Are clusters rejected with significant probability?
  Do worms/clusters reflect underlying physics?
- Composition of clusters should reflect long-wavelength correlations of the system...
  Algorithm needs to “know” of the physics of geometric frustration?

Example of sign-free but challenging models

- Ising models of quantum frustration (Moessner-Sondhi 2000)
  Triangular lattice Ising antiferromagnet in a transverse field
  $H_{\mathrm{TFIM}} = J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x + \ldots$
- Quantum cluster algorithm available in SSE representation for unfrustrated quantum Ising models
  (Sandvik 2003)

Challenge: Low but not zero temperatures

- Classical frustrated Ising models:
  Thermal fluctuations need to be captured in efficient way
  Standard (Wolff-inspired) classical cluster constructions accurately reflect long-wavelength physics of ferromagnetic correlations, but not of frustration
  Coddington & Han 1994, Zhang and Yang 1994
- Frustrated transverse field Ising models
  Quantum cluster algorithm reduces to variant of Swendsen-Wang clusters in $\Gamma = 0$ limit $\rightarrow$ frustrated J_{ij} again cause problem at low temp.
  Need to "teach" cluster algorithms structure of minimally frustrated landscape(?)

Difficult even in classical case

- Dual worm construction (Wang,Sterck & Melko 2012) Uses worms to update dual variables (*a la* Hitchcock,Sorenson,Alet 2004)
- Works when $T = 0$ limit is dual to non-interacting dimers
- Involves rejection of significant fraction of worms

Our recent progress

- Quantum cluster construction for *frustrated* TFIM
  (Sounak Biswas, R. Geet, & KD, unpublished)
- Stochastic Series Expansion Quantum Monte Carlo in basis of total spin eigenstates of clusters of spins
  (F. Alet, KD, & S. Pujari, unpublished)
- Cluster algorithm for frustrated two-dimensional $H_{\rm Ising}$ with up to third neighbour interactions
  (KD & R. Geet, unpublished)

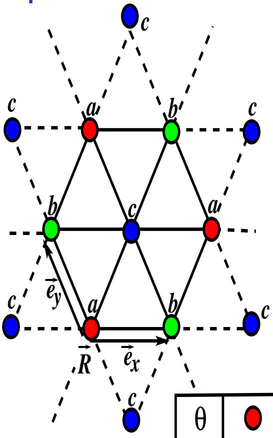
Ingredients

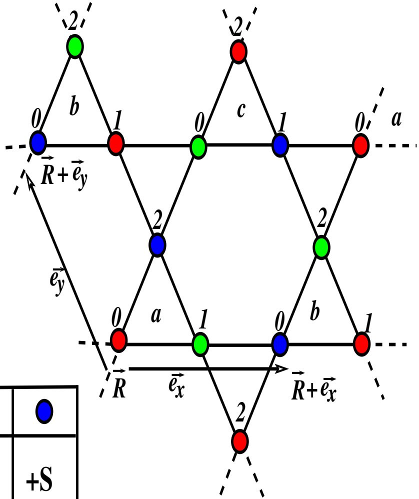
- Cluster constructions
- (Dual) “loop-like” (dimer) representations
- Directed worm constructions

Quantum cluster algorithm for frustrated TFIM

- Example: Transverse field Ising antiferromagnet on triangular lattice (also with further neighbour (J_2, J_3) couplings...)
- Interesting physics questions
  Thermodynamic signature of two-step melting of three-sublattice order
  Transition from plaquette to columnar three-sublattice order

Order parameter





θ	🔴	🟢	🔵
0	−S	+S	+S
$\frac{\pi}{6}$	−S	0	+S

For triangular lattice: $\Psi = \sum_r e^{i\mathbf{Q}\cdot r}\sigma_r^z$

Columnar vs Plaquette type orders

$\Psi = |\Psi| e^{i\theta}$

$\theta = 2\pi m/6$: Columnar three-sublattice order ($m = 0, 1, 2 \ldots 6$)

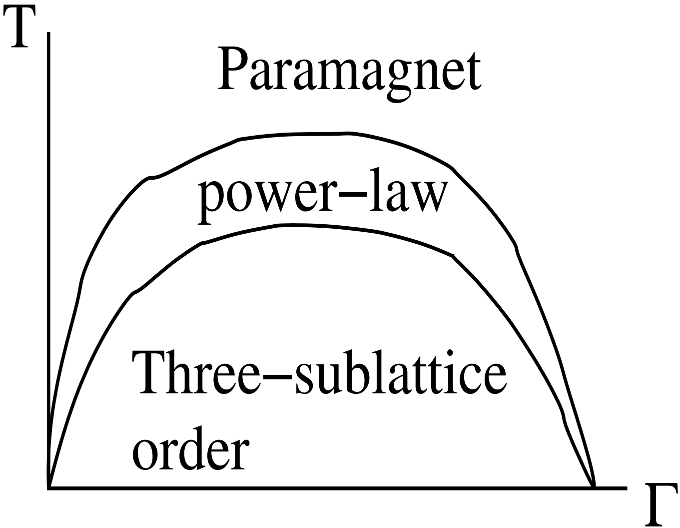
$\theta = (2m + 1)\pi/6$: Plaquette three-sublattice order ($m = 0, 1, 2 \ldots 6$)

