Cluster Monte Carlo method with a conserved order parameter

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- Combining cluster methods with fixed-magnetisation ensembles was soon identified as a key (but probably intractable) challenge.
- We present a working cluster algorithm with a globally conserved order parameter.
- We work in the Tethered Monte Carlo framework (introduced at CompPhys08), an (almost) fixed-magnetisation ensemble.

Introduction (II)

Main features

- Tethered Ensemble: original d.o.f. + Gaussian *magnetostat*:
  - Micromagnetic ensemble: fixed β and order parameter (m).
  - Tethered ensemble: fixed β and $\hat{m} = m +$ [Gaussian bath].
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- Independent simulations at fixed $\hat{m}$. Later, reconstruction of *canonical* effective potential Ω_N.
- Canonical averages are recovered for any value of the external field h without new simulations.
- Local algorithm (e.g. Metropolis) straightforward.
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  - No critical slowing down for magnetic observables.
  - Other quantities have typical $z = 2$ behavior.
- Here we implement a Swendsen-Wang update scheme and present our results for the $D = 2, 3$ Ising model.

Notations: Ising model

- Standard benchmark for MC simulation methods.
- Partition function and main observables ($N = L^D$):

$$Z = \sum_{\{\sigma_{\boldsymbol{x}}\}} \exp\Big[\beta \sum_{\langle \boldsymbol{x},\boldsymbol{y}\rangle} \sigma_{\boldsymbol{x}}\sigma_{\boldsymbol{y}} + h \sum_{\boldsymbol{x}} \sigma_{\boldsymbol{x}}\Big], \qquad \sigma_{\boldsymbol{x}} = \pm 1,$$

$$E = Ne = -\sum_{\langle \boldsymbol{x},\boldsymbol{y}\rangle} \sigma_{\boldsymbol{x}}\sigma_{\boldsymbol{y}}, \qquad M = Nm = \sum_{\boldsymbol{x}} \sigma_{\boldsymbol{x}}.$$

- We denote canonical averages by $\langle \cdots \rangle_\beta$:

$$C = N[\langle e^2\rangle_\beta - \langle e\rangle_\beta^2], \qquad \chi = N[\langle m^2\rangle_\beta - \langle m\rangle_\beta^2].$$

The Tethered Ensemble (I)

- Canonical pdf for order parameter ($h = 0$),

$$p_1(m) = \frac{1}{Z} \sum_{\{\sigma_{\boldsymbol{x}}\}} \exp[-\beta E] \delta\Big(m - \sum_i \sigma_i / N \Big)$$

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- A smooth $p(\hat{m})$ has an effective potential $\Omega_N(\hat{m}, \beta)$

$$p(\hat{m}) = \frac{1}{Z} \int_{-\infty}^{\infty} \prod_{i=1}^{N} \mathrm{d}\eta_i \sum_{\{\sigma_{\boldsymbol{x}}\}} \mathrm{e}^{-\beta E - \sum_i \frac{\eta_i^2}{2}} \delta\Big(\hat{m} - m - \sum_i \frac{\eta_i^2}{2N}\Big) = \mathrm{e}^{N\Omega_N(\hat{m},\beta)}$$

The tethered ensemble (II)

- Integrating demons out in the *constrained* (fixed $\hat{m}$) partition function → tethered expectation values:

$$\langle O \rangle_{\hat{m},\beta} = \frac{\sum_{\{\sigma_{\boldsymbol{x}}\}} O(\hat{m};\{\sigma_{\boldsymbol{x}}\})\,\omega(\beta,\hat{m},N;\{\sigma_{\boldsymbol{x}}\})}{\sum_{\{\sigma_{\boldsymbol{x}}\}} \omega(\beta,\hat{m},N;\{\sigma_{\boldsymbol{x}}\})},$$

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$$\hat{h}(\hat{m};\{\sigma_{\boldsymbol{x}}\}) = -1 + \frac{N/2-1}{\hat{M}-M} \quad \Longrightarrow \quad \langle \hat{h} \rangle_{\hat{m},\beta} = \frac{\partial \Omega_N(\hat{m},\beta)}{\partial \hat{m}}.$$

