Cluster algorithms for frustrated Ising models

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Ingredients

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

Particularly appropriate setting...

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

Example

- $S = 1$ easy-axis triangular lattice antiferromagnet with large single-ion anisotropy
  $H = \sum_{\langle rr' \rangle} \vec{S}_r \cdot \vec{S}_{r'} - D \sum_r (S^z_r)^2$
- Reduction to: $S = 1/2$
  $H_{XXZ} = J_z \sum_{\langle rr' \rangle} \sigma^z_r \sigma^z_{r'} - J_\perp \sum_{\langle rr' \rangle} (\sigma^+_r \sigma^-_{r'} + h.c.)$
  (KD & Senthil 2006)
- QMC of H_{XXZ} using SSE
  (Heidarian & KD 2005, Melko *et.al.* 2005, Wessel & Troyer 2005, Boninsegni & Prokofev 2005 ...)

Key challenge for algorithm

- Needs to "know" structure of minimally frustrated landscape
  Within stochastic Series Expansion (SSE): Directed-loop updates must be able to move system within minimally frustrated subspace
- Solution: Cluster decomposition of H_{XXZ} in triangle Hamiltonians (Kim & Gross, KD & Heidarian 2004)
- advantage: incorporates $\Delta E = 0$ changes & $\Delta E \neq 0$ on equal footing

Another example

- $S \geq 3/2$ easy axis antiferromagnets on triangular and Kagome lattices
- Reduction to frustrated Ising model with further-neighbour/multi-spin interactions
  $H_{\text{Ising}} = J\sum_{\langle ij \rangle} \sigma_i \sigma_j + J' \sum_{\langle\langle ij \rangle\rangle} \sigma_i \sigma_j + \ldots$

Challenge for algorithm

- At $T = 0$, formulate as interacting dimer model and use dimer worm algorithm of Alet *et. al.*.
  (Sen *et. al.*,2008,09)
- Difficulty at small nonzero temperature: Need to include higher-energy configurations with correct weight in efficient way
  Standard (Wolff-inspired) cluster constructions don't work so well with frustration
  Coddington & Han 1994, Zhang and Yang 1994

More recent attempt

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

Third example

- 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 (Sandvik 2003)
  Clusters reduce to variant of Swendsen-Wang clusters in $\Gamma = 0$ limit $\rightarrow$ frustrated J_{ij} again leads to problems(?)
  Need to "teach" algorithm physics of minimally frustrated configurations(?)

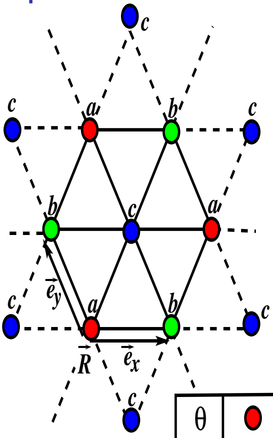
In this talk...

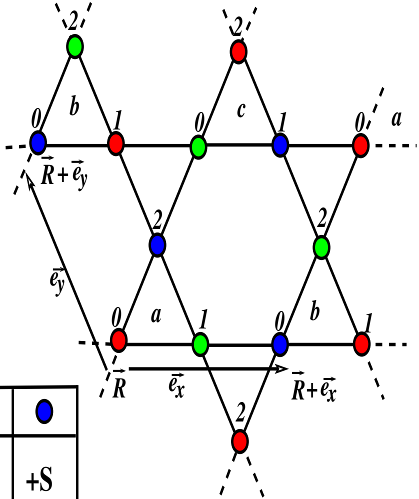
- Quantum cluster construction for *frustrated* TFIM
- Cluster algorithm for frustrated two-dimensional H_{Ising} with up to third neighbour interactions

SSE 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	red	green	blue
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 ($m = 0, 1, 2 \ldots 6$)

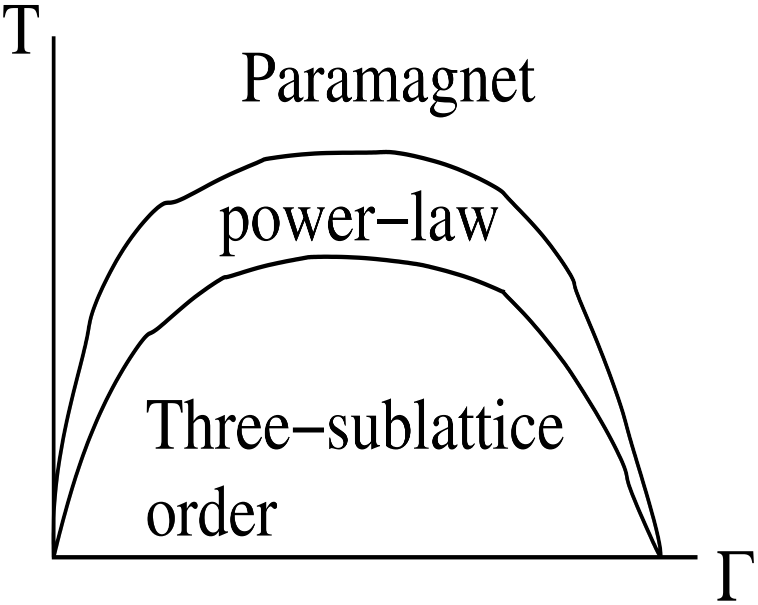
$\theta = (2m+1)\pi/6$: Plaquette three-sublattice order ($m = 0, 1, 2 \ldots 6$)