In ordered state: θ pinned to these values

Columnar phase is ferrimagnetic $m \propto \cos(3\theta)$

In power-law phase: θ has gaussian fluctuations with no pinning

Physics summary



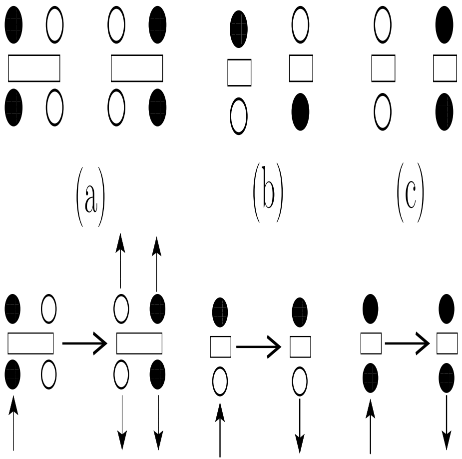
(Isakov & Moessner 2003) for $J_2 = 0$

(D. P. Landau 1985) for J_2 ferromagnetic

Conventional quantum cluster algorithm

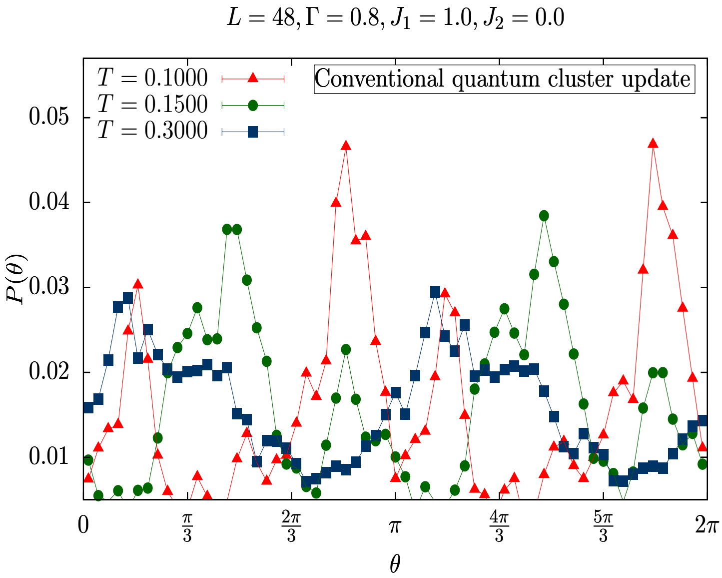
$H_{\text{TFIM}} = \sum_{\text{link}} H_{\text{link}} + \sum_{\text{sites}} H_{\text{sites}}$
trick: $H_{\text{site}} = -\Gamma\sigma^x_{\text{site}} - \Gamma\mathbf{1}_{\text{site}}$

Conventional quantum cluster algorithm

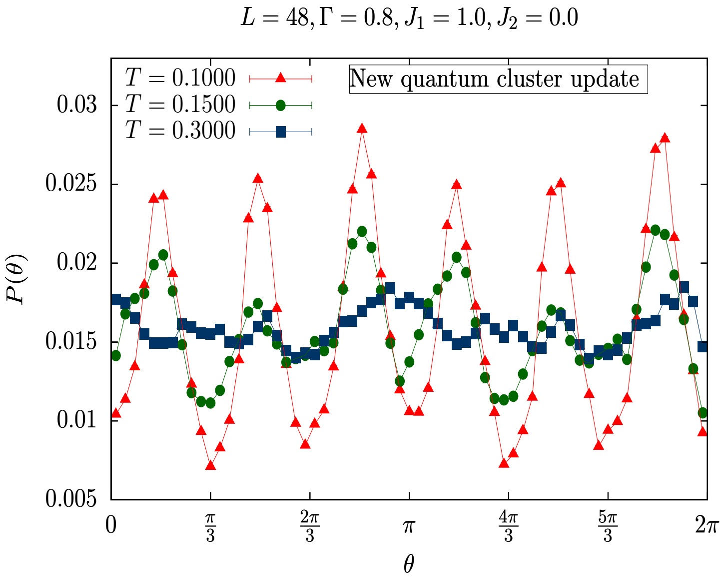


: Also add or remove diagonal operators to change length of operator string

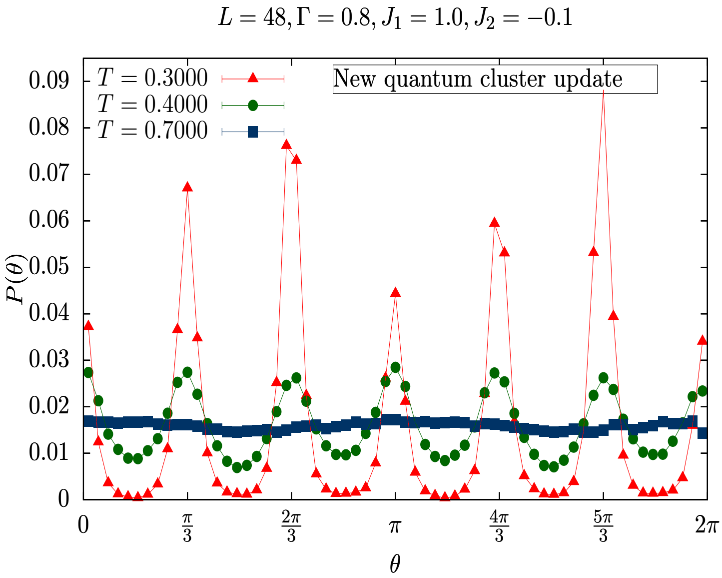
Loss of ergodicity in conventional approach



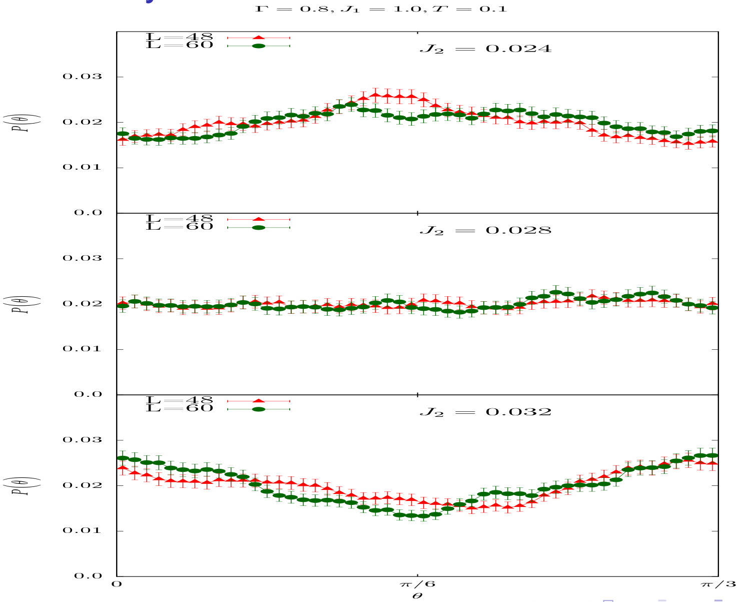
Improvement achieved:



