Simulated tempering and magnetizing simulations of a Potts model

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Background

- Monte Carlo (MC) and molecular dynamics (MD) simulations are extensively used in computational physics.

- To enhance the sampling efficiency, the generalized-ensemble (aka extended-ensemble) algorithms are developed and applied, such as the multicanonical algorithm (MUCA) [*], simulated tempering (ST) [**], and replica-exchange method [***] (REM) (aka parallel tempering).

[*] BA Berg and T. Neuhaus: Phys. Lett. B **267**, 249 (1991) BA Berg and T. Neuhaus: Phys. Rev. Lett. **68**, 9 (1992)
[**] AP Lyubartsev et al: JCP **96**, 1776 (1992); E. Marinari and G. Parisi: EPL **19**, 451 (1992)
[***] K. Hukushima and K. Nemoto: JPSJ **65**, 1604 (1996)

Motivation

- Whether the dimensional generalization of ST helps perform simulations better.

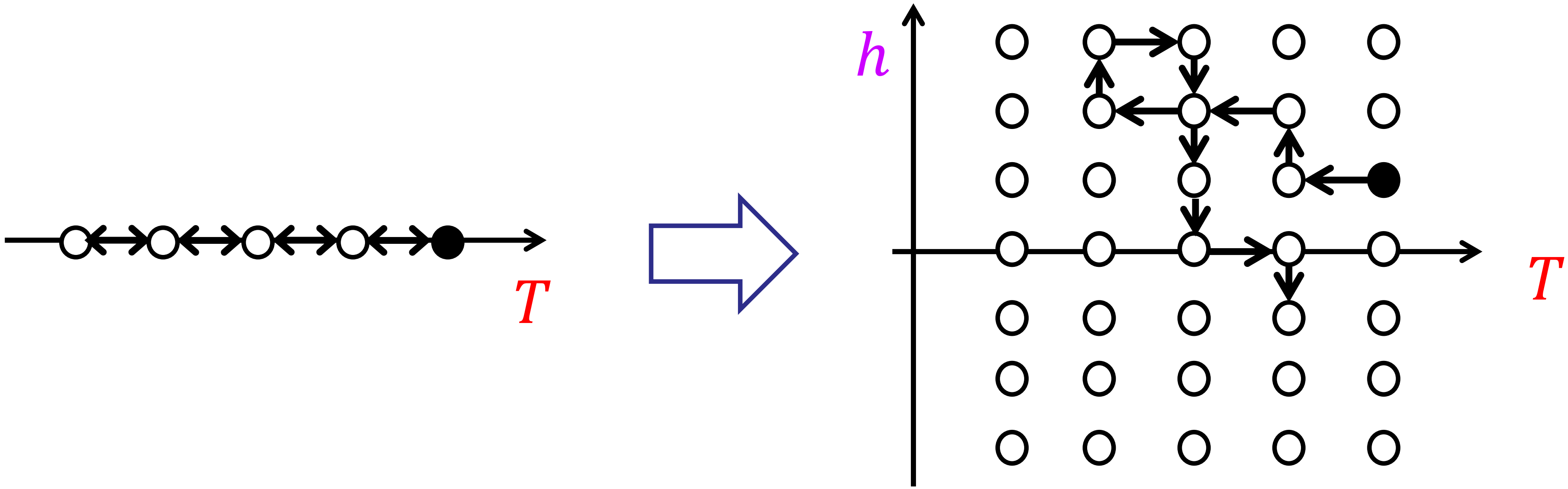
$$P(E, T) \propto e^{-\beta E + a(T)}$$

$$P(E, T, h) \propto e^{-\beta(E + hM) + a(T, h)}$$

We addressed this question by applying the two-dimensional ST method to the two-dimensional Potts model (and Ising model).

A. Mitsutake and Y. Okamoto.: J. Chem. Phys. **130**, 214105 (2009)
T.Nagai and Y. Okamoto: Phys Rev E **86,** 056705 (2012); arXiv: 1205:2523 arXiv:[cond-mat.stat-mech]
T.Nagai, Y. Okamoto, and W. Janke,: in preparation.

"Simulated Tempering and Magnetizing" (STM)



$$P(E, T) \propto e^{-\beta E + a(T)}$$

$$P(E, T, h) \propto e^{-\beta(E + hM) + a(T, h)}$$

Reconstruction of canonical ensembles

One can reconstruct the canonical ensemble via the conditional probability.

$$P(\{\sigma_l\}, T, h) \propto e^{-(E-hM)/T + a(T,h)},$$

$$P(\{\sigma_l\} | T_i, h_j) \propto e^{-\frac{(E-h_jM)}{T_i}}$$

(Accordingly, the conditional expectation gives the canonical average.)

Reweighting techniques

They give free energy values (necessary as STM parameters $a(T,h)$) with preliminary simulations.