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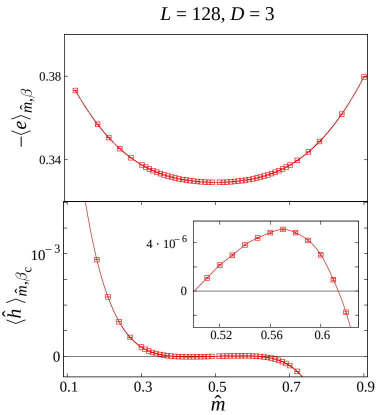
- Tethered mean values $\langle O \rangle_{\hat{m},\beta}$ ↔ canonical mean values $\langle O \rangle_\beta(h)$, for any external field h:

$$\langle O \rangle_\beta(h) = \int \mathrm{d}\hat{m}\; \langle O \rangle_{\hat{m},\beta} \exp[N(\Omega_N(\hat{m}, \beta) + h\hat{m})].$$

Numerical methods



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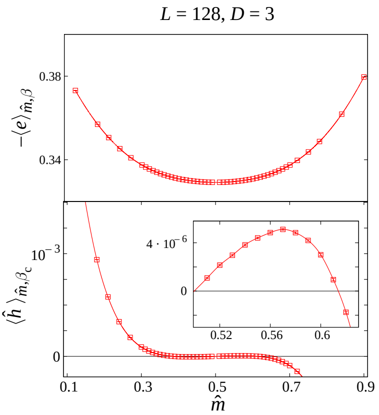

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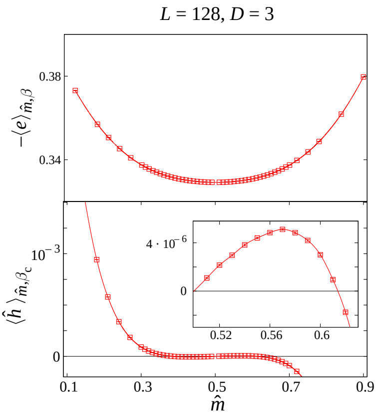

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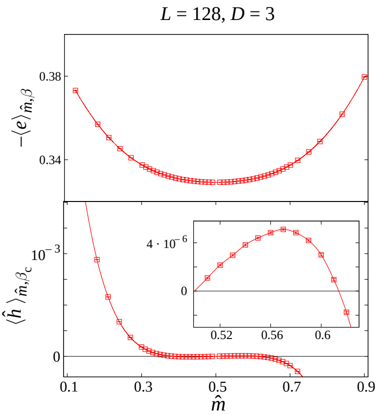

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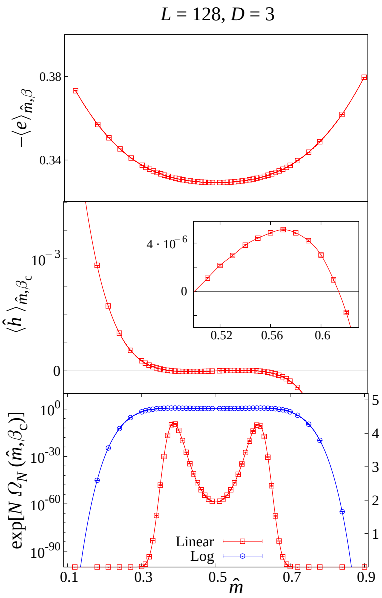

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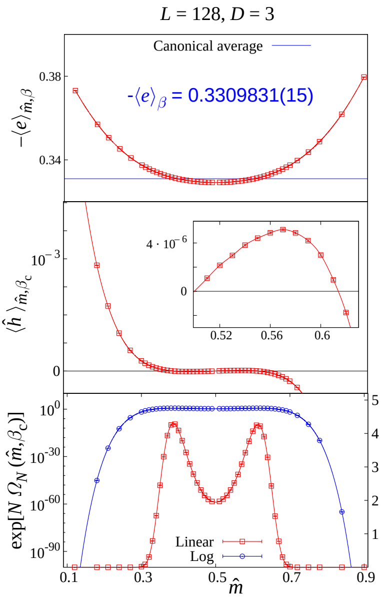