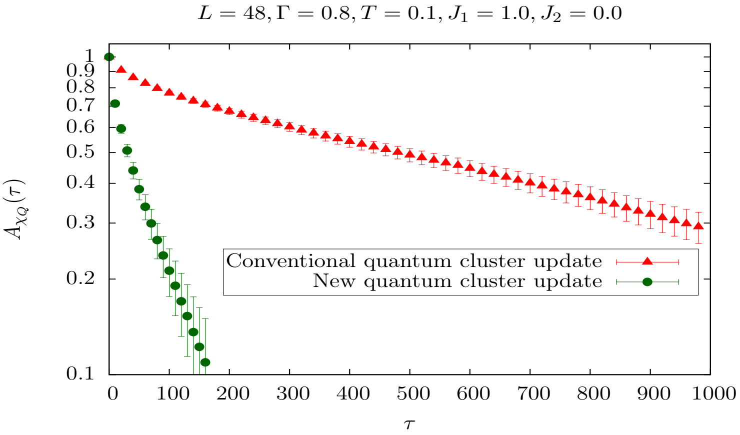
Clean signature of ferrimagnetic phase



Pinpointing transition to ferrimagnetic phase algorithmically



Improvement achieved:



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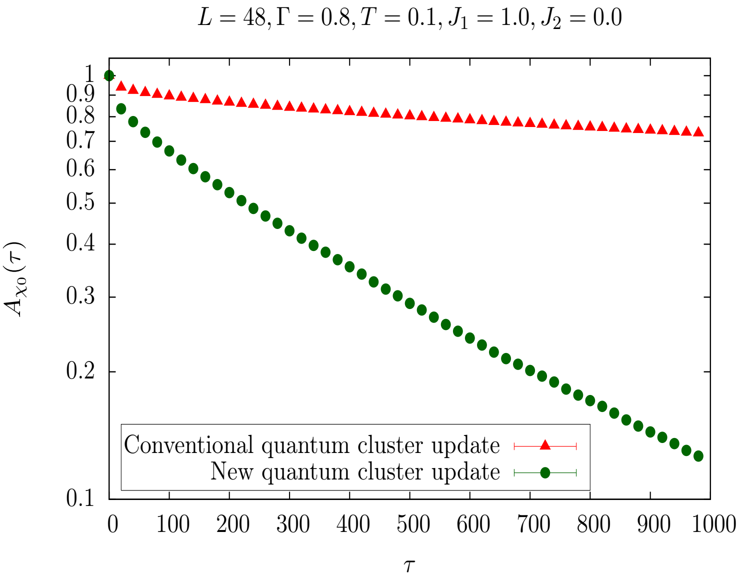

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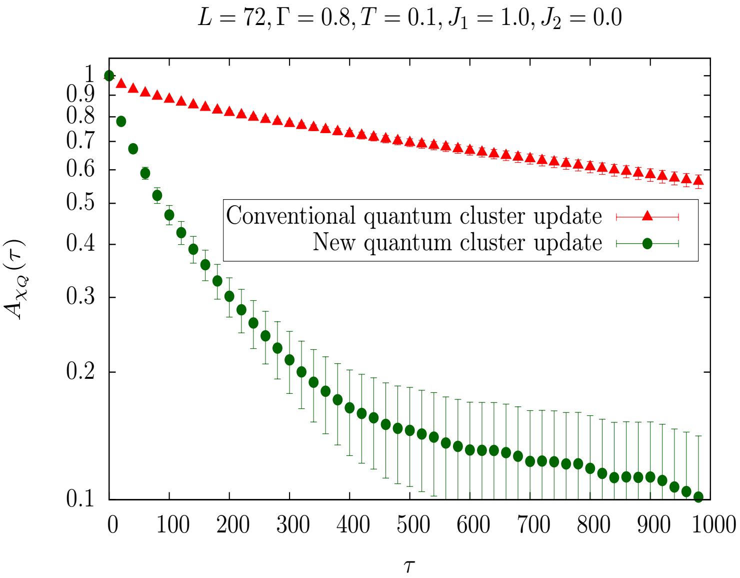

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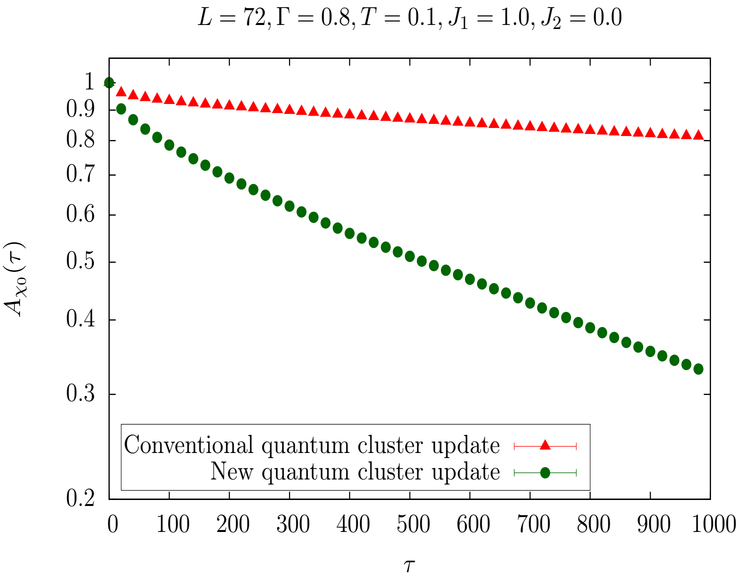