WHAM

$$n(E,M) = \frac{\sum_{T_i,h_j} n_{T_i,h_j}(E,M)}{\sum_{T_i,h_j} N_{T_i,h_j} \exp(f(T_i,h_j) - (E - h_j M)/T_i)}$$

$$f(T_i,h_j) = -\log \sum_{E,M} n(E,M) \exp(-(E - h_j M)/T_i)\,,$$

A. Mitsutake and Y. O.: J. Chem. Phys. **130**, 214105 (2009)
S. Kumar, et al.: J. Computational Chemistry **13,** 1011 (1992)

MBAR

$$f(T_i,h_j) = -\log \sum_{n=1}^{N} \frac{\exp(-(E_n - h_j M_n)/T_i)}{\sum_{k=1}^{N_T} \sum_{l=1}^{N_h} N_{T_k,h_l} \exp(f(T_k,h_l) - (E_n - h_l M_n)/T_k)}$$

M. Shirts and J. Chodera: J. Chem. Phys. **129**, 124105 (2008)

Reweighting techniques

Thermal quantity

$$\langle A \rangle_{T,h} = \sum_{n=1}^{N} W_{na} A(x_n)\,,$$

$$W_{na} = \frac{1}{\langle c_a \rangle} \frac{\exp(-(E_n - hM_n)/T)}{\sum_{k=1}^{N_T} \sum_{l=1}^{N_h} N_{T_k,h_l} \exp(f(T_k,h_l) - (E_n - h_l M_n)/T_k)}\,,$$

$$\langle c_a \rangle = \sum_{n=1}^{N} \frac{\exp(-(E_n - hM_n)/T)}{\sum_{k=1}^{N_T} \sum_{l=1}^{N_h} N_{T_k,h_l} \exp(f(T_k,h_l) - (E_n - h_l M_n)/T_k)}\,.$$

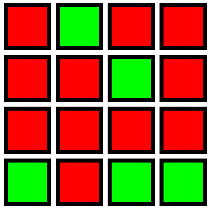
M. Shirts and J. Chodera: J. Chem. Phys. **129**, 124105 (2008)
A. Mitsutake, Y. Sugita, and Y. Okamoto.: J. of Chem. Phys **118**, 6664 (2003).

Review of application to Ising model

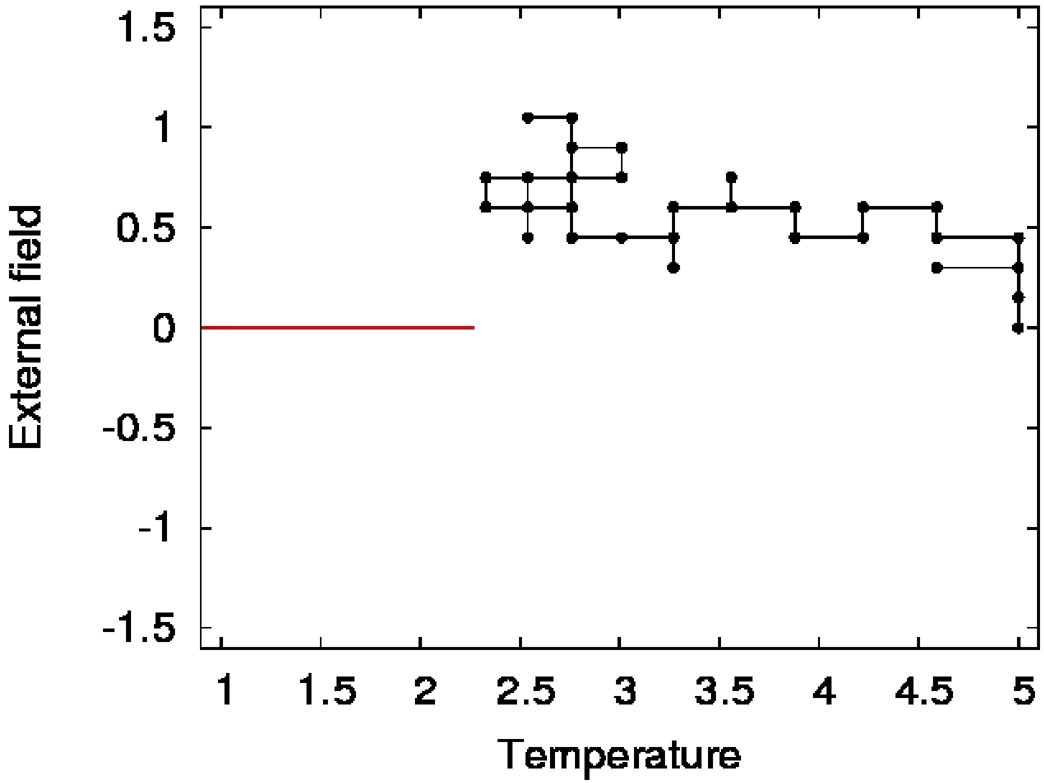
Hamiltonian: $H = E - hM$,

where $E = \sum_{<i,j>} \sigma_i \sigma_j$, $M = \sum_i \sigma_i$.

Weight: $P(\{\sigma_i\}, T, h) \propto e^{-(E-hM)/T+a(T,h)}$,



Two-dimensional Ising model (4X4)