In ordered state: θ pinned to these values

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

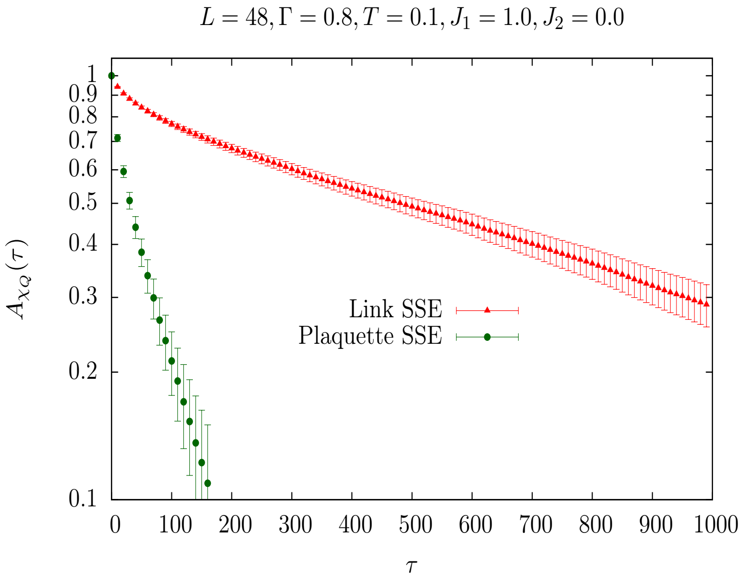
In power-law phase: θ has gaussian fluctuations with no pinning

Physics with $J_2 = 0$



(Isakov & Moessner 2003)

New ideas needed?



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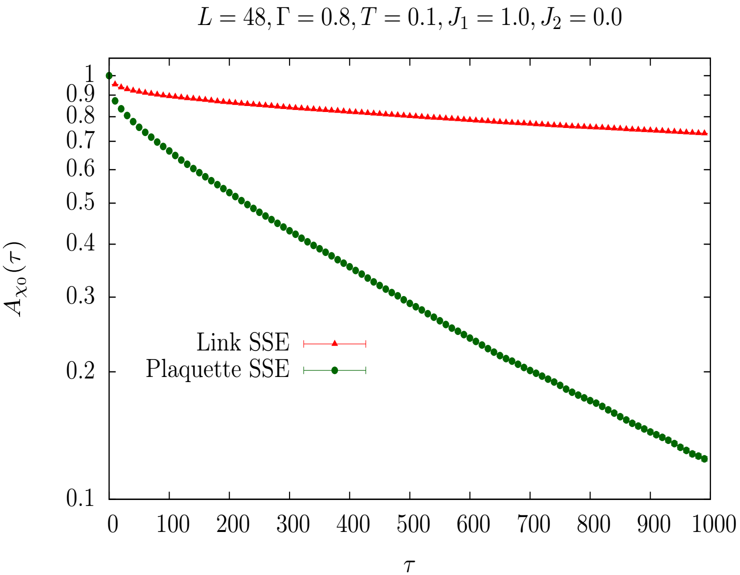

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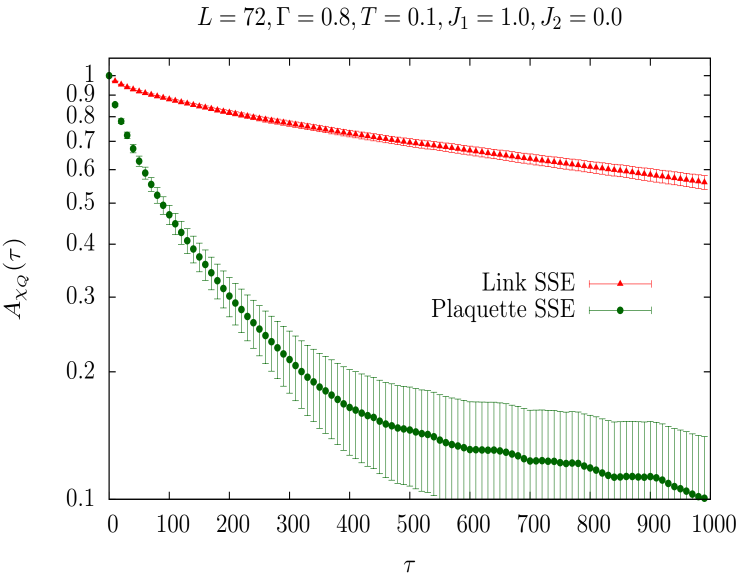

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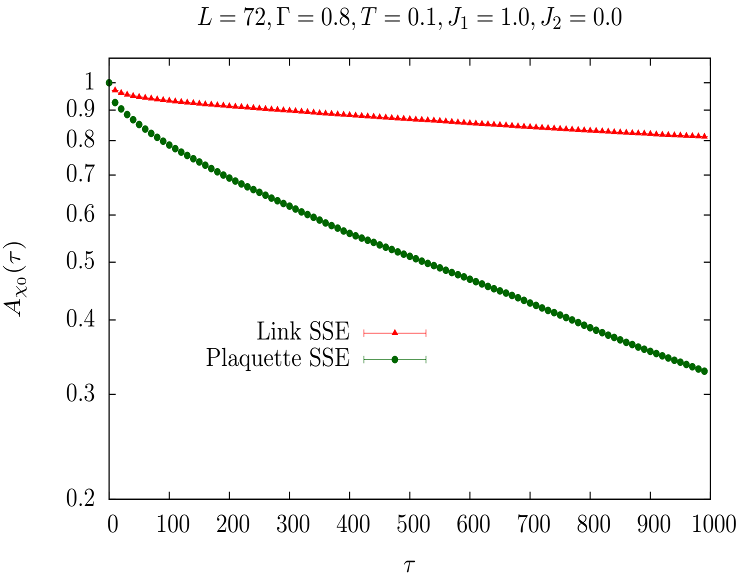

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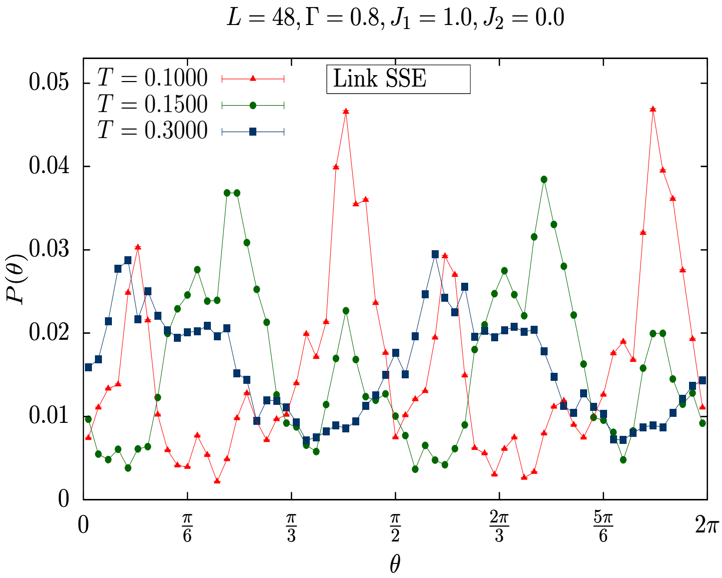