How: Our approach

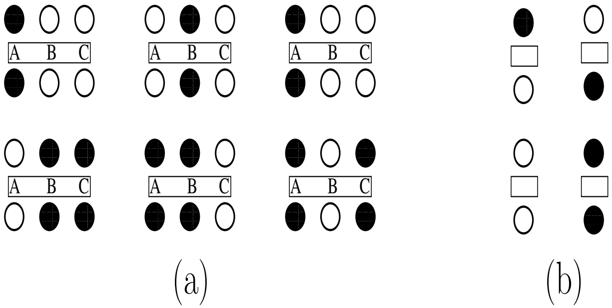
$H_{\text{TFIM}} = \sum_{\Delta} H_{\Delta} + \sum_{\text{link}} H_{\text{link}} + \sum_{\text{sites}} H_{\text{sites}}$

H_{Δ}: Triangle decomposition of all antiferromagnetic couplings

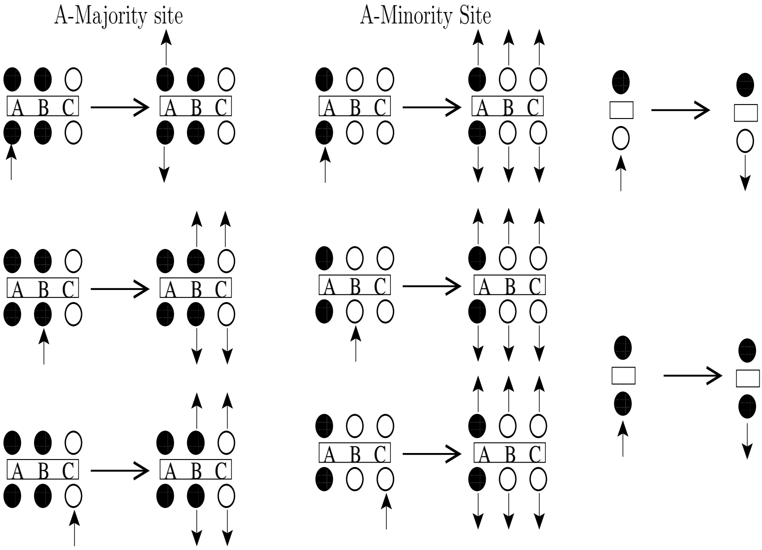
H_{Link}: Bond decomposition of all ferromagnetic couplings

H_{sites}: site decomposition of transverse field term

Quantum-cluster construction for frustrated TFIM

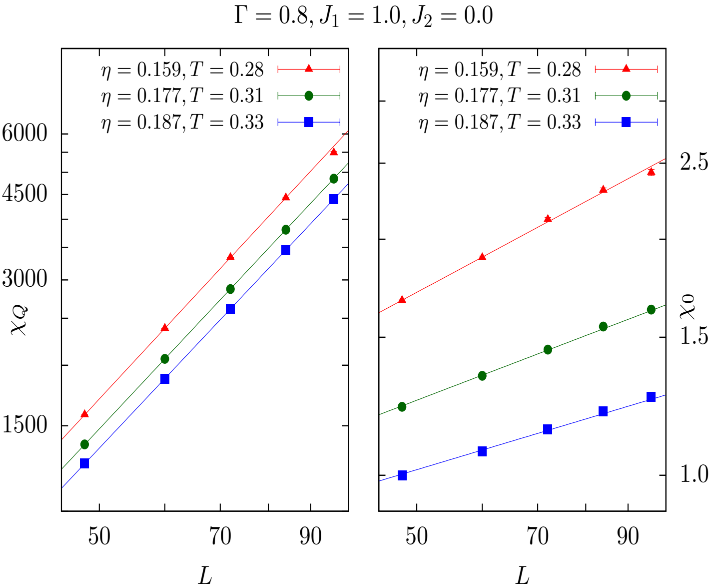


Quantum-cluster construction for frustrated TFIM

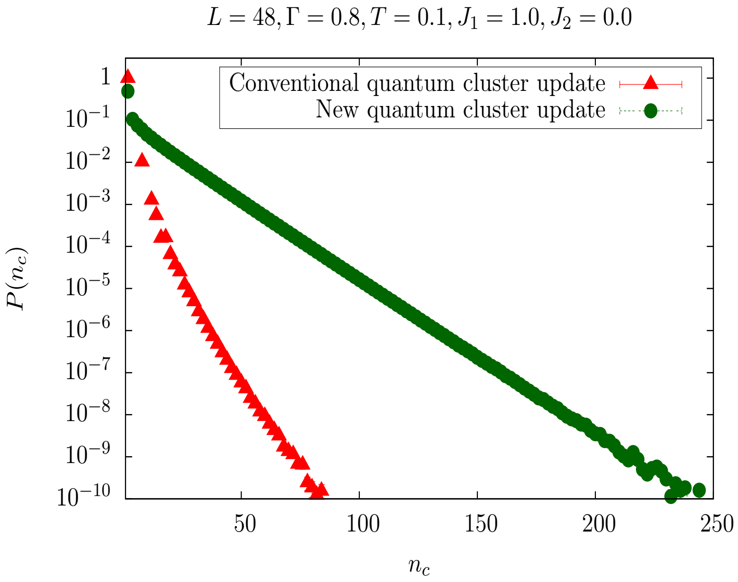


‘A’ Update

Physics: Divergent ferromagnetic susceptibility of antiferromagnet



Why does it work?