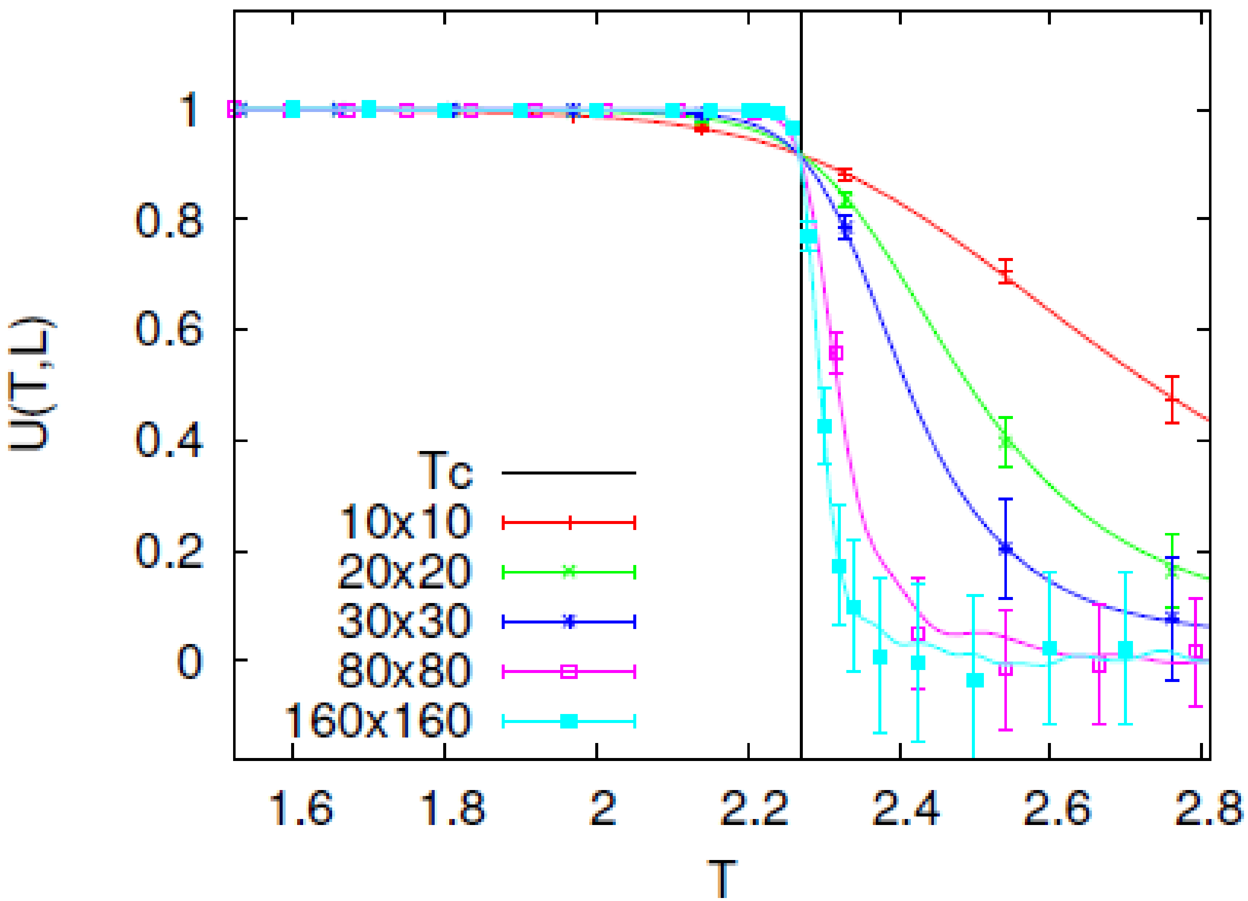
At every flame, 5000 MC sweeps.
Change by 1000 MC sweeps.

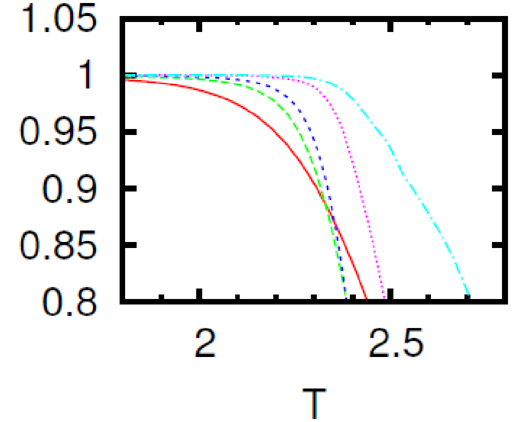
ST-Freq: 50
TvsH=0.5
L=20

T.Nagai and Y. Okamoto: Phys Rev E **86,** 056705 (2012); arXiv: 1205:2523 arXiv:[cond-mat.stat-mech]

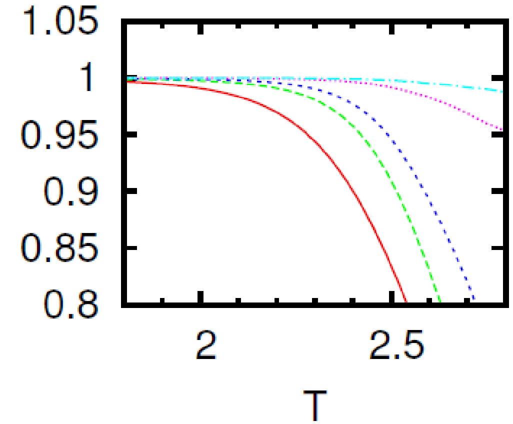
Binder Cumlant

Those lines can be obtained by a single run for each.