Approach

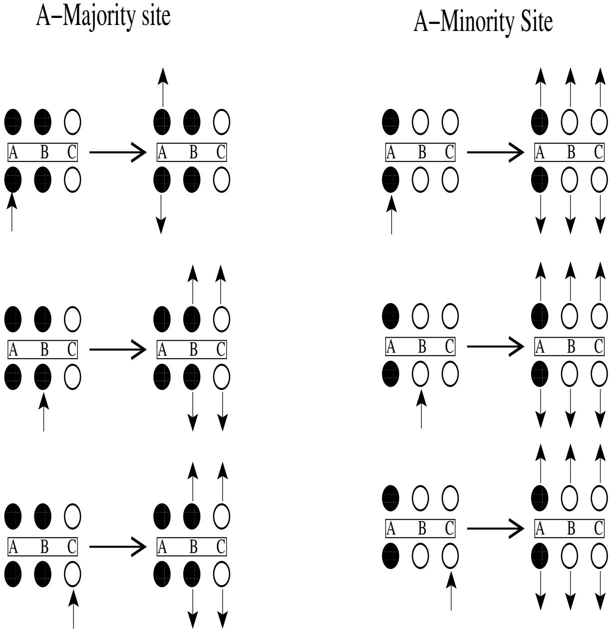
$H_{\text{TFIM}} = \sum_{\Delta} H_{\Delta} + \sum_{\text{link}} H_{\text{link}} + \sum_{\text{sites}} H_{\text{sites}}$

H_{Δ}: Triangle decomposition of all antiferromagnetic couplings

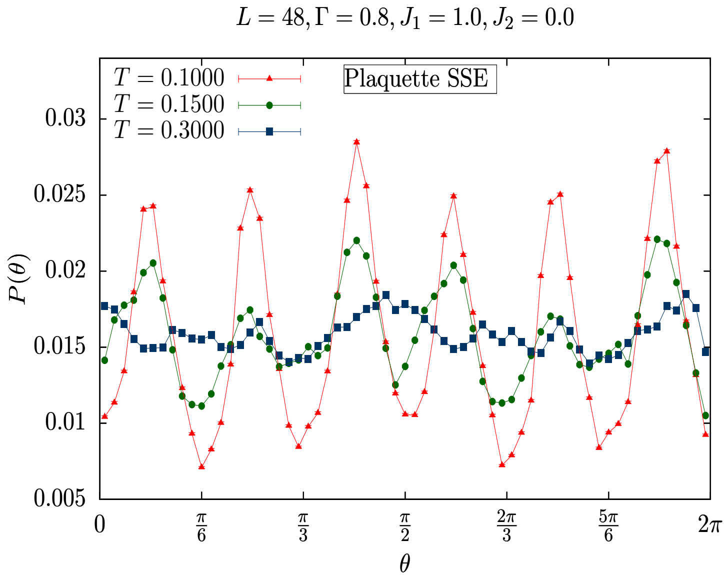
H_{Link}: Bond decomposition of all ferromagnetic couplings

H_{sites}: site decomposition of transverse field term

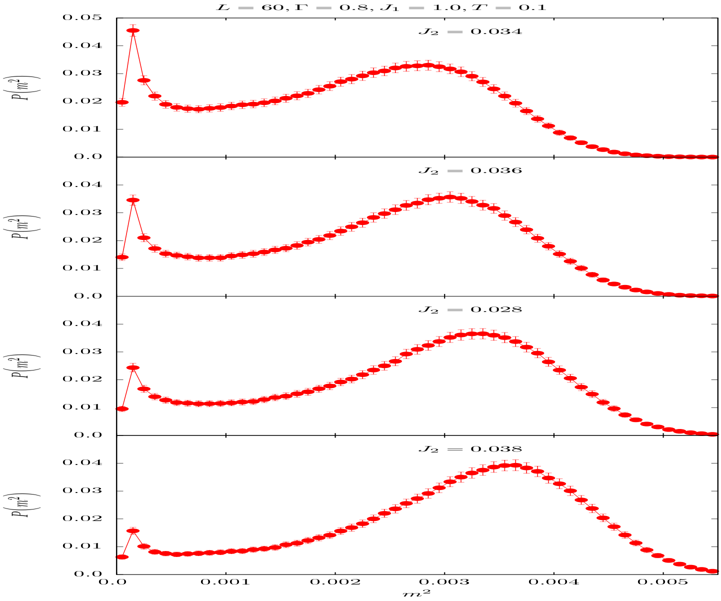
Quantum-cluster construction for frustrated TFIM



