Meron-Cluster and Nested Cluster Algorithms: Addressing the Sign Problem in Quantum Monte Carlo Simulations

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Collaborators:

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F.-J. Jiang and M. Nyfeler (Bern University),
F. Kämpfer (MIT), M. Pepe (Milano University)

Outline

The Nature of the Sign Problem

Avoiding a Sign Problem by an Unconventional Regularization:
Application to $\mathbb{C}P(N-1)$ θ-Vacua using $SU(N)$ Quantum Spin Ladders

The Meron-Cluster Algorithm:
Application to some Strongly Correlated Electron Systems

The Nested Cluster Algorithm:
Application to Frustrated Antiferromagnets

Conclusions

Outline

Fermionic path integral

$$Z_f = \mathrm{Tr}\exp(-\beta H) = \sum_{[n]} \mathrm{Sign}[n]\exp(-S[n]) \ , \quad \mathrm{Sign}[n] = \pm 1$$

Path integral of a corresponding bosonic model

$$Z_b = \sum_{[n]} \exp(-S[n])$$

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Fermionic observable $O[n]$ from the bosonic ensemble

$$\langle O \rangle_f = \frac{1}{Z_f} \sum_{[n]} O[n]\mathrm{Sign}[n]\exp(-S[n]) = \frac{\langle O \ \mathrm{Sign} \rangle}{\langle \mathrm{Sign} \rangle}$$

Average sign in the simulated bosonic ensemble

$$\langle \mathrm{Sign} \rangle = \frac{1}{Z_b} \sum_{[n]} \mathrm{Sign}[n]\exp(-S[n]) = \frac{Z_f}{Z_b} = \exp(-\beta V \Delta f)$$

Using

$$\langle \mathrm{Sign} \rangle = \exp(-\beta V \Delta f) \ , \quad \Delta f = f_f - f_b \ ,$$

the estimated statistical error is

$$\frac{\sigma_{\mathrm{Sign}}}{\langle \mathrm{Sign} \rangle} = \frac{\sqrt{\langle \mathrm{Sign}^2 \rangle - \langle \mathrm{Sign} \rangle^2}}{\sqrt{N} \langle \mathrm{Sign} \rangle} = \frac{\exp(\beta V \Delta f)}{\sqrt{N}} \ .$$

Hence, the required number of independent measurements is

$$N = \exp(2\beta V \Delta f) \ .$$

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Academic "solution" of the sign problem:

$$UHU^\dagger = \text{diag}(E_1, E_2, ...) \ \Rightarrow \ Z_f = \sum_n \exp(-\beta E_n) \ \Rightarrow \ Sign[n] > 0 \ .$$

Of course, if one could diagonalize the Hamiltonian — which is generally exponentially hard for large systems — one would not even need Monte Carlo simulations.

Outline

$\mathbb{C}P(N-1)$ models are $(1+1)$-dimensional toy models for QCD formulated in terms of $N \times N$ projection matrices

$$P(x)^\dagger = P(x), \quad \mathrm{Tr}P(x) = 1, \quad P(x)^2 = P(x)$$

with the Euclidean action

$$S[P] = \int_0^\beta dt \int_0^L dx \, \frac{1}{g^2} \mathrm{Tr}\left[\partial_x P \partial_x P + \frac{1}{c^2}\partial_t P \partial_t P\right] + i\theta Q[P]$$

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that contains the topological charge

$$Q[P] = \frac{1}{\pi i} \int_0^\beta dt \int_0^L dx \, \mathrm{Tr}[P\partial_x P \partial_t P] \in \Pi_2[SU(N)/U(N-1)] = \mathbb{Z} \, .$$

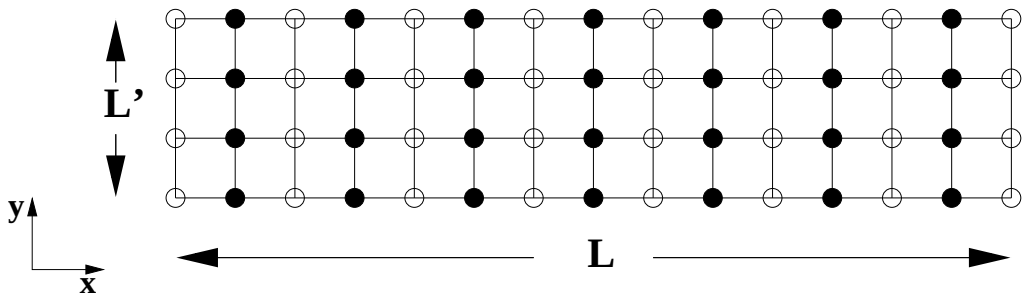
The complex action of a θ-vacuum causes a severe sign problem.

$SU(N)$ quantum spins

$$T^a_x, \quad a \in \{1, 2, ..., N^2 - 1\}, \quad [T^a_x, T^b_y] = i\delta_{xy} f_{abc} T^c_x$$

Spin ladder Hamiltonian

$$H = -J \sum_{x \in A} [T^a_x T^{a*}_{x+\hat{1}} + T^a_x T^a_{x+\hat{2}}] - J \sum_{x \in B} [T^{a*}_x T^a_{x+\hat{1}} + T^{a*}_x T^{a*}_{x+\hat{2}}]$$



Conserved $SU(N)$ spin

$$T^a = \sum_{x \in A} T^a_x - \sum_{x \in B} T^{a*}_x, \quad [T^a, H] = 0$$

Spontaneous symmetry breaking $SU(N) \to U(N-1)$ implies Goldstone boson fields $P(x) \in \mathbb{C}P(N-1) = SU(N)/U(N-1)$ with the low-energy effective action

$$\begin{aligned} S[P] &= \int_0^\beta dt \int_0^L dx \int_0^{L'} dy \ \mathrm{Tr} \left\{ \rho_s' \partial_y P \partial_y P \right. \\ &+ \left. \rho_s \left[\partial_x P \partial_x P + \frac{1}{c^2} \partial_t P \partial_t P \right] - \frac{1}{a} P \partial_x P \partial_t P \right\} \ . \end{aligned}$$

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Very large correlation length

$$\xi \propto \exp(4\pi L' \rho_s / cN) \gg L'$$

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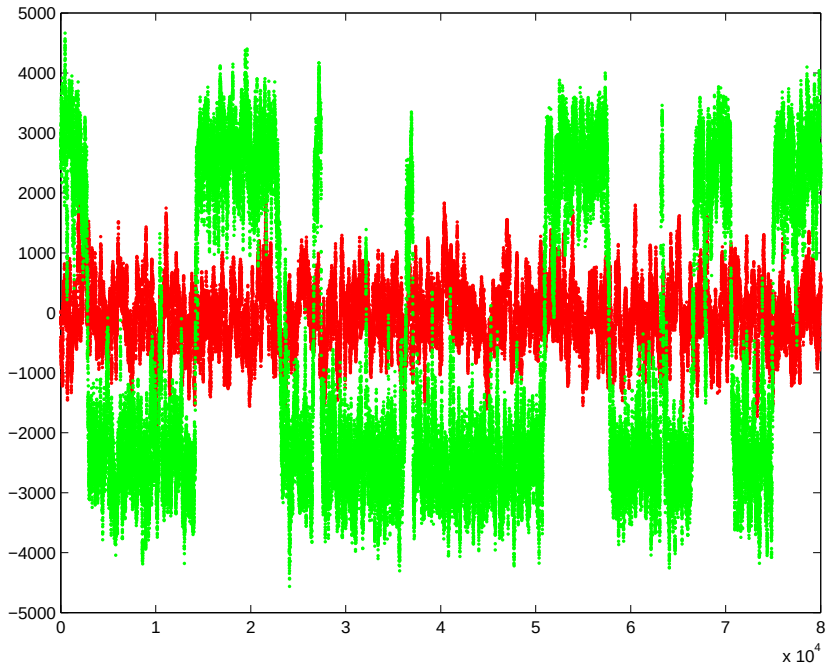
implies dimensional reduction to $(1+1)$-d $\mathbb{C}P(N-1)$ model

$$S[P] = \int_0^\beta dt \int_0^L dx \ \mathrm{Tr} \left\{ \frac{1}{g^2} \left[\partial_x P \partial_x P + \frac{1}{c^2} \partial_t P \partial_t P \right] - n P \partial_x P \partial_t P \right\} .$$