$h = 0.01$



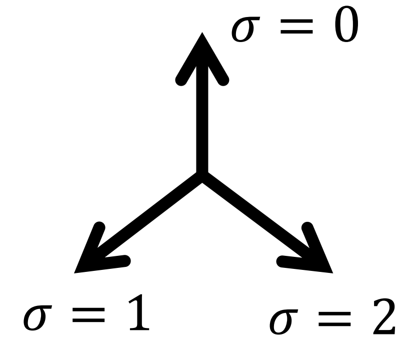
$h = 0.05$

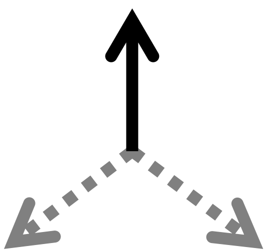
K. Binder, Z. f. Phys. B **43**, 119 (1981).

Potts Model

Hamiltonian: $H = E - hM$,

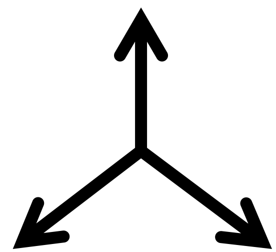
where $E = \sum_{<i,j>} \delta_{\sigma_i,\sigma_j}$, $M = \sum_i \delta_{0,\sigma_i}$.





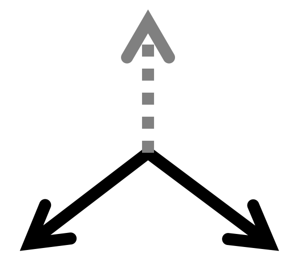
$h > 0$

State 0 is favored. No phase transitions.



$h = 0$

All the three states are equivalent.

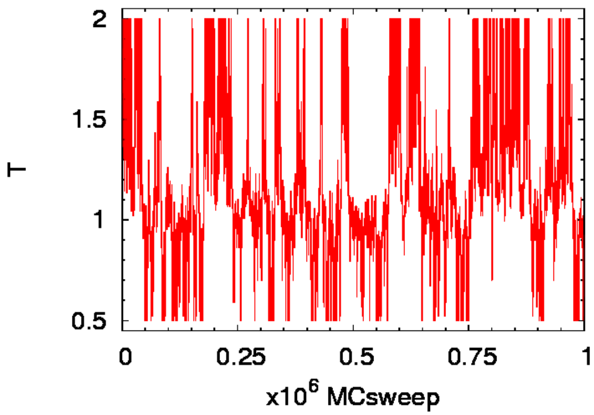


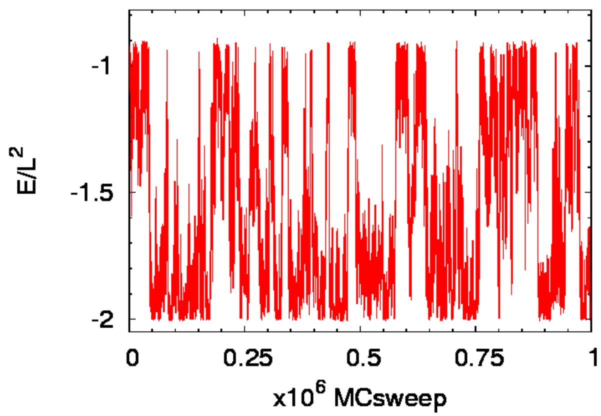
$h < 0$

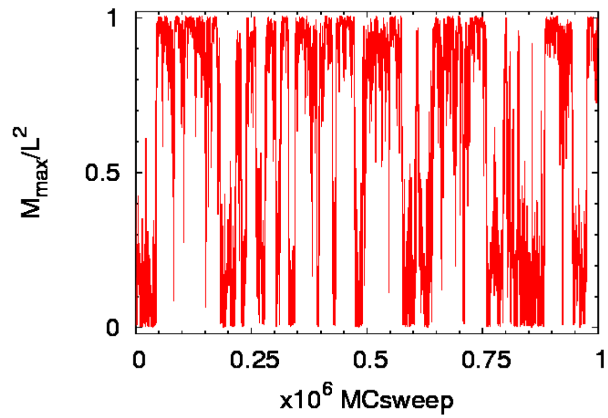
State 0 is disfavored. Behave like an Ising model.

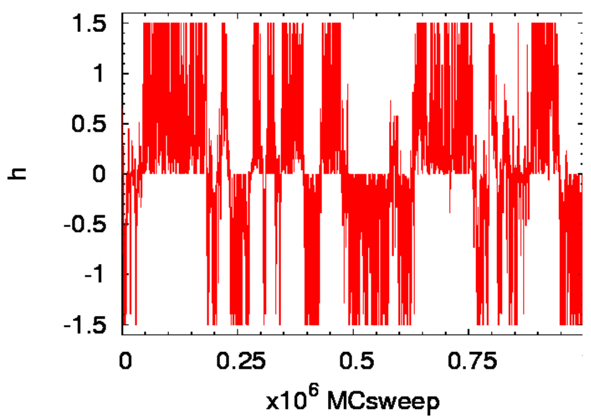
Results

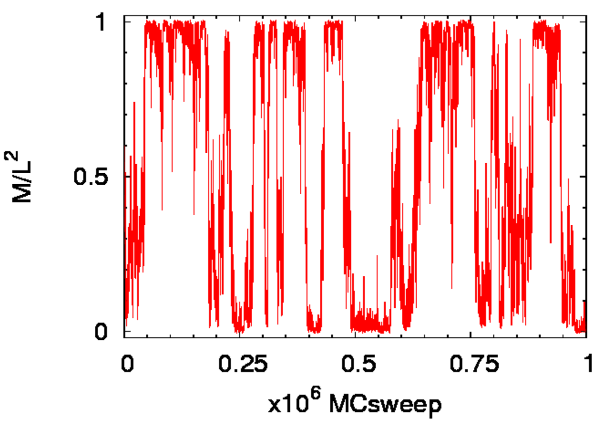
- Random walks realized in $T, h, E, M, M_{\max}$