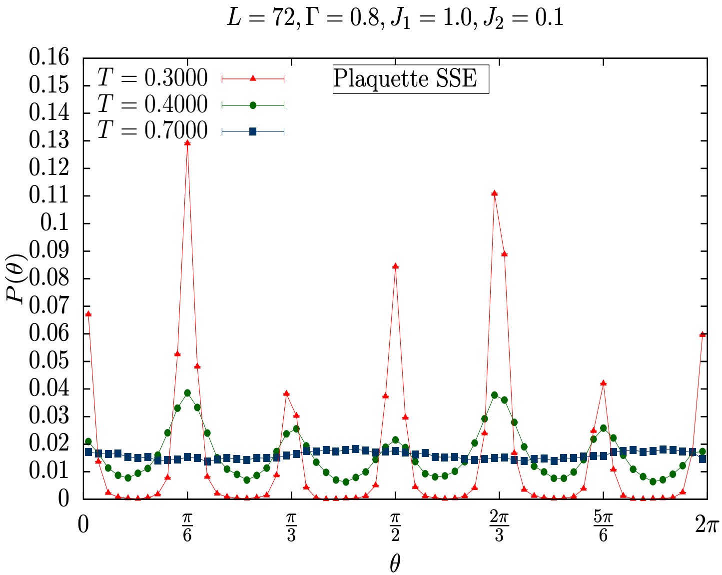
Improvement



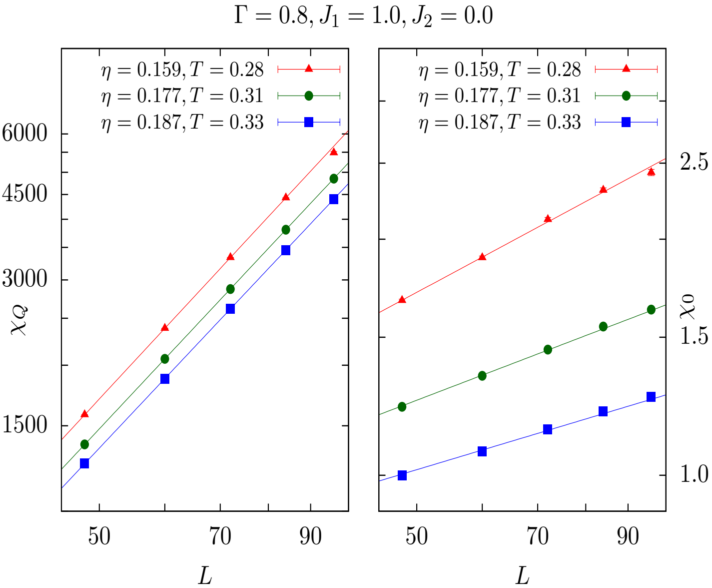
Going into columnar phase



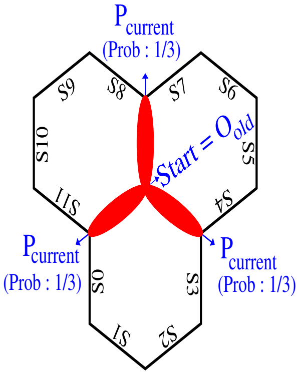
In columnar phase

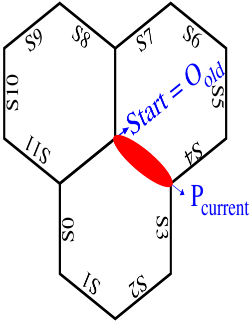


Divergent ferromagnetic susceptibility of antiferromagnet



Algorithm for H_{Ising}





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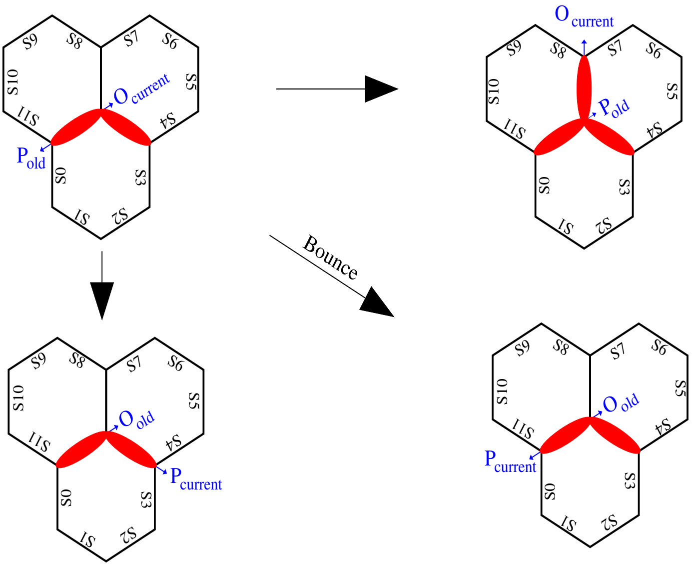

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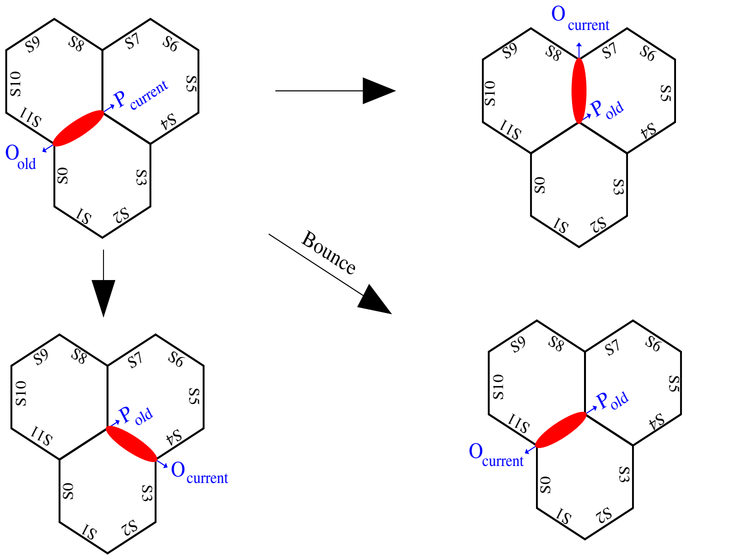

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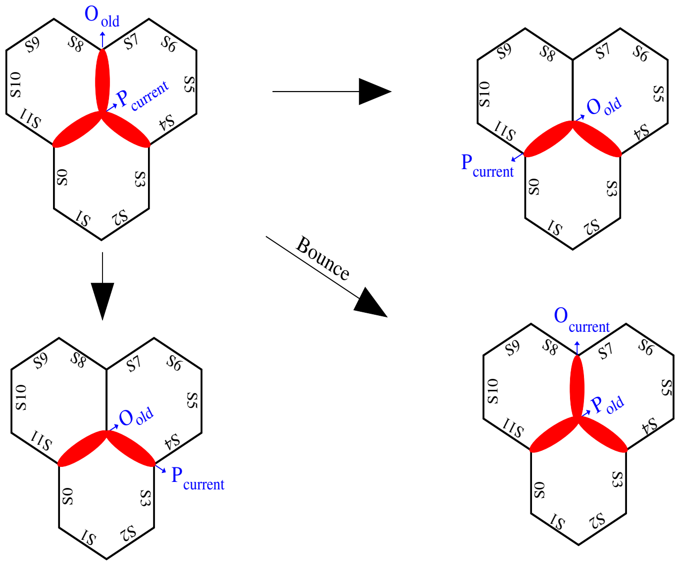