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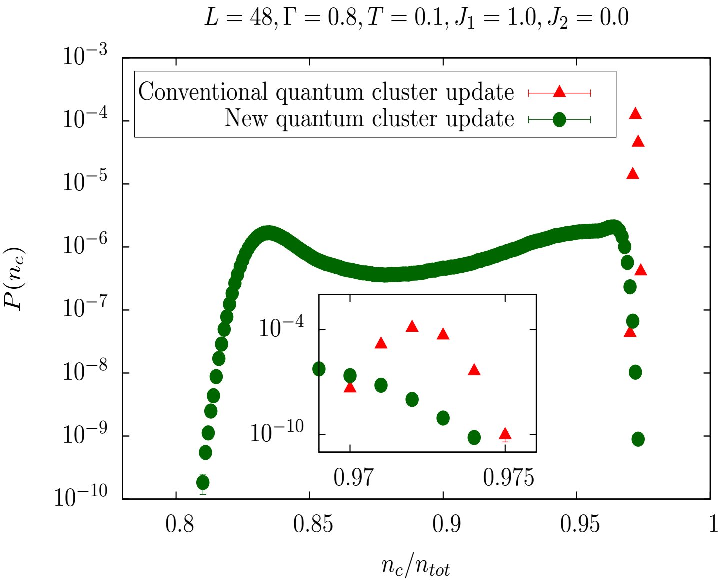

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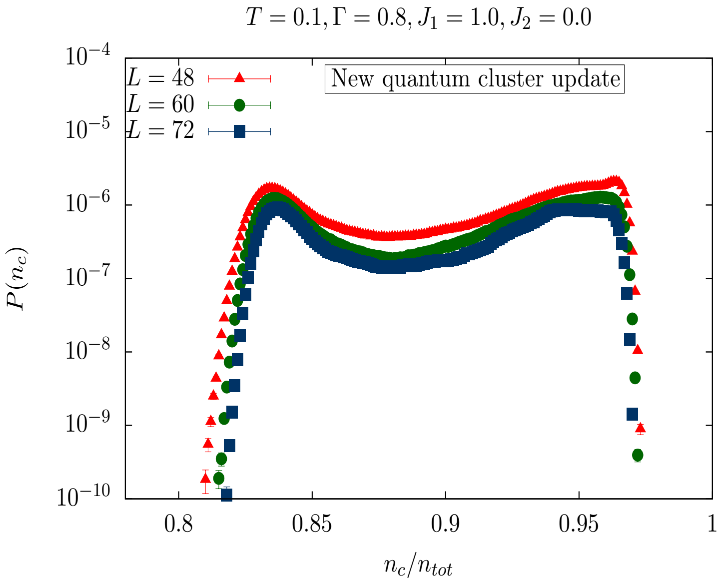

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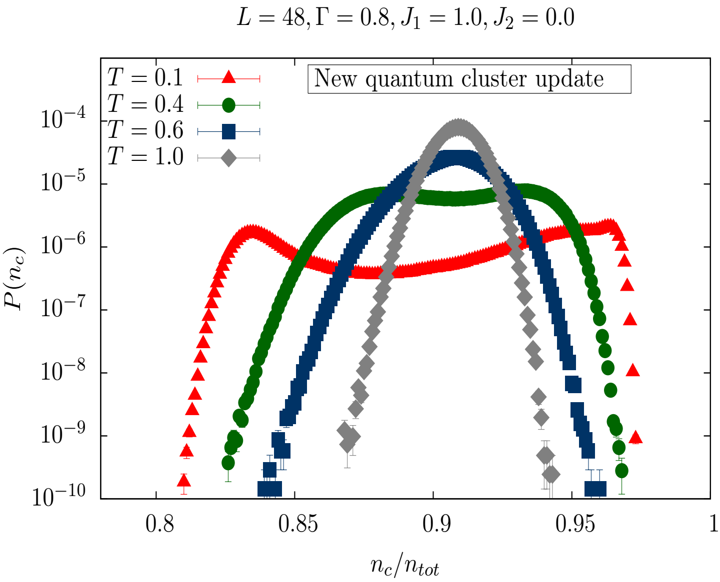
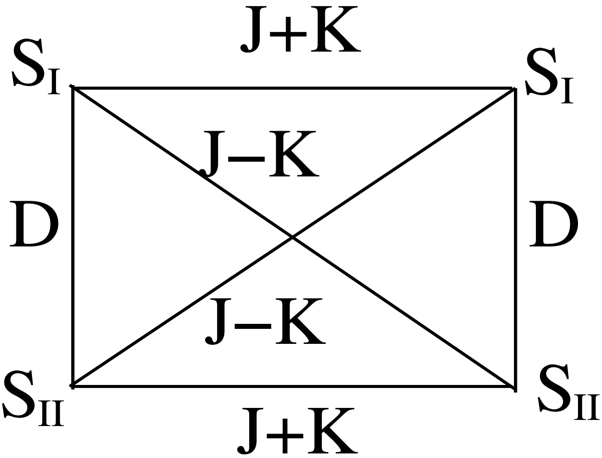


Solution of sign problem for frustrated bilayer magnets

- $\vec{S}_{\mathrm{I}r}$ and $\vec{S}_{\mathrm{II}r}$ located on the two *layers* at sites r of a bipartite Bravais lattice in any spatial dimension



General frustrated bilayer Hamiltonian

$$H_{\text{bilayer}} = \sum_r \mathcal{D}_z S^z_{\text{I}r} S^z_{\text{II}r} + \mathcal{D}_\perp \vec{S}^\perp_{\text{I}r} \cdot \vec{S}^\perp_{\text{II}r} + \sum_{\langle r_a r_b \rangle} (\mathcal{J}_z S^z_{\text{I}r_a} S^z_{\text{I}r_b} + \mathcal{J}_\perp \vec{S}^\perp_{\text{I}r_a} \cdot \vec{S}^\perp_{\text{I}r_b} + \text{I} \leftrightarrow \text{II}) + \sum_{\langle r_a r_b \rangle} (\mathcal{K}_z S^z_{\text{I}r_a} S^z_{\text{II}r_b} + \mathcal{K}_\perp \vec{S}^\perp_{\text{I}r_a} \cdot \vec{S}^\perp_{\text{II}r_b} + \text{I} \leftrightarrow \text{II})$$