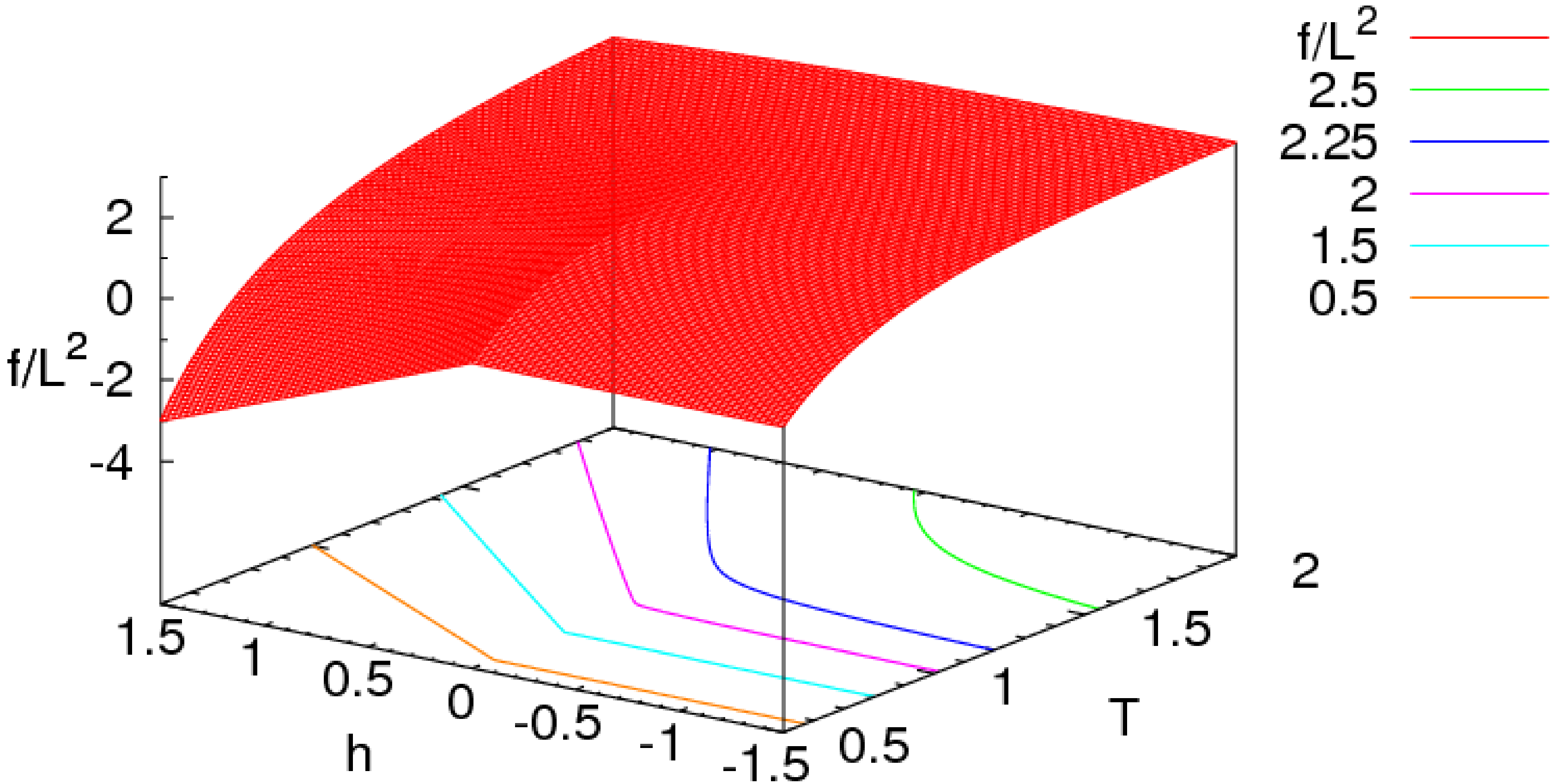




$$M_{\max} \equiv \left\{ \max_{j=0,1,2} \left[\sum_{i}^{L^2} \delta_{j,\sigma_i} \right] - \frac{L^2}{3} \right\} \times \frac{3}{2}$$