Emergent θ-vacuum angle $\theta = n\pi$

Monte Carlo history of the order parameter



- For $n = 3$ (green curve) there is a first order phase transition with spontaneous CP breaking in the $(1 + 1)$-d $\mathbb{C}P(3)$ model at $\theta = \pi$.
- For $n = 4$ (red curve) there is no phase transition at $\theta = 0$.

H. G. Evertz, G. Lana, and M. Marcu, Phys. Rev. Lett. 70 (1993) 875.

B. B. Beard and U.-J. W., Phys. Rev. Lett. 77 (1996) 5130.

B. Beard, M. Pepe, S. Riederer, and U.-J. W., Phys. Rev. Lett. 94 (2005) 010603.

Outline

Strategy of the meron-cluster algorithm:

S. Chandrasekharan and U.-J. W., Phys. Rev. Lett. 83 (1999) 3116.

- 1. Rewrite Z_f using cluster variables such that all negative configurations are matched with positive ones. Then effectively one obtains Sign $\in \{0, 1\}$, such that $\text{Sign}^2 = \text{Sign}$, and hence

$$\frac{\sigma_{\text{Sign}}}{\langle \text{Sign} \rangle} = \frac{\sqrt{\langle \text{Sign}^2 \rangle - \langle \text{Sign} \rangle^2}}{\sqrt{N} \langle \text{Sign} \rangle} = \frac{1}{\sqrt{N} \sqrt{\langle \text{Sign} \rangle}} = \frac{\exp(\beta V \Delta f / 2)}{\sqrt{N}} \ .$$

  This solves one half of the sign problem.

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- 2. Never generate configurations that have been canceled analytically. This solves the sign problem completely.

Like any other method for solving the sign problem, the meron-cluster algorithm is not generally applicable. This is unavoidable because some sign problems are NP-hard.

M. Troyer and U.-J. W., Phys. Rev. Lett. 94 (2005) 170201.

Spinless fermion Hamiltonian with nearest-neighbor repulsion

$$H = \sum_{x,i} h_{x,i}, \quad h_{x,i} = -\frac{t}{2}(c_x^\dagger c_{x+\hat{i}} + c_{x+\hat{i}}^\dagger c_x) + U(n_x - \frac{1}{2})(n_{x+\hat{i}} - \frac{1}{2})$$

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Suzuki-Trotter decomposition of the partition function

$$\begin{aligned} Z_f &= \mathrm{Tr}\{\exp[-\beta(H - \mu N)]\} \\ &= \lim_{M\to\infty} \mathrm{Tr}\left\{\exp[-\epsilon(H_1 - \frac{\mu}{2d}N)] \ldots \exp[-\epsilon(H_{2d} - \frac{\mu}{2d}N)]\right\}^M \end{aligned}$$

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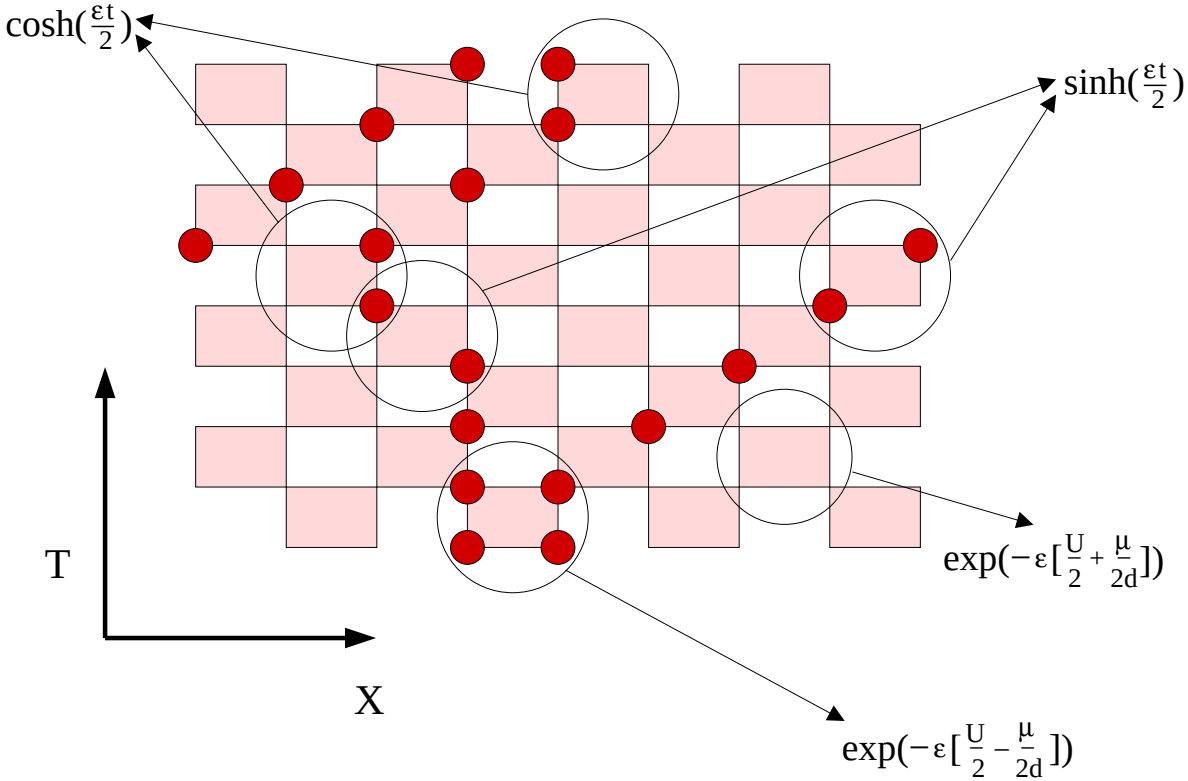
Two-spin transfer matrix

$$\exp[-\epsilon(h_{x,i} - \frac{\mu}{2d}(n_x + n_{x+\hat{i}}))] = \exp[\epsilon(\frac{U}{4} + \frac{\mu}{2d})]$$

$$\times \begin{pmatrix} \exp[-\epsilon(\frac{U}{2} + \frac{\mu}{2d})] & 0 & 0 & 0 \\ 0 & \cosh(\frac{\epsilon t}{2}) & \Sigma\sinh(\frac{\epsilon t}{2}) & 0 \\ 0 & \Sigma\sinh(\frac{\epsilon t}{2}) & \cosh(\frac{\epsilon t}{2}) & 0 \\ 0 & 0 & 0 & \exp[-\epsilon(\frac{U}{2} - \frac{\mu}{2d})] \end{pmatrix}$$