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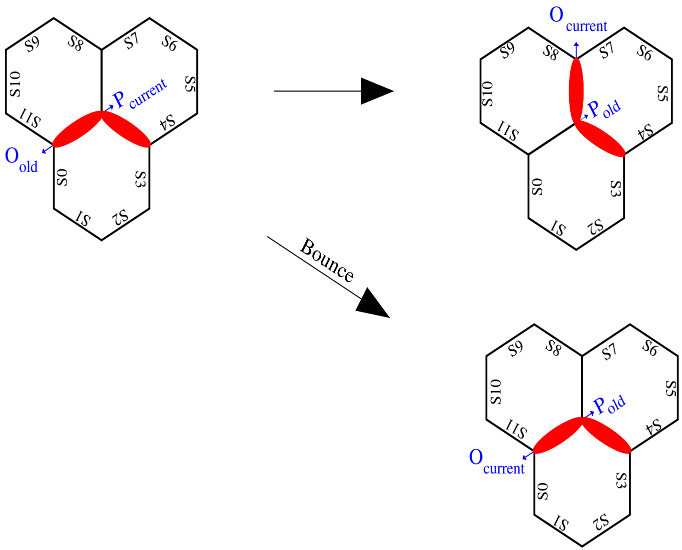
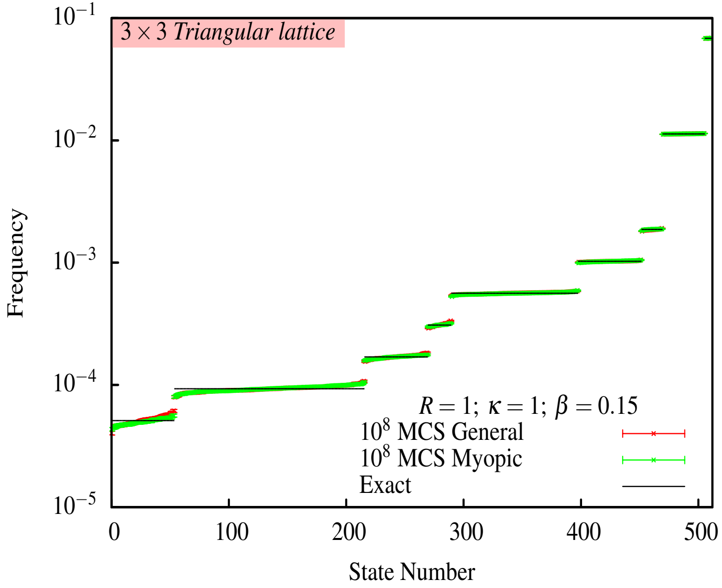
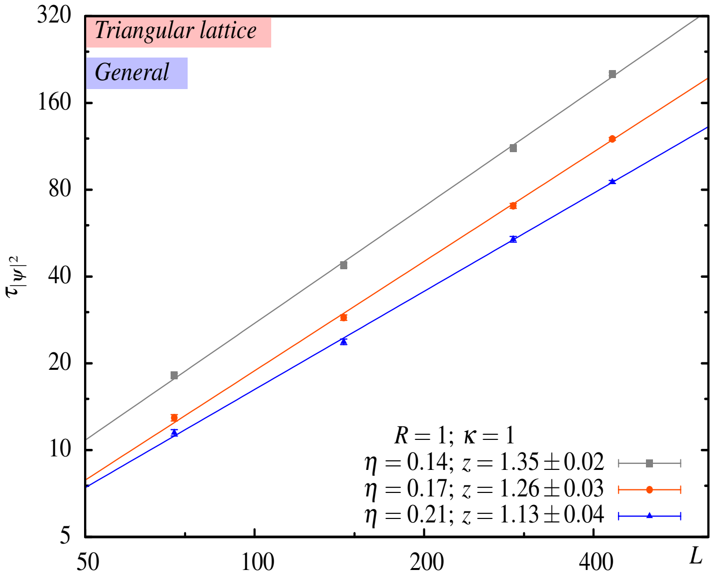