L=80

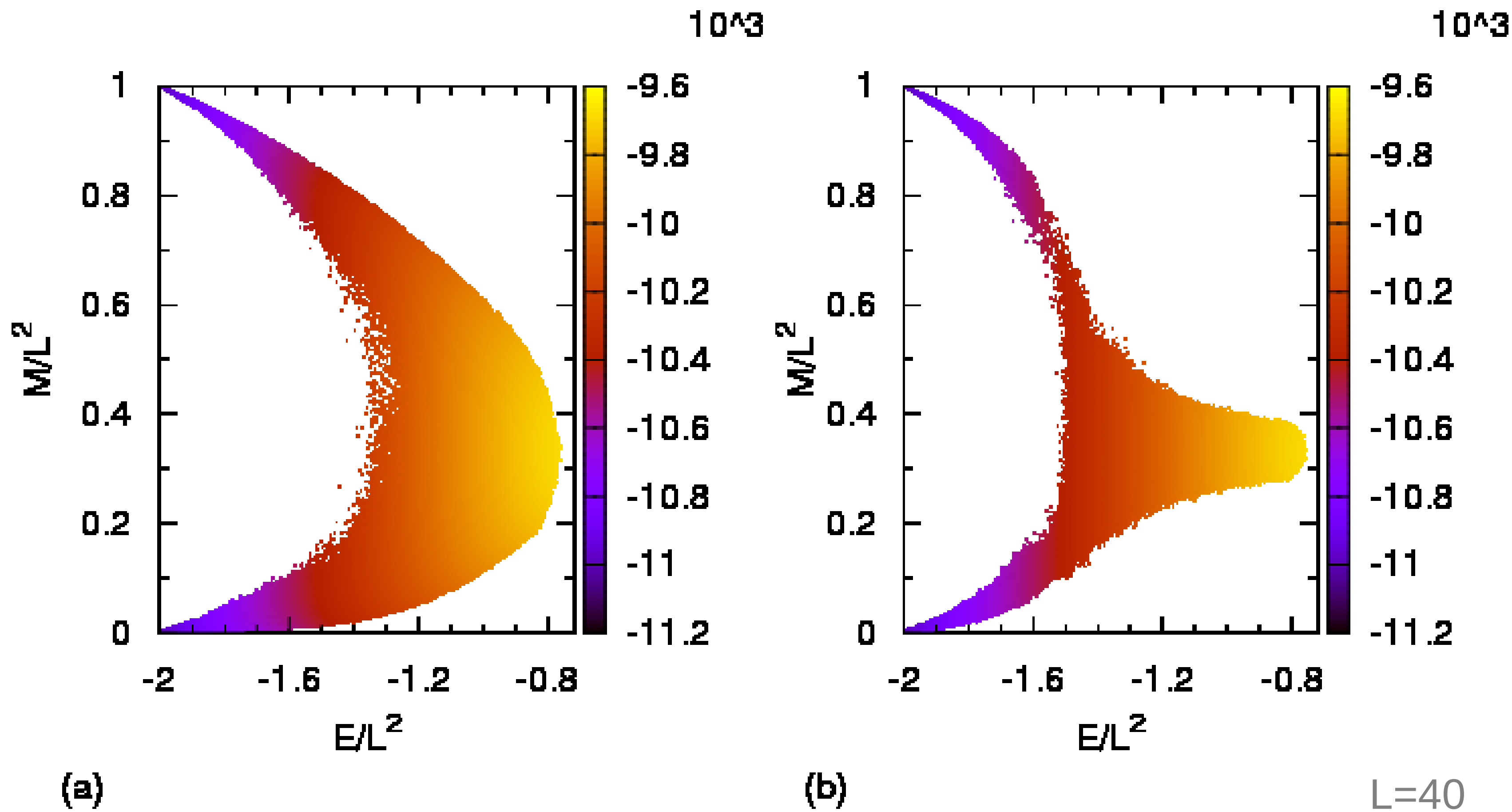
Dimensionless free energy



L=80

Density of states

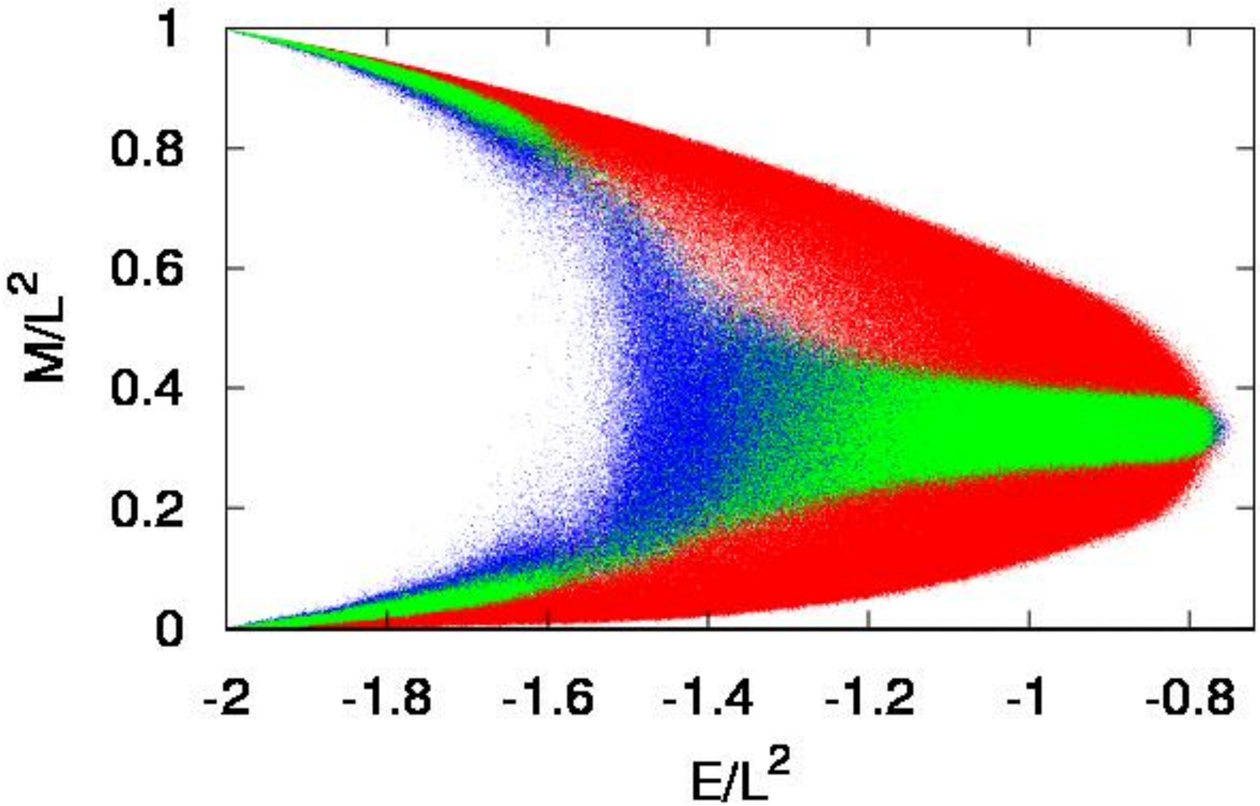
Wider areas of DOS were gained by STM than by ST.