Path integral (in discrete time $\beta = \epsilon M$)

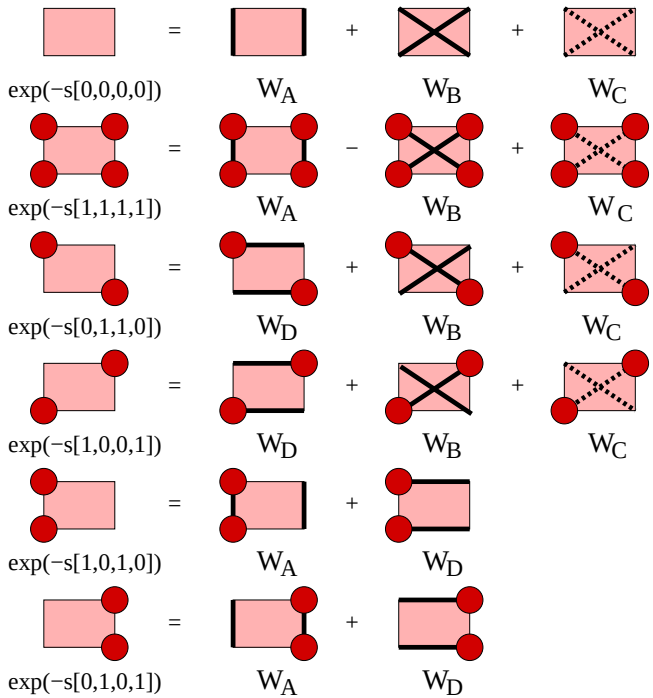
$$\begin{aligned} Z_f &= \mathrm{Tr}[\exp(-\varepsilon H_1)\exp(-\varepsilon H_2)\ldots\exp(-\varepsilon H_{2d})]^M \\ &= \sum_{[n]} \mathrm{Sign}[n]\exp(-S[n]) \end{aligned}$$



Here two fermions interchange their positions. $\Rightarrow$ $\mathrm{Sign}[n] = -1$.

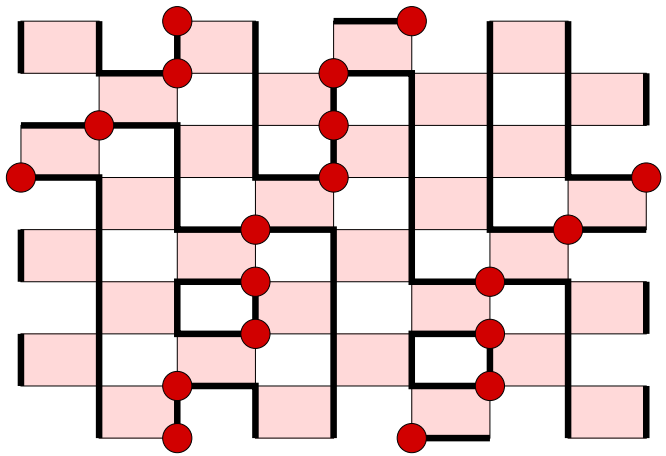
Two-spin transfer matrix and cluster bonds

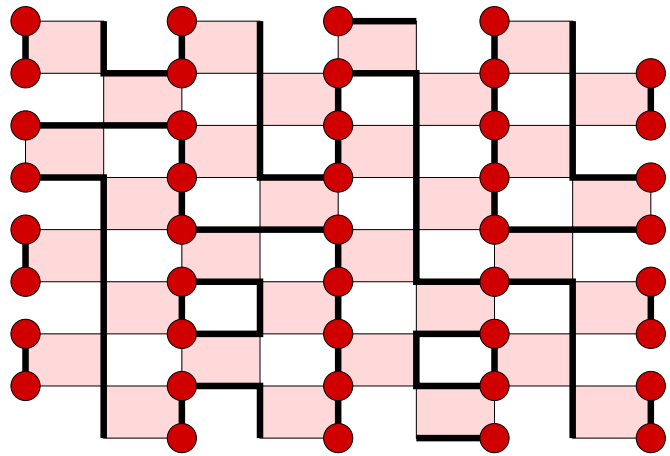
$$\exp(-\varepsilon h_{xy}) = \begin{pmatrix} W_A & 0 & 0 & 0 \\ 0 & W_A + W_D & -W_D & 0 \\ 0 & -W_D & W_A + W_D & 0 \\ 0 & 0 & 0 & W_A \end{pmatrix}$$



Here $W_A = \exp(-\varepsilon U/2)$, $W_B = W_C = 0$, $W_D = \sinh(\varepsilon t/2)$.

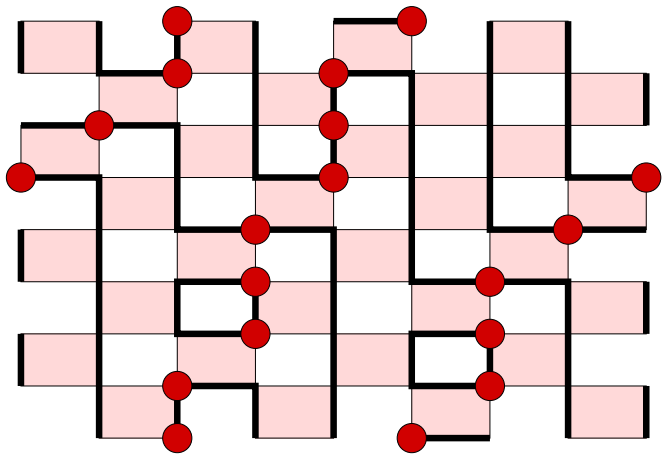
Cluster decomposition and reference configuration

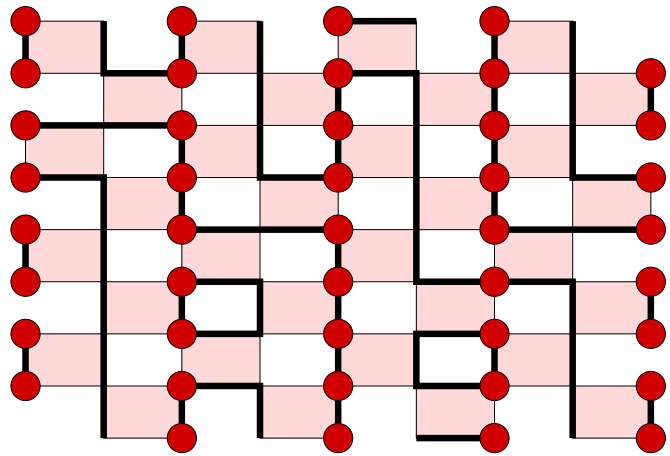




- All spins in a cluster are flipped simultaneously with probability $\frac{1}{2}$.

Cluster decomposition and reference configuration





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- The flip of a meron-cluster changes the fermion sign.