Test against exact enumeration



In power-law three-sublattice ordered phase



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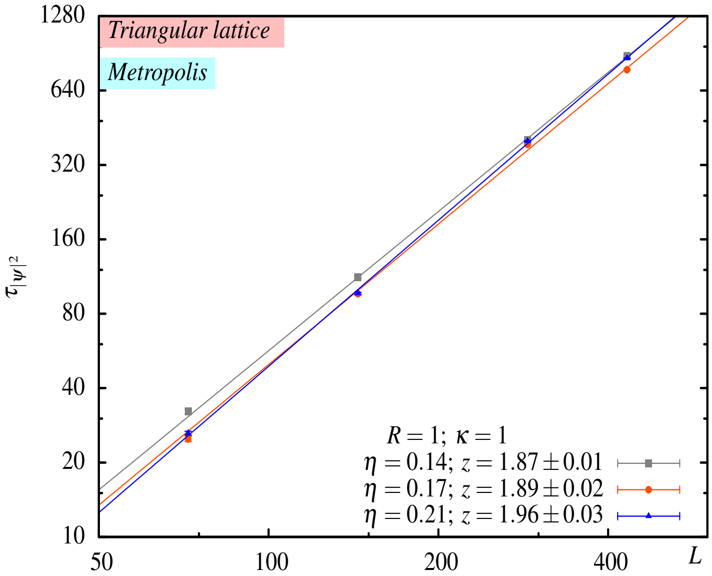
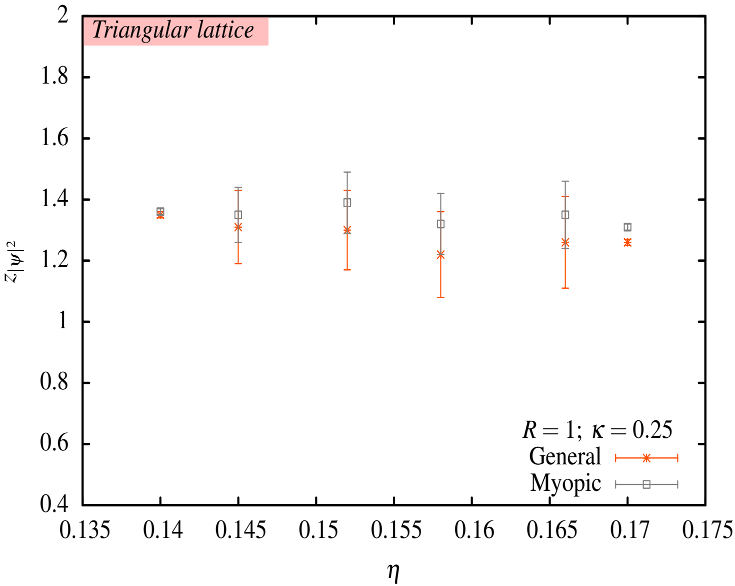


In power-law three-sublattice ordered phase



Acknowledgements

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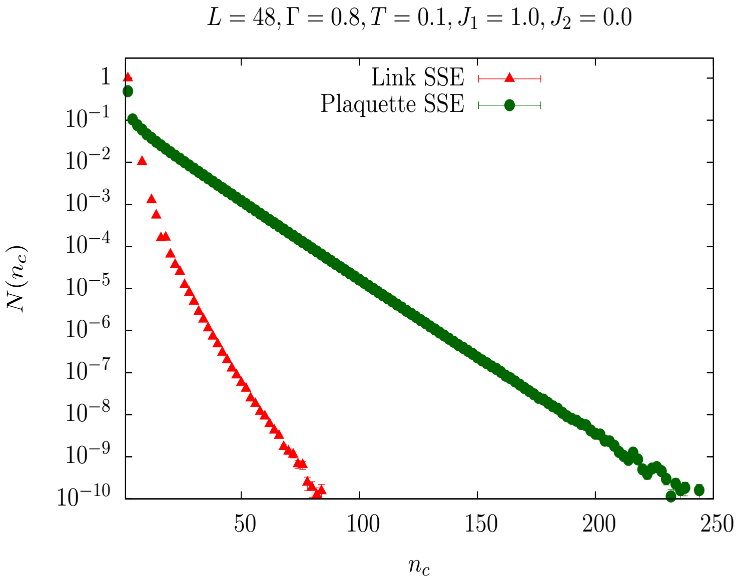
  Sounak Biswas & Geet Ghanshyam TIFR
- Computational resources: funded by DTP TIFR

Cluster size distribution



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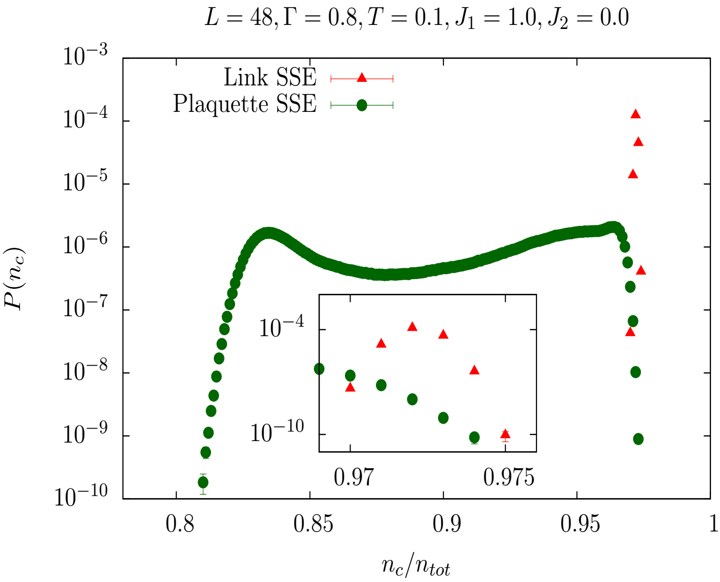

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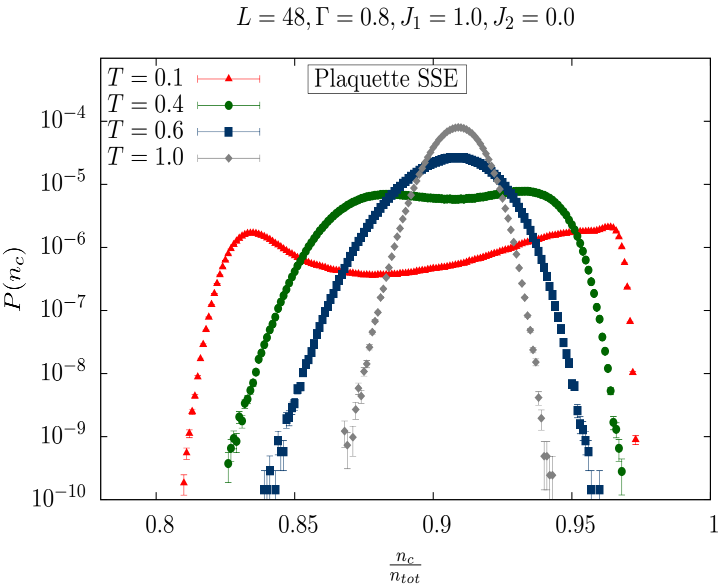