L=40

Area really enlarged?

How the area sampled is exactly different?

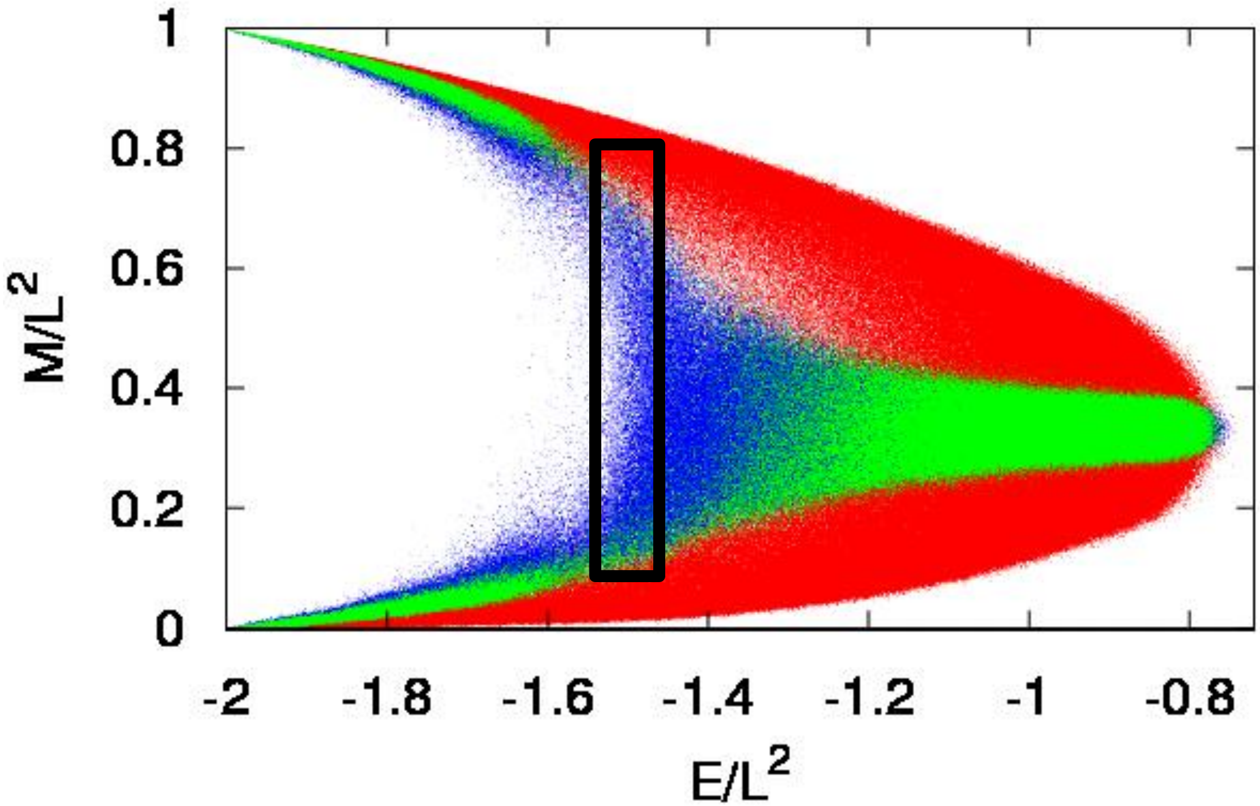


red: by STM only
green: by both
blue: by ST only
L=40

THERE ARE AREAS IN BLUE AREN’T THERE?

Area really enlarged?

How the area sampled is exactly different?