Severe sign problem for conventional SSE

- Triangles in lattice structure

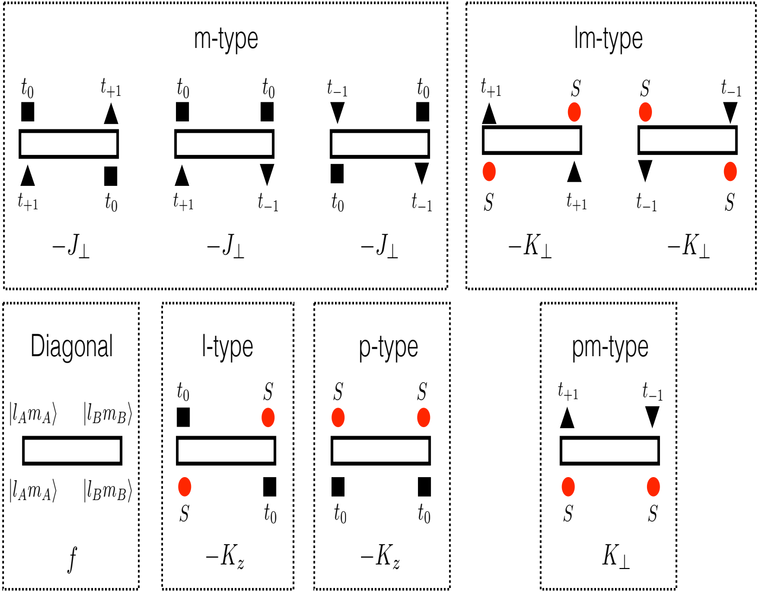
  $\rightarrow$

- Severe sign problem in z basis for SSE

Basic idea

- Stochastic Series Expansion in basis of total spin eigenstates of two spins at Bravais lattice site r

Vertices and weights

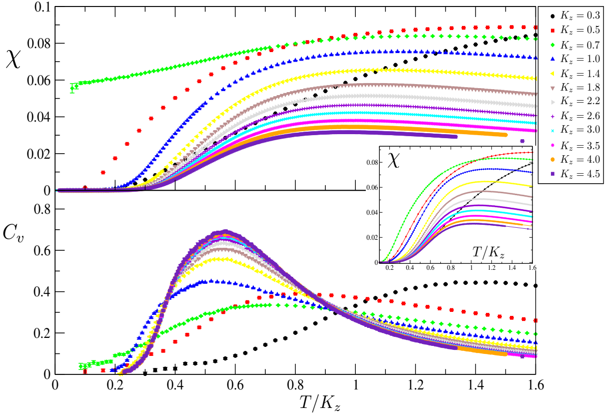


Proof of sign-free nature

Periodicity and bipartiteness implies constraints

- $\mathcal{N}_p + \mathcal{N}_{pm}$ must at least be even.
- $\mathcal{N}_m + \mathcal{N}_{pm} + \mathcal{N}_{lm}$ must also be even.
- $\mathcal{N}_l + \mathcal{N}_{lm}$ must also be even.
- If $K_\perp = 0$, we have $\mathcal{N}_{lm} = \mathcal{N}_{pm} = 0$.
  No sign problem
- If $K_z = 0$, we have $\mathcal{N}_l = \mathcal{N}_p = 0$.
  No sign problem

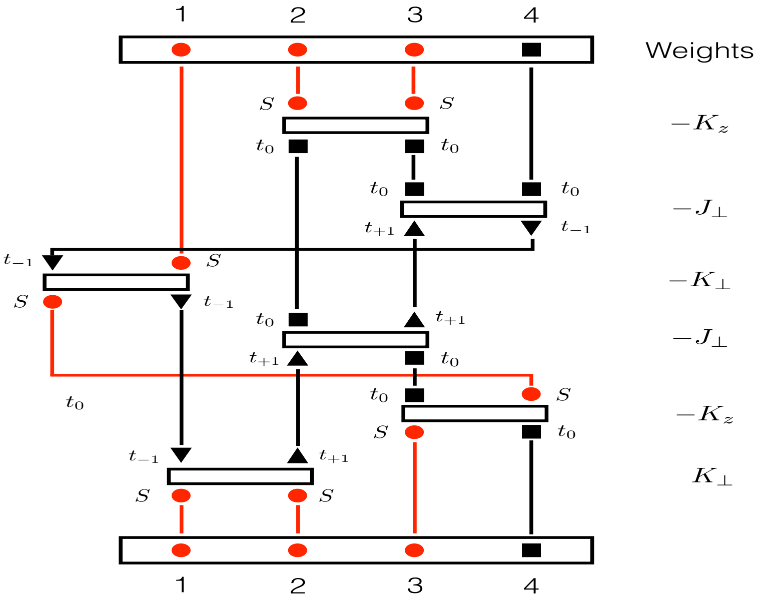
Illustration: Fully frustrated ladder with $K_z \neq 0$



H_{bilayer} in $d = 1$ with $\mathcal{D}_z = \mathcal{D}_\perp = 1$, $\mathcal{J}_\perp = \mathcal{K}_\perp = 1$, $\mathcal{J}_z = 1 + K_z$, $\mathcal{K}_z = 1 - K_z$, as a function of rescaled temperature T/K_z with linear size (number of unit-cells) $L = 64$.

The inset shows the perfect agreement between QMC data (symbols) and exact diagonalization results (lines) for a system of linear size $L = 6$.