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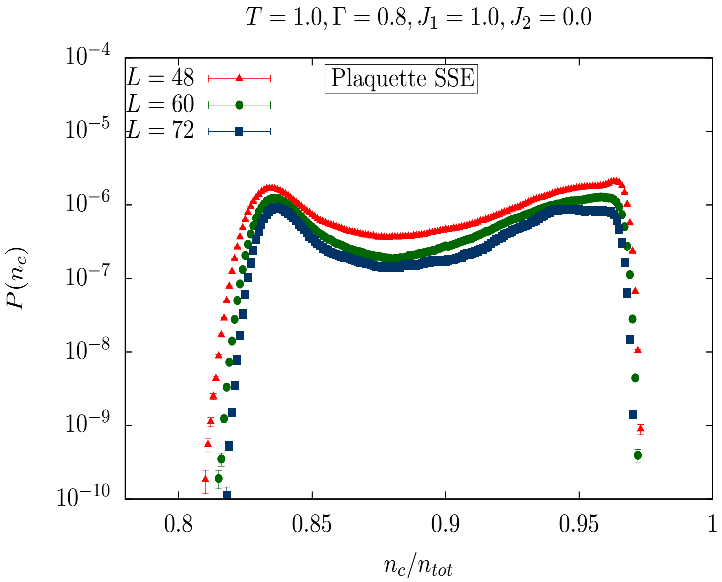
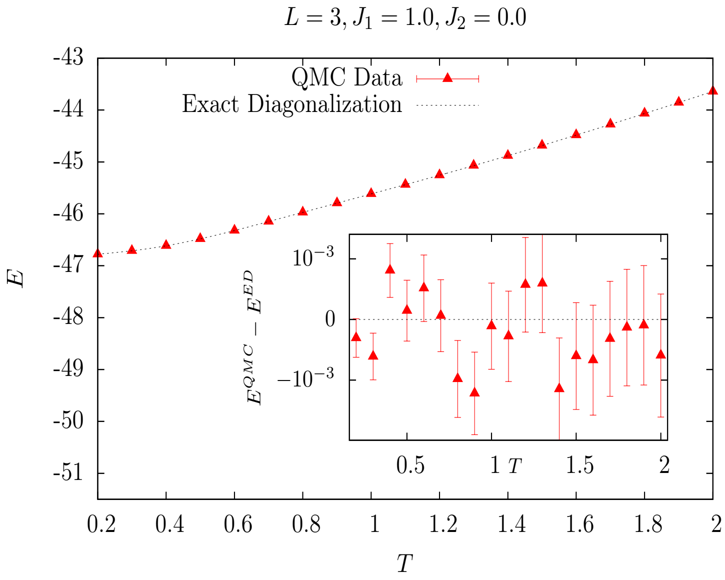
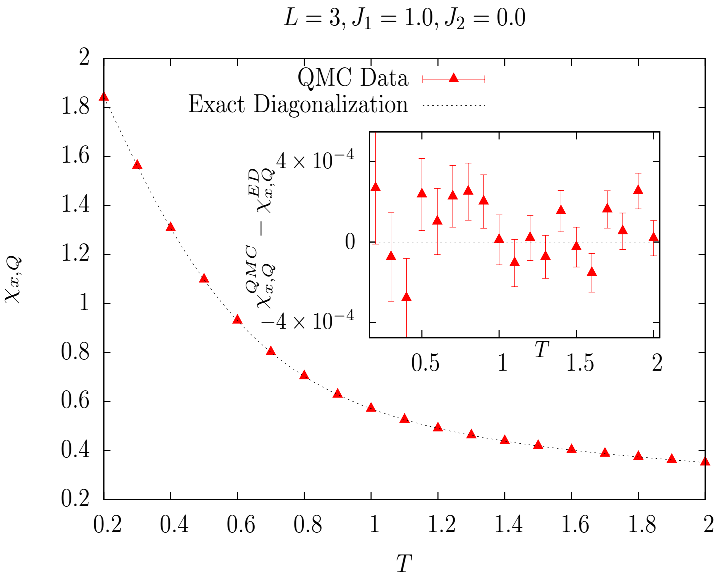


ED tests

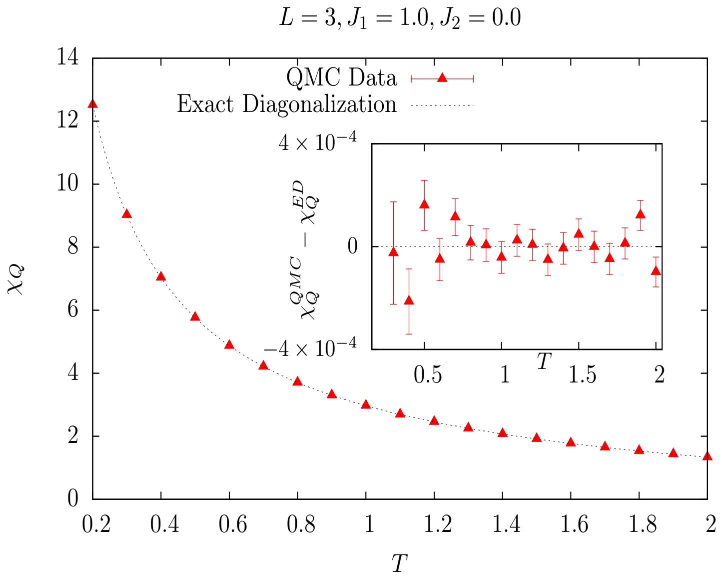

$L = 3, J_1 = 1.0, J_2 = 0.0$
QMC Data
Exact Diagonalization
E
T
-43
-44
-45
-46
-47
-48
-49
-50
-51
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
$E^{QMC} - E^{ED}$
10^{-3}
0
-10^{-3}
0.5
1 T
1.5
2