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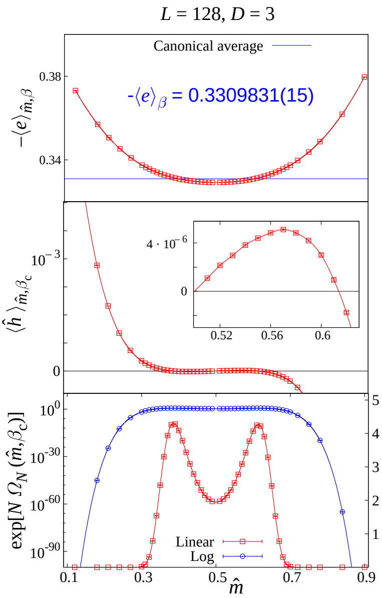

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7. Systematic errors: refine $\hat{m}$ grid.

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- We can follow the Fortuin-Kasteleyn construction.
- Introduce bond-occupation variables n_{xy} $(= 0, 1)$:

$$\mathrm{e}^{\beta(\sigma_x \sigma_y - 1)} = \sum_{n_{xy}=0,1} [(1-p)\delta_{n_{xy},0} + p\delta_{\sigma_x,\sigma_y}\, \delta_{n_{xy},1}], \quad p = 1-\mathrm{e}^{-2\beta}.$$

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  - Given $\{n_{xy}\}$, the spins within cluster i are equal to $S_i = \pm 1$. Not all $\{S_i\}$ configurations have the same probability:

$$p(\{S_i\}) \propto \mathrm{e}^{M-\hat{M}}(\hat{M}-M)^{(N-2)/2}\,\theta(\hat{M}-M).$$

The cluster update algorithm (II)

a) Cluster tracing

b) Cluster flipping:

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b) Cluster flipping: It is impossible to consider all 2^{N_C} cluster orientations

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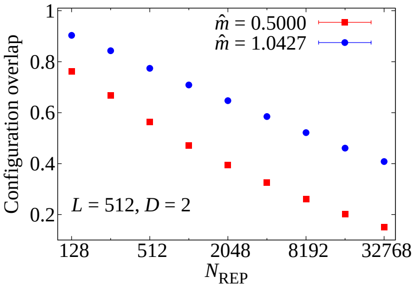

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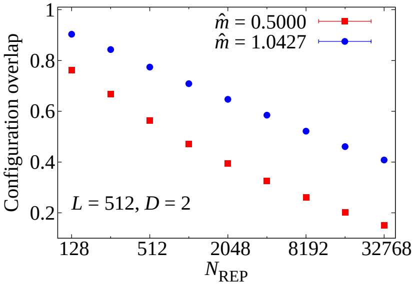
- Measuring $\hat{h}$ at each of the N_{REP} steps reduces errors by up to a factor 25.



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Integrated autocorrelation times

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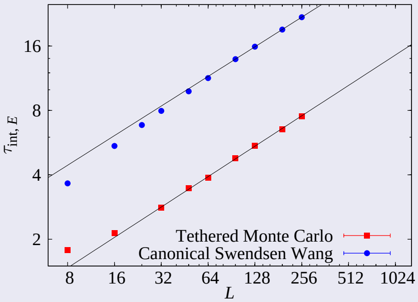

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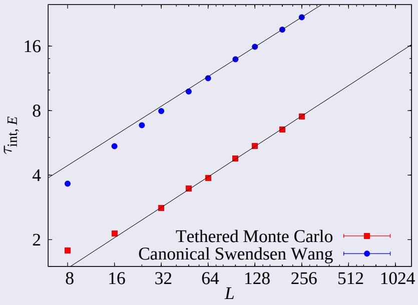