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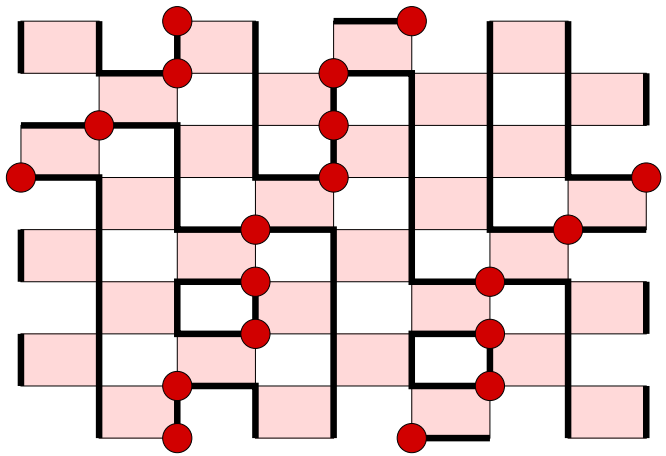
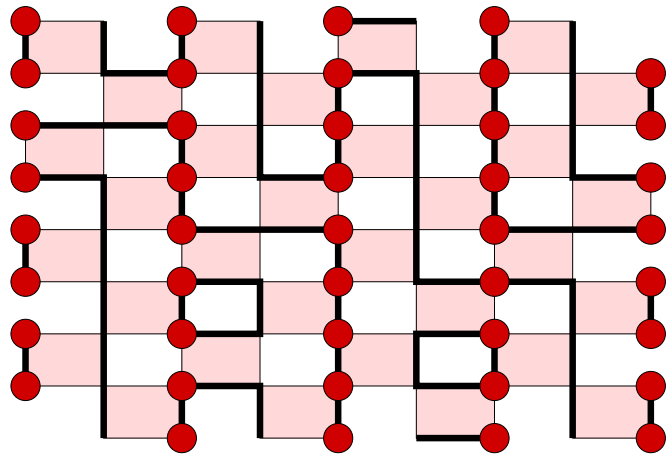
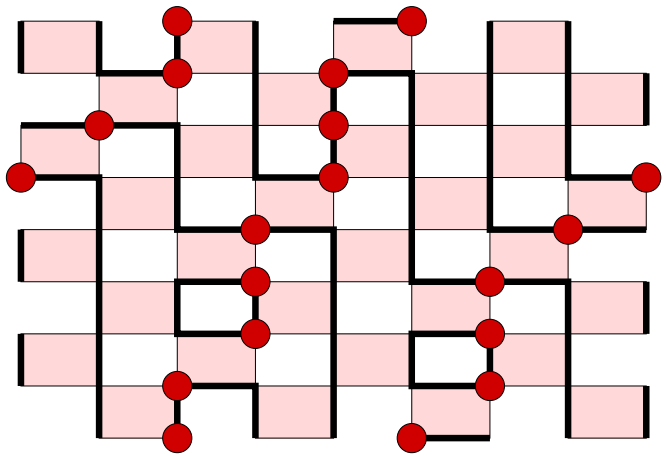
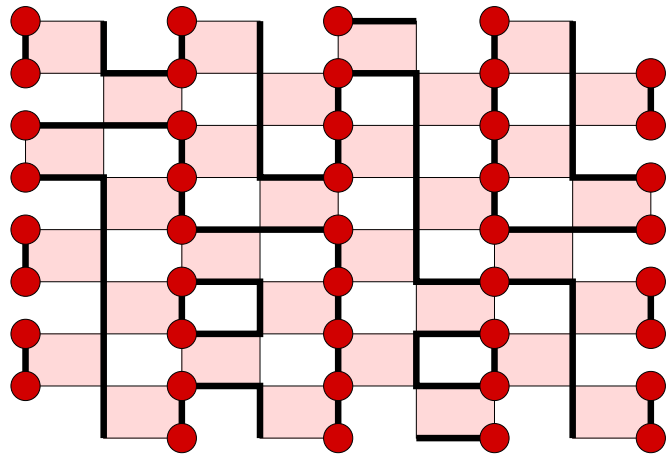




- All spins in a cluster are flipped simultaneously with probability $\frac{1}{2}$.
- The flip of a meron-cluster changes the fermion sign.
- Only the 0-meron sector (which contains configurations without merons) contributes to the partition function.

Cluster decomposition and reference configuration





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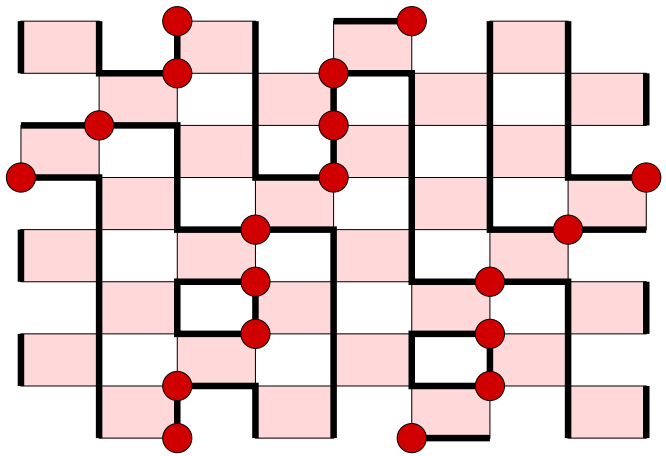