ED tests

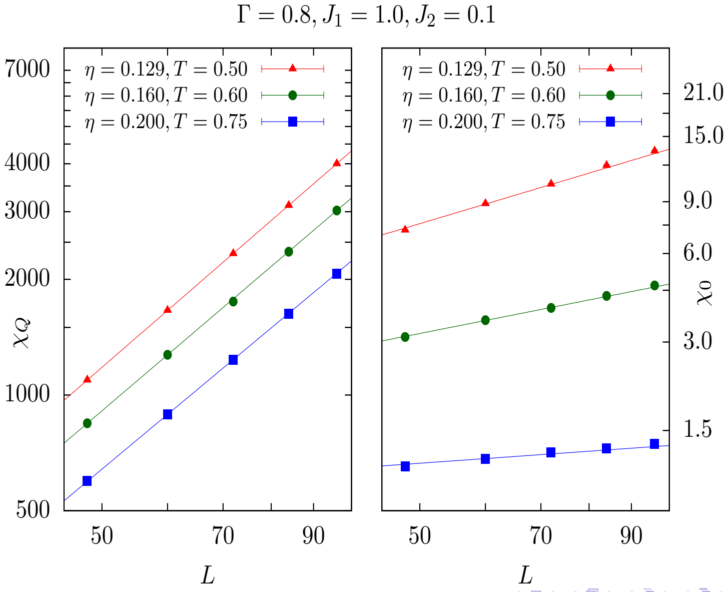


$L = 3, J_1 = 1.0, J_2 = 0.0$
QMC Data
Exact Diagonalization
$\chi_{x,Q}$
T
$\chi_{x,Q}^{QMC} - \chi_{x,Q}^{ED}$
4×10^{-4}
0
-4×10^{-4}
0.5
1
1.5
2
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

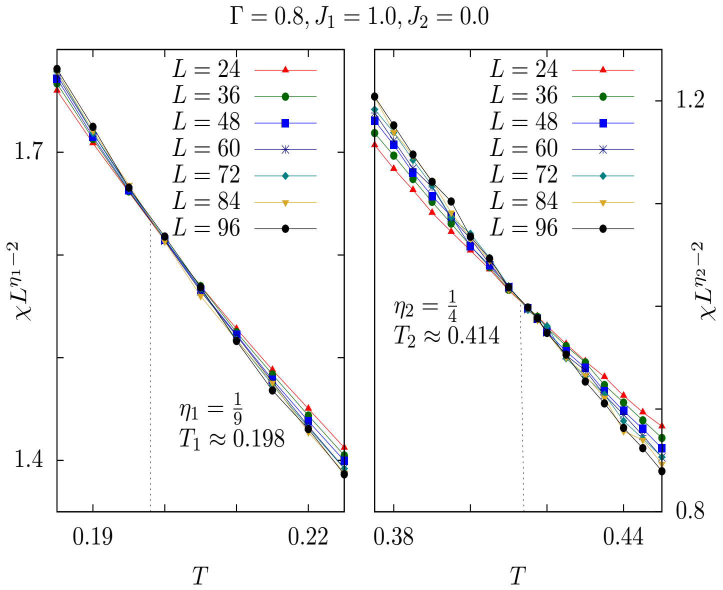
ED tests


$L = 3, J_1 = 1.0, J_2 = 0.0$
QMC Data
Exact Diagonalization
χ_Q
T
0
2
4
6
8
10
12
14
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
4×10^{-4}
0
-4×10^{-4}
$\chi_Q^{QMC} - \chi_Q^{ED}$
0.5
1
1.5
2
T

Thermodynamic signature of melting of columnar order



Scaling for two step transition



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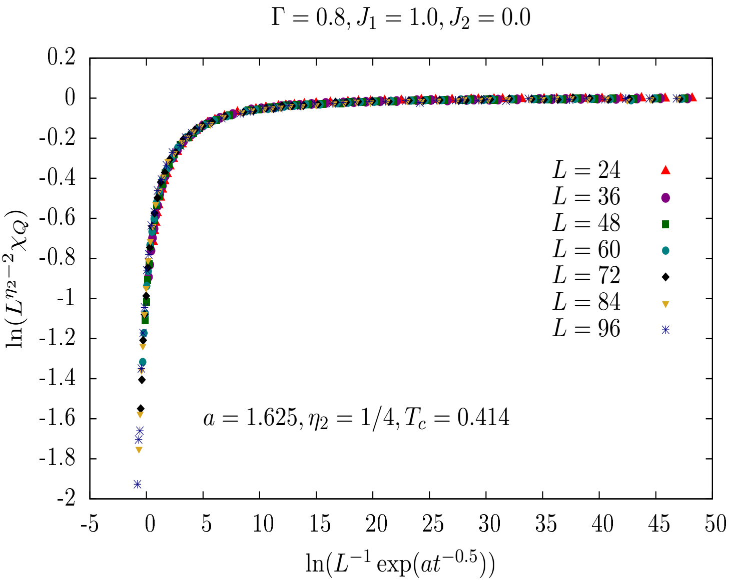

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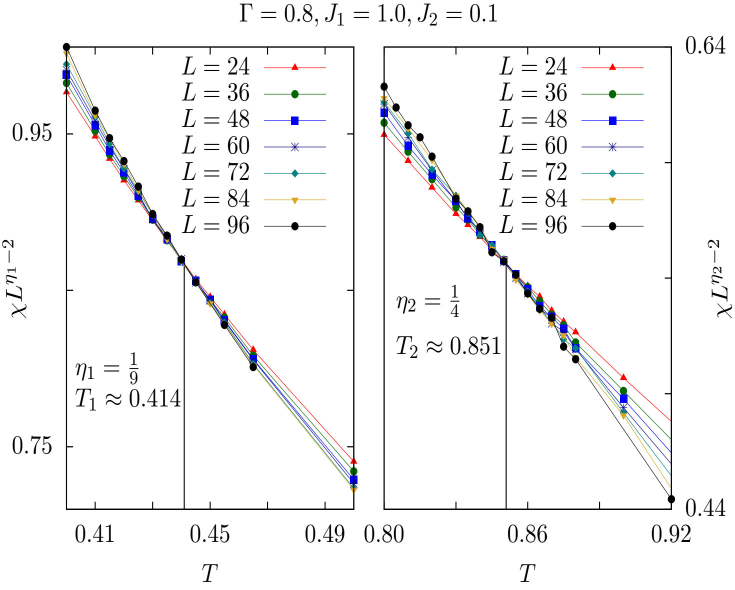

Scaling for two step transition