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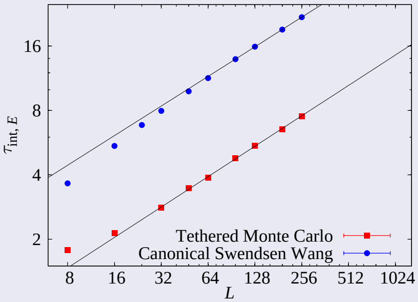
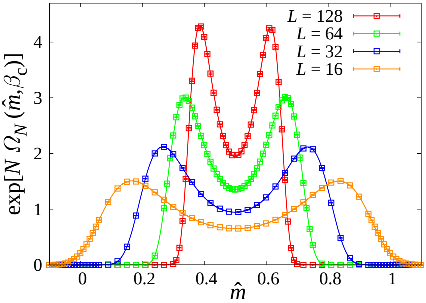


Canonical averages for $L = 128$, $D = 3$

	MCS	$-\langle e \rangle_\beta$	C	χ	ξ
SW	48×10^6	0.3309822(16)	22.155(18)	21193(13)	82.20(3)
TMC	50×10^6	0.3309831(15)	22.174(13)	21202(13)	82.20(5)

A funny way of computing the anomalous dimension



L	$\hat{m}_{\text{peak}} - \frac{1}{2}$
48	0.18956(4)
64	0.16341(4)
96	0.13240(4)
128	0.114083(24)
192	0.09246(4)
256	0.07959(12)
η	0.0360(7)

- $p(\hat{m}, \beta_{\text{c}}, L) = L^{\frac{\beta}{\nu}} f\left(L^{\frac{\beta}{\nu}}(\hat{m} - \frac{1}{2})\right)$

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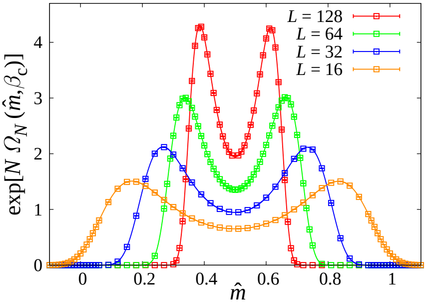

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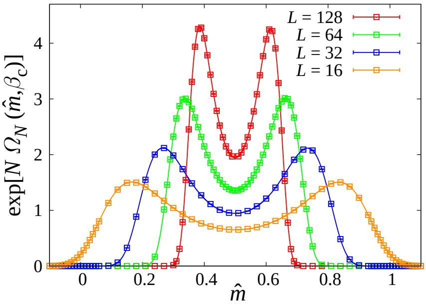

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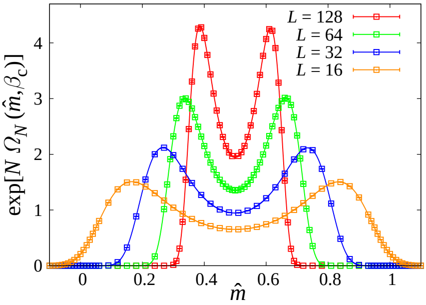

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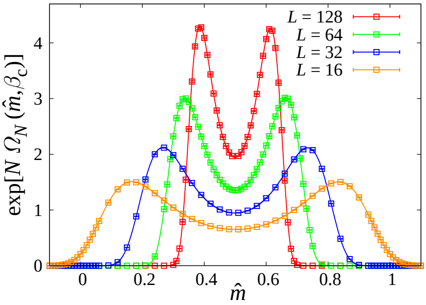

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- Previous determinations for $D = 3$:
  - HT-expansion: $\eta = 0.03639(15)$ (Campostrini et al., 2002).
  - MC + perfect action: $\eta = 0.0362(8)$ (Hasenbusch, 2001).

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- Current and future work
  - Diluted Antiferromagnet in a Field (TMC + Metropolis).
  - Condensation transition (TMC + cluster).