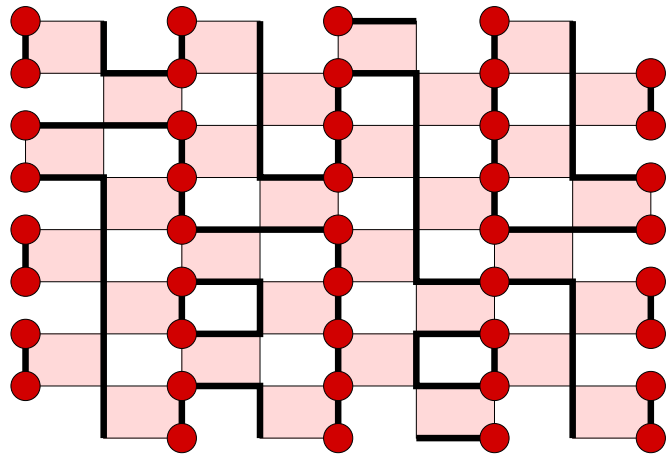

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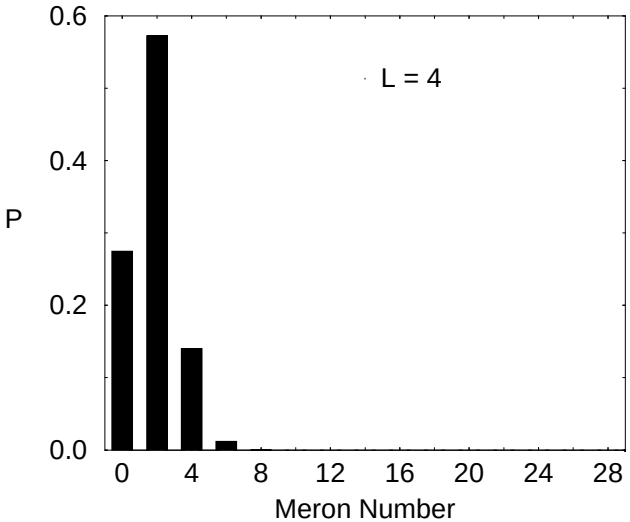
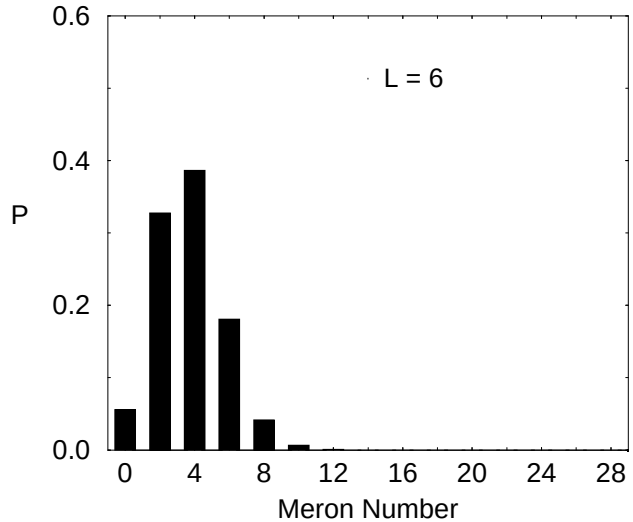
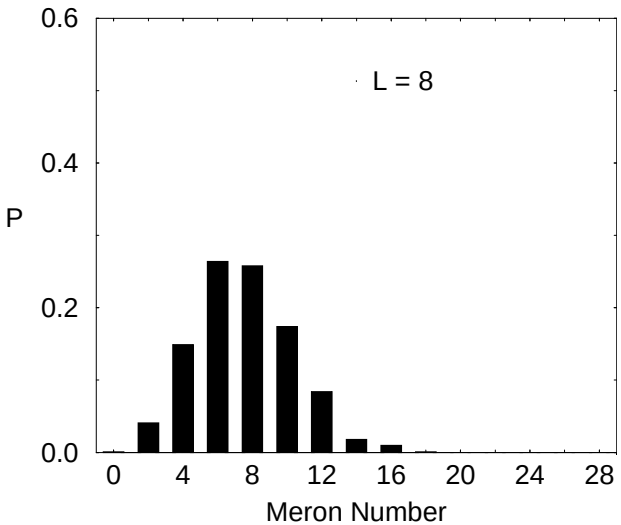
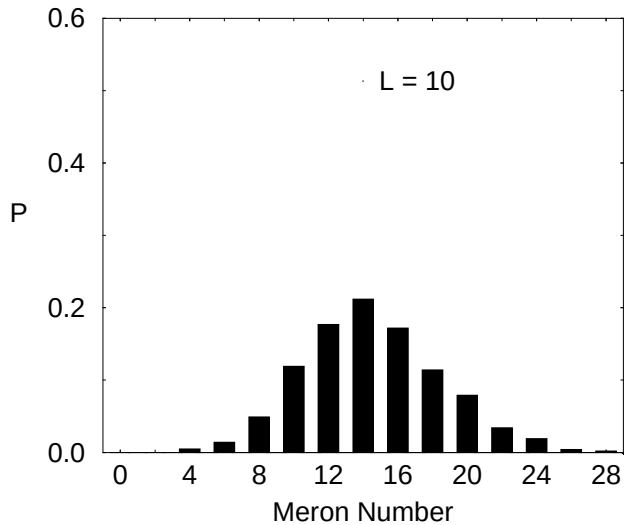
- The flip of a meron-cluster changes the fermion sign.
- Only the 0-meron sector (which contains configurations without merons) contributes to the partition function.
- By appropriate cluster flips one can reach a reference configuration.
- The measurement of 2-point functions also requires sampling the 2-meron sector.

Population of different meron sectors



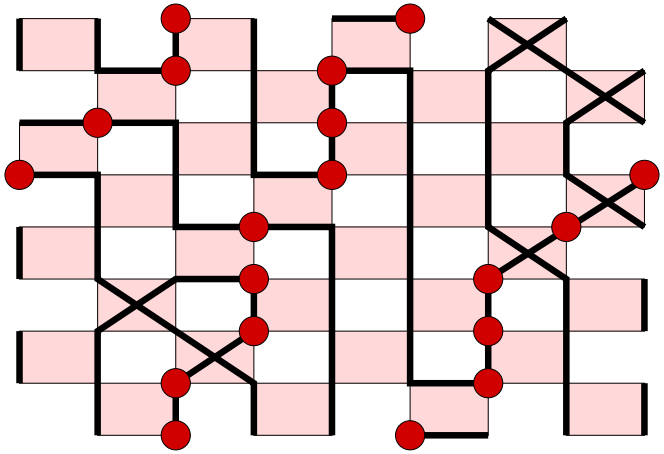




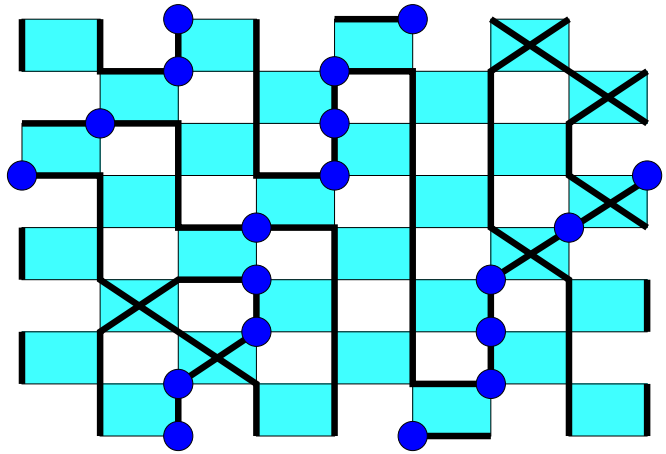


Restricting oneself to the 0-meron sector yields an exponential improvement which completely solves the sign problem.

Class of reference configurations for fermions with spin



Spin up Layer



Spin down Layer

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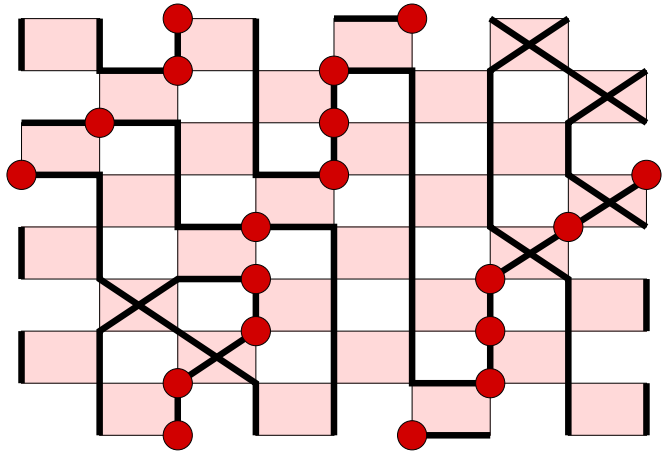

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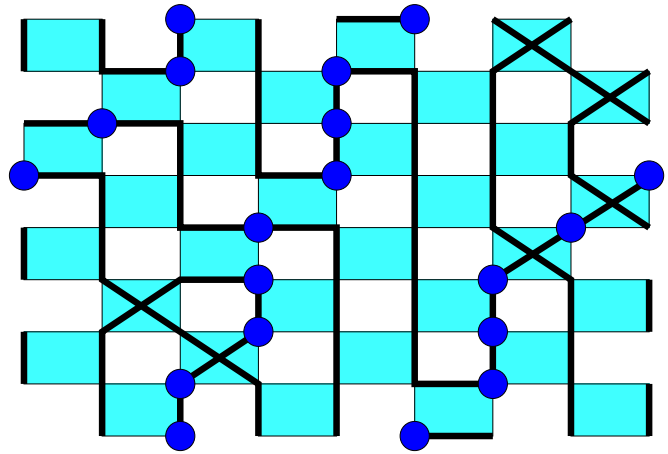

