Tethered Monte Carlo: computing the effective potential without critical slowing down

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- All known Monte Carlo methods suffer critical or *exponential* slowing down when applied to important problems:
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- We present here Tethered Monte Carlo, a general method to reconstruct the effective potential for the order parameter.
- Even if we do *not* work in the canonical ensemble, canonical expectation values are recovered with high accuracy.

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- Local algorithm (e.g. Metropolis) straightforward.
- Method demonstrated in the two dimensional Ising model.
- Currently implementing cluster methods: improved estimators promising.

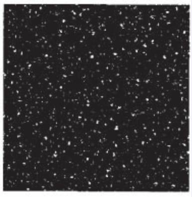
Notations: $D = 2$ Ising model

- Exact results available even for *finite* lattices.
- Partition function and main observables:

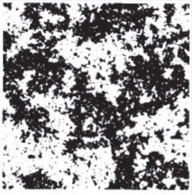
$$Z = \sum_{\{\sigma_{\boldsymbol{x}}\}} \mathrm{e}^{\beta \sum_{\langle \boldsymbol{x},\boldsymbol{y}\rangle} \sigma_{\boldsymbol{x}}\sigma_{\boldsymbol{y}} + h \sum_{\boldsymbol{x}} \sigma_{\boldsymbol{x}}}, \qquad \sigma_{\boldsymbol{x}} = \pm 1,$$

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

- Second order phase transition at $\beta_c = 0.440\,686\ldots$.



$\beta \gg \beta_c$



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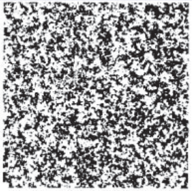

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The Tethered Ensemble (I)

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

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

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- Extend configuration space with N decoupled Gaussian demons

$$Z = \int_{-\infty}^{\infty} \prod_{i=1}^{N} \mathrm{d}\eta_i \sum_{\{\sigma_{\boldsymbol{x}}\}} \exp\left[-\beta U - \sum_i \eta_i^2 / 2 \right], \qquad R = Nr = \sum_i \eta_i^2 / 2.$$

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

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

The tethered ensemble (II)

- Integrating demons out in the *constrained* (fixed $\hat{m}$) partition function $\rightarrow$ 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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- The *canonical* Ω_N follows from Fluctuation-Dissipation

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

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- Tethered mean values $\langle O \rangle_{\hat{m},\beta}$ ↔ canonical mean values $\langle O \rangle_{\beta}$,

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

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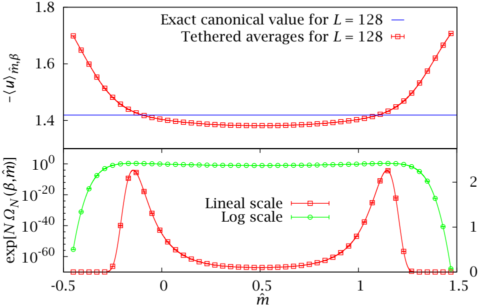

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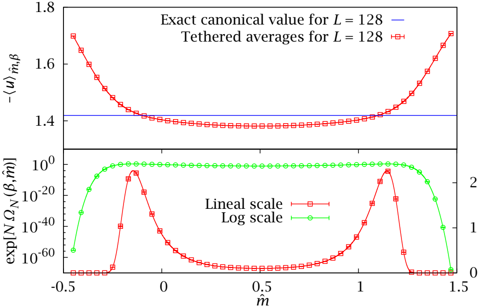
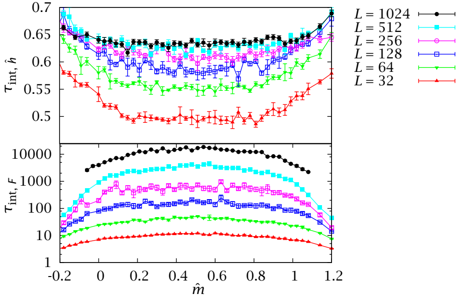


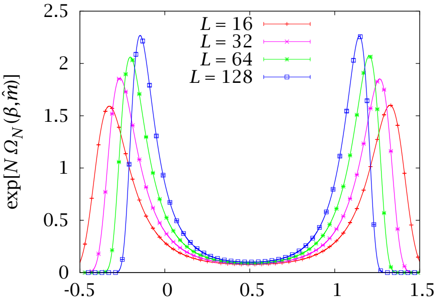
Tethered: $\langle u \rangle_{\beta_c} = -1.419\,05(5)$
Exact: $\langle u \rangle_{\beta_c} = -1.419\,076\ldots$

Autocorrelation times



- τ_{int}: dramatic dependence on observable, and on $\hat{m}$.
- Functions of m (e.g. $\hat{h}$): no measurable critical slowing down.
- Energy or propagator's Fourier transform ($\vec{k} \neq 0$) $\tau_{\text{int}}(\hat{m} = 0.5) \approx L^2$ Worst case: $m \sim 0$ or $\hat{m} = \frac{1}{2}$.