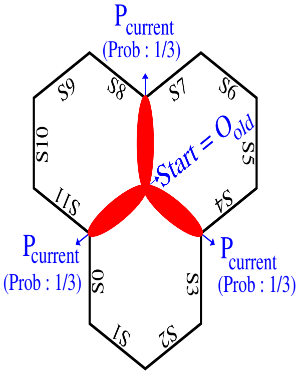
Can we access SU(2) symmetric frustrated bilayers?

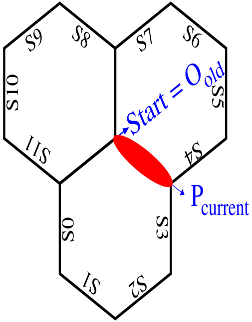


Cluster algorithm for classical frustrated Ising models

- Map configuration to dual (bond-energy) representation.
  "Generalized dimer model"
- Devise a rejection-free worm algorithm to update bond-energies
  Subtlety: Allowing for excursions outside minimally frustrated subspace with correct weight
- Transform back to spins

Algorithm for H_{Ising} on triangular lattice





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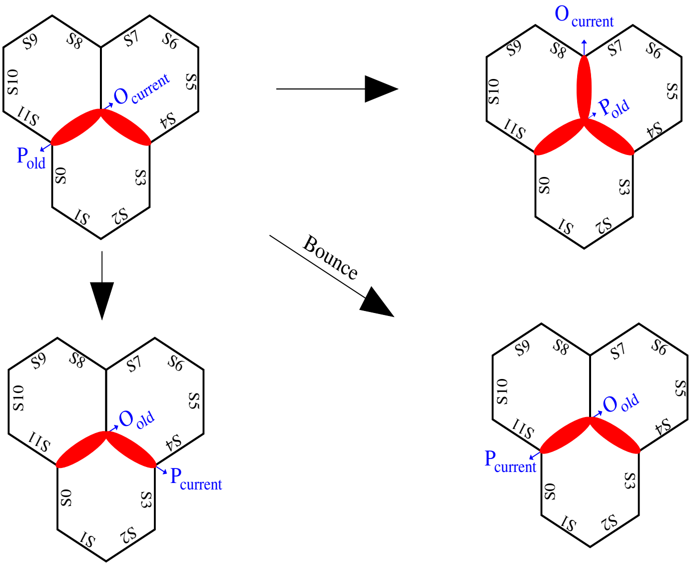

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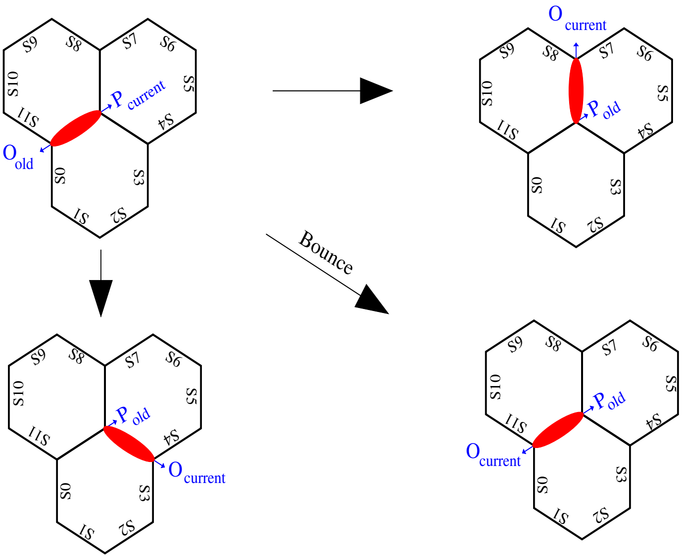

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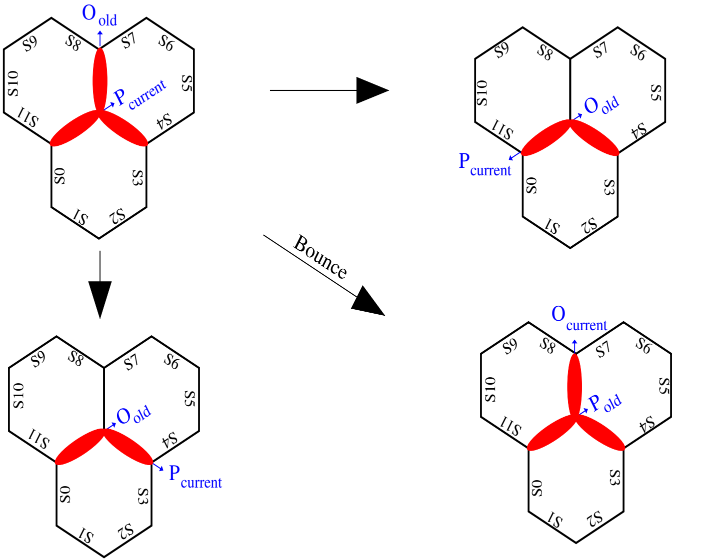
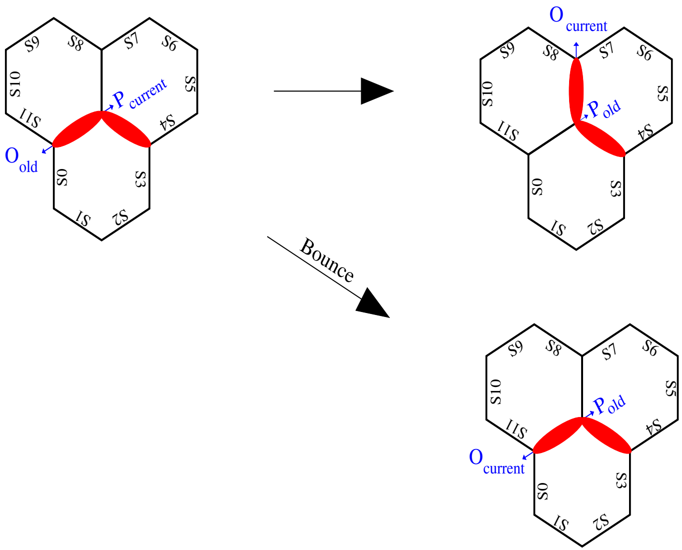
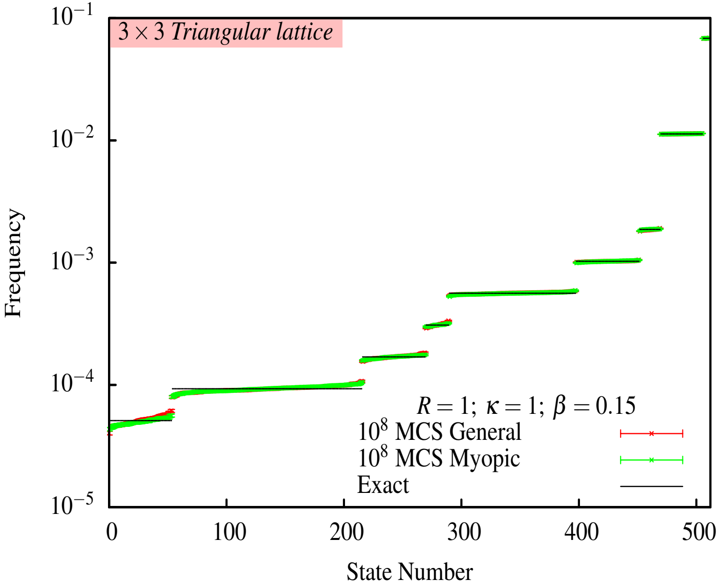