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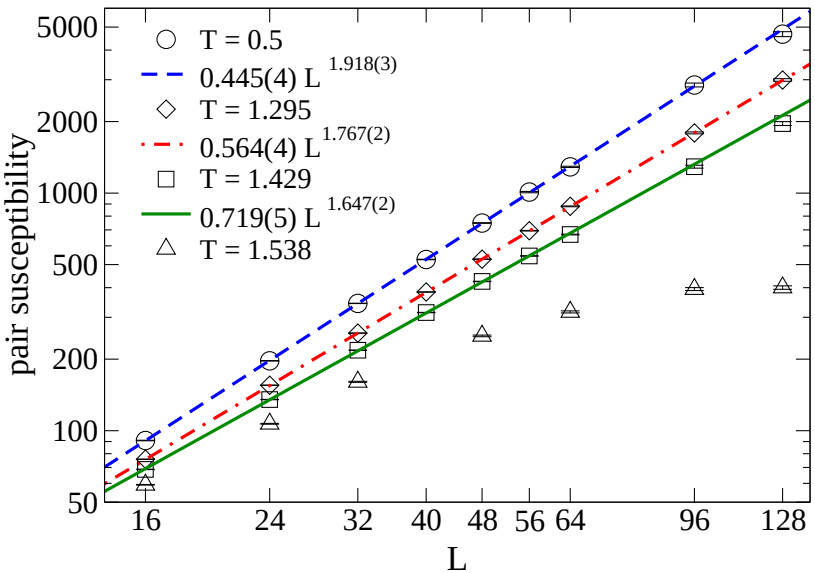
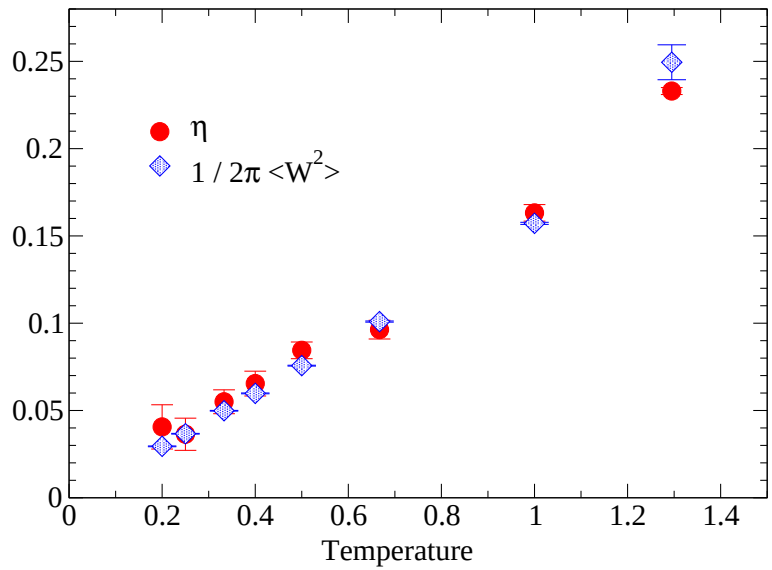




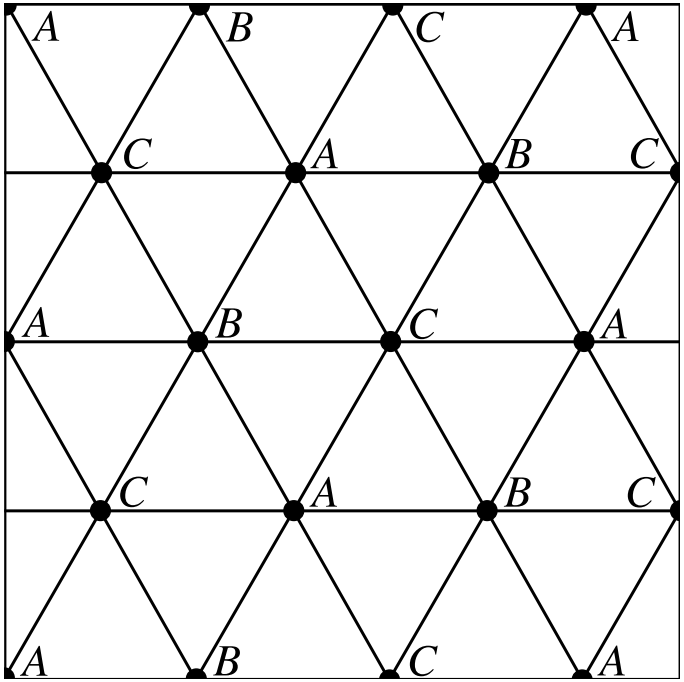
One finds accurate Kosterlitz-Thouless behavior for $L \leq 128$.

S. Chandrasekharan, J. Cox, J. Osborn, and U.-J. W., Nucl. Phys. B673 (2003) 405.

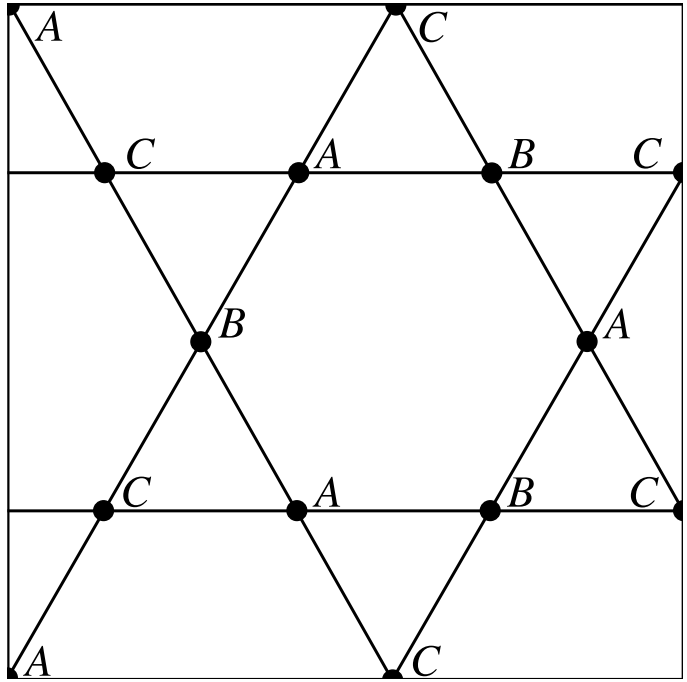
S. Chandrasekharan and J. Osborn, Phys. Rev. B66 (2002) 045113.