Results at the critical point



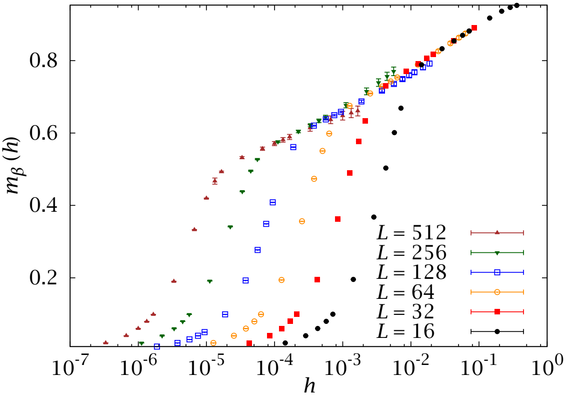
Parameters

- 51 points in $\hat{m}$ mesh for $L \leq 256$.
- 77 points in $\hat{m}$ mesh for $L \geq 512$.
- 10^7 Metropolis sweeps per $\hat{m}$.
- Comparison with Ferdinand and Fisher's exat results for finite L.

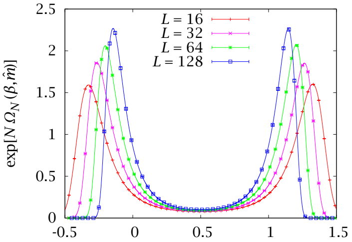
L	**Energy**		**Specific heat**	
	TMC	**Exact**	**TMC**	**Exact**
32	-1.433 69(4)	-1.433 659...	9.509(3)	9.509 4...
64	-1.423 97(4)	-1.423 938...	11.285(6)	11.288 1...
128	-1.419 05(5)	-1.419 076...	13.063(10)	13.060 1...
256	-1.416 63(5)	-1.416 645...	14.83(2)	14.829...
512	-1.415 42(4)	-1.415 429...	16.57(3)	16.595...
1024	-1.414 89(5)	-1.414 821...	18.28(8)	18.361...

Results in an external field: magnetization $m(h)$

- No new simulations needed to obtain results in a field
- Just shift $\Omega_N(\hat{m},\beta) \to \Omega_N(\hat{m},\beta) - \hat{m}h$, and normalize $p(\hat{m},\beta,h)$.

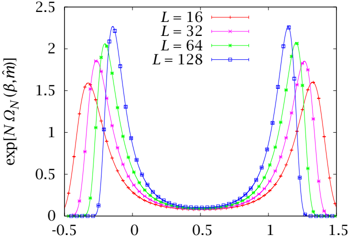


A funny way of computing the anomalous dimension



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

A funny way of computing the anomalous dimension



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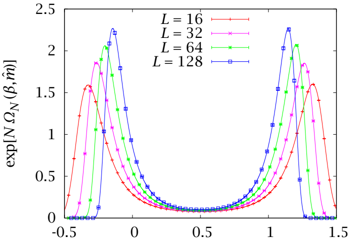

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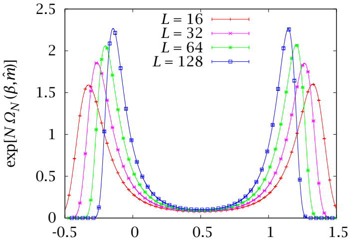

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- Finding maxima numerically ill conditioned. Finding roots is OK: $0 = \langle \hat{h} \rangle_{\frac{1}{2}+m^{\pm},\beta_c}$ (byproduct, simulation not optimized to this aim)

$$m^{\pm} = L^{-\frac{1}{8}}[A + BL^{-\frac{7}{4}}],\ \chi^2/\mathrm{dof} = 0.98/4^{(-)}, 2.85/4^{(+)}$$

L	$-m^{-}_{\mathbf{peak}}$	$m^{+}_{\mathbf{peak}}$
32	0.764 01(10)	0.764 31(11)
64	0.702 86(18)	0.703 0(2)
128	0.645 3(3)	0.645 1(4)
256	0.592 1(7)	0.591 0(7)
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- Promising when suffering from large tunneling barriers associated to the order parameter: Random Field Ising Model, Diluted antiferromagnets on a field, Condensation transition,. . .