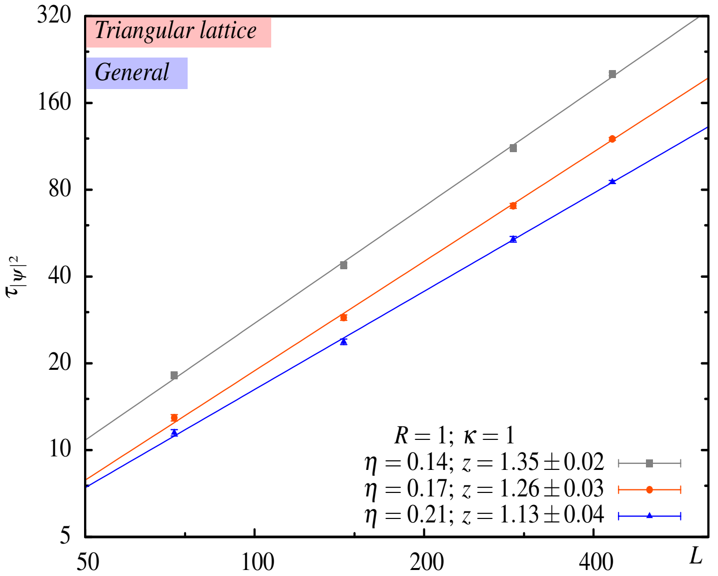
Algorithm for H_{Ising}



Test against exact enumeration



In power-law three-sublattice ordered phase



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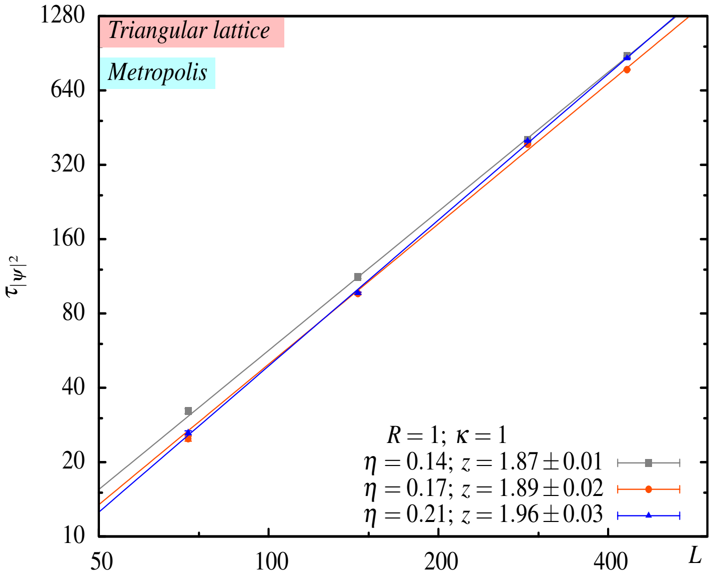

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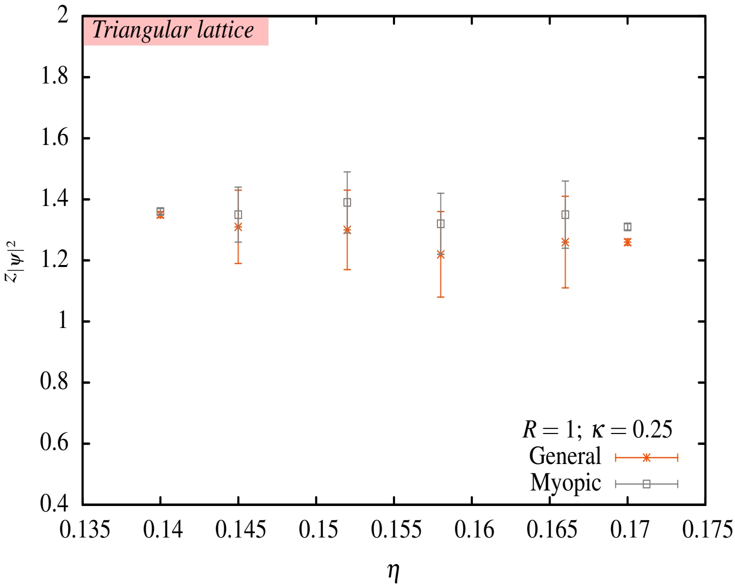

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