Outline

Geometrically frustrated lattices



Triangular lattice



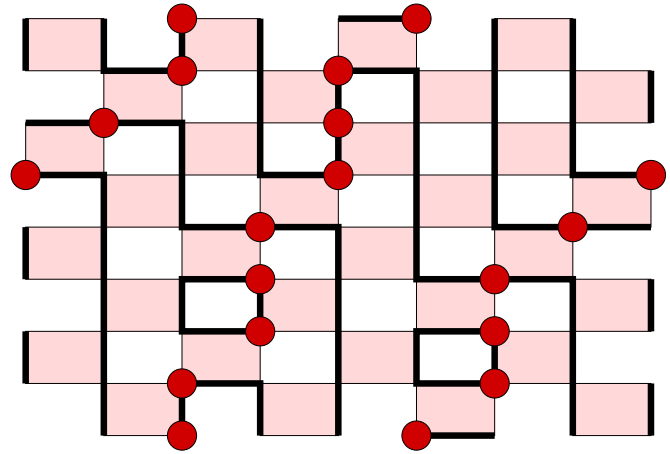
Kagomé lattice

Antiferromagnetic spin $\frac{1}{2}$ Heisenberg Hamiltonian

$$H = J \sum_{x,i} \vec{S}_x \cdot \vec{S}_{x+\hat{i}}$$

Integrating out the spins

$$Z = \sum_{[b]} \mathrm{Sign}[b] W_A^{n_A} W_D^{n_D} 2^{N_C}$$



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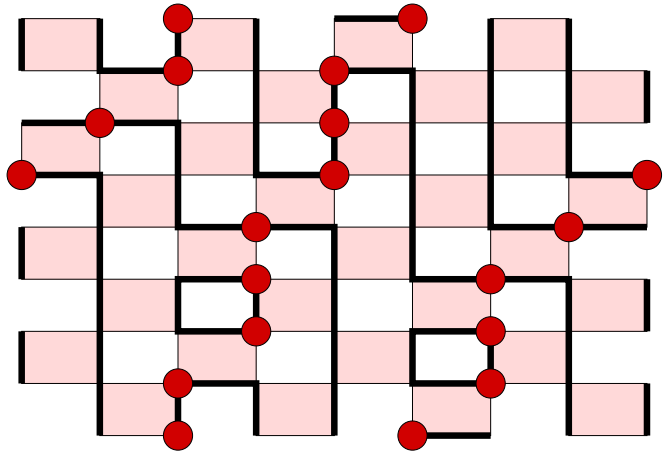

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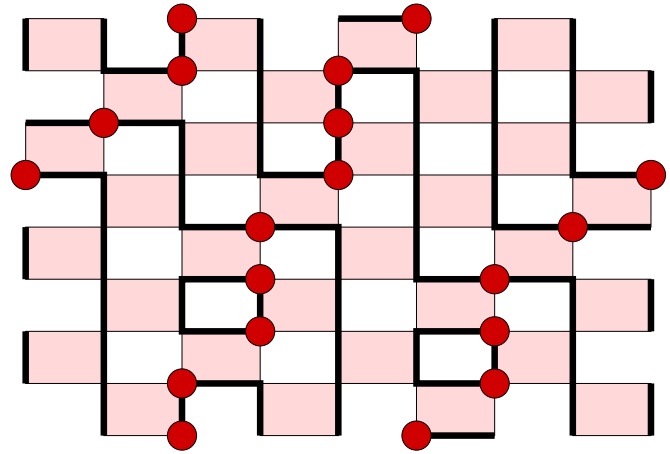

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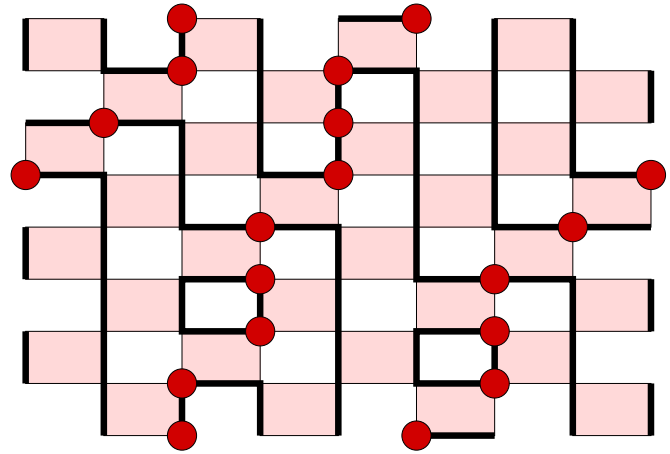

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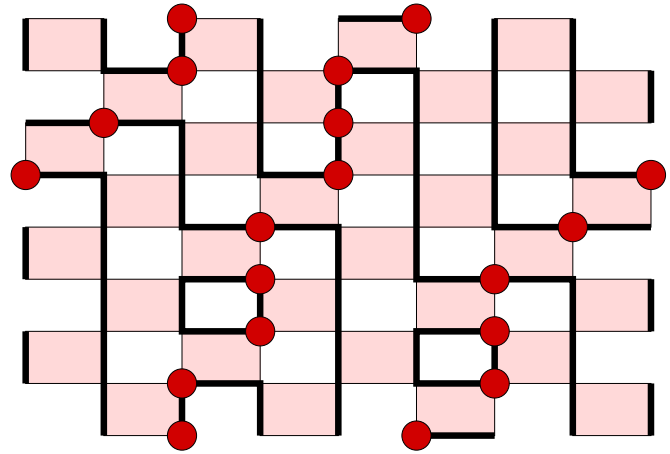

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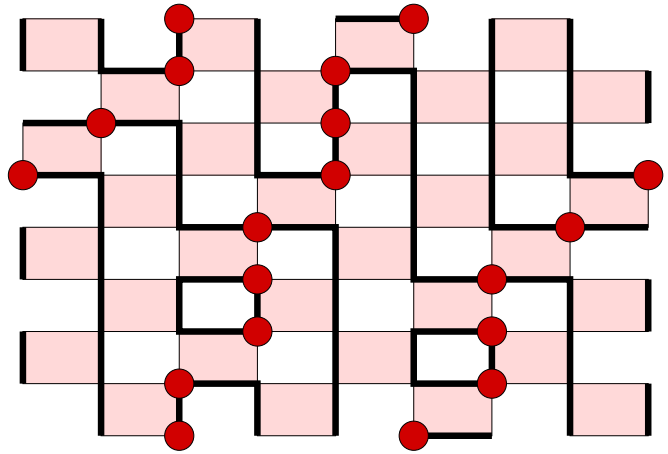
- In this process, break-ups that lead to the decomposition of $\Lambda_{\mathcal{C}}$ into separate clusters must be rejected.

Updating independent regions $\Lambda_{\mathcal{C}}$



Since the different regions $\Lambda_{\mathcal{C}}$ are independent, the improved estimator of the sign factorizes.

Improved estimator for the sign

$$\langle \mathrm{Sign} \rangle_i = \prod_{\Lambda_{\mathcal{C}}} \langle \mathrm{Sign}_{\mathcal{C}} \rangle_i$$

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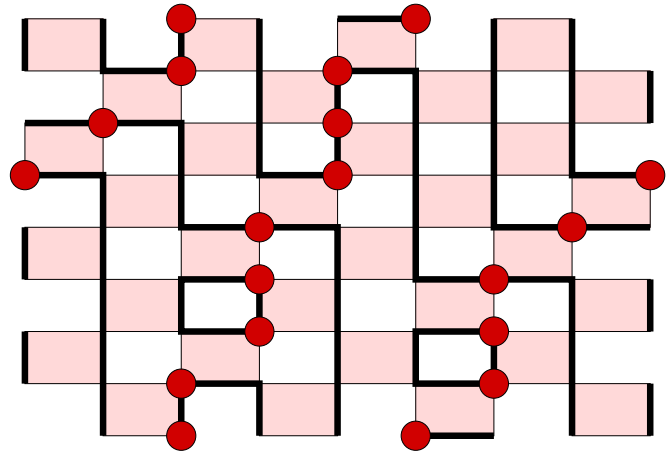