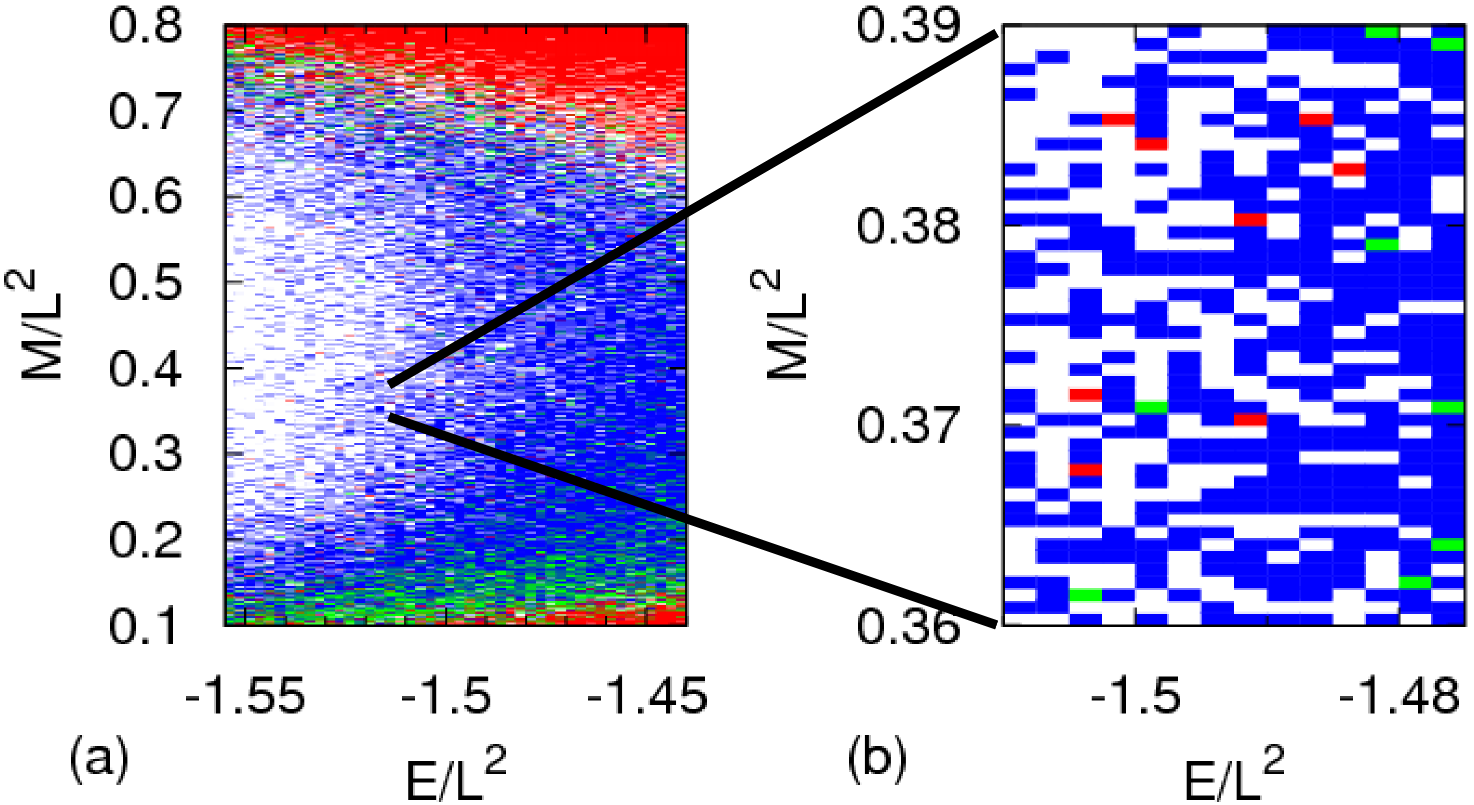


red: by STM only
green: by both
blue: by ST only
L=40

THERE ARE AREAS IN BLUE AREN’T THERE?

The difference zoomed up

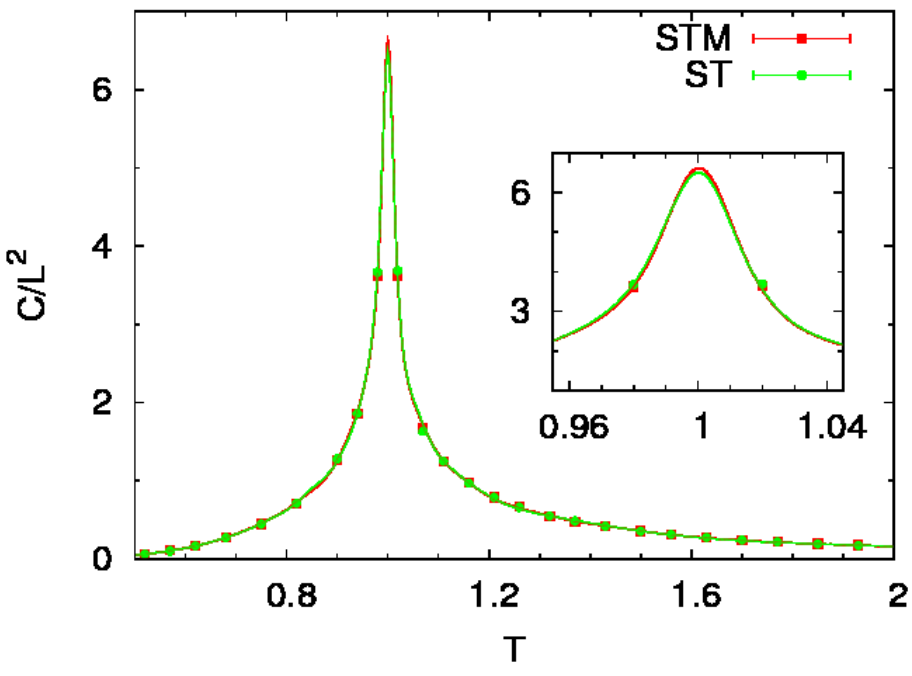
Yes, but the red and green segments are among blue regions!