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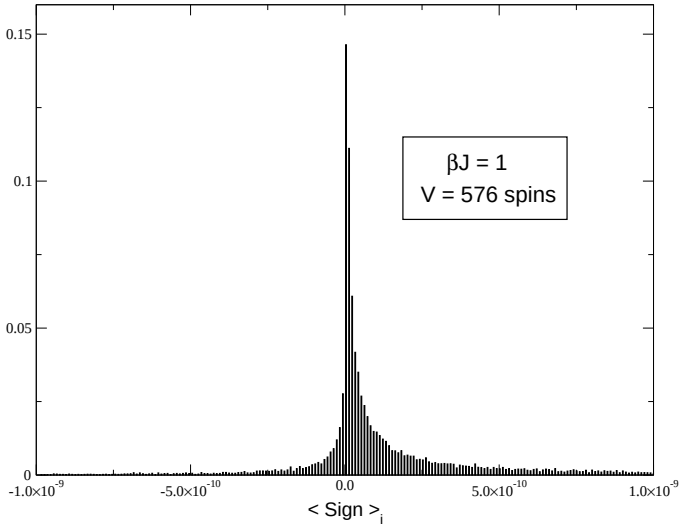
$$\langle \mathrm{Sign} \rangle_i = \prod_{\Lambda_{\mathcal{C}}} \langle \mathrm{Sign}_{\mathcal{C}} \rangle_i$$

Improved estimator for the staggered susceptibility

$$\langle M_s^2 \mathrm{Sign} \rangle_i = \sum_{\Lambda_{\mathcal{C}}} \langle M_{s\mathcal{C}}^2 \mathrm{Sign}_{\mathcal{C}} \rangle_i \prod_{\Lambda_{\mathcal{C}'} \neq \Lambda_{\mathcal{C}}} \langle \mathrm{Sign}_{\mathcal{C}'} \rangle_i$$

Probability distribution of $\langle \text{Sign} \rangle_i$



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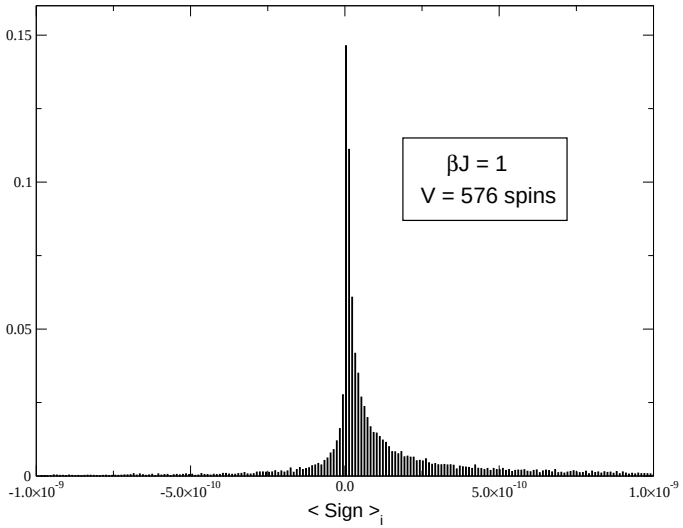
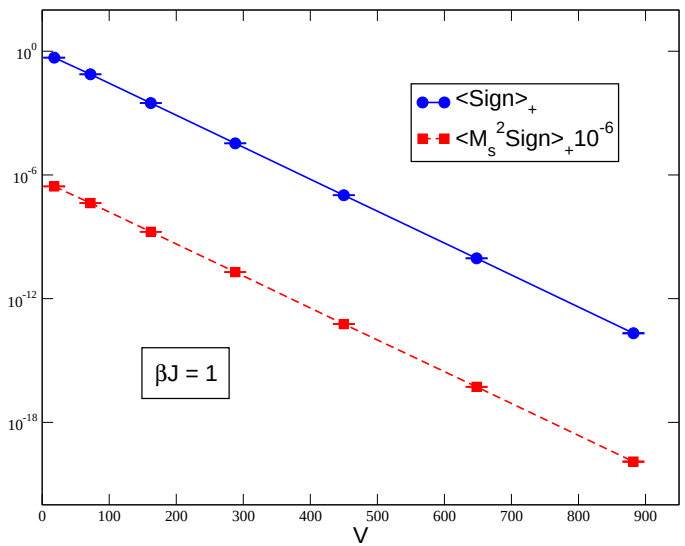
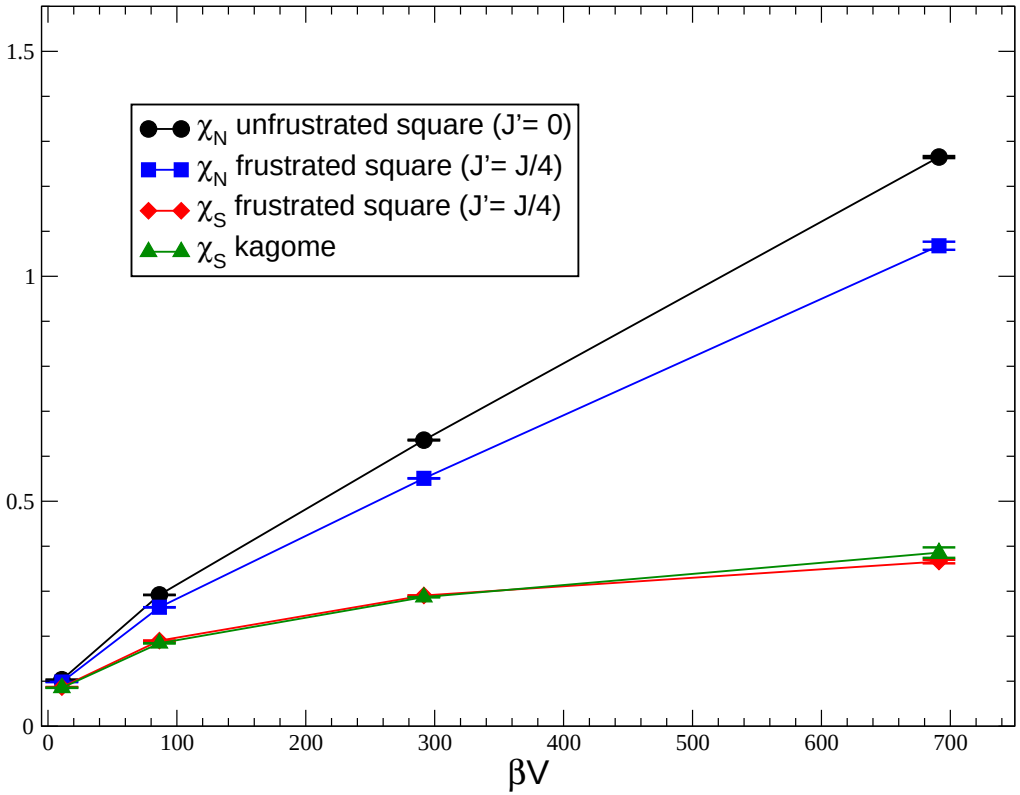


Volume dependence of $\langle \text{Sign} \rangle_i$ and $\langle \mathcal{M}_s^2 \text{Sign} \rangle_i$



Coplanar susceptibility χ_s and collinear Néel susceptibility χ_N



- Susceptibilities can be measured on volumes never reached before.
- However, the nested cluster algorithm works efficiently only at moderate temperatures, when the regions $\Lambda_{\mathcal{C}}$ are not too large.

M. Nyfeler, F.-J. Jiang, F. Kämpfer, and U.-J. W., Phys. Rev. Lett. 100 (2008) 247206.

Outline

Sign Problem and Meron-Cluster Algorithm

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- The meron-cluster algorithm has been applied successfully to relativistic field theories at non-zero chemical potential and at non-zero vacuum angle, to theories of relativistic staggered fermions, as well as to specific models for non-relativistic strongly correlated electrons.

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This workshop is a great opportunity to make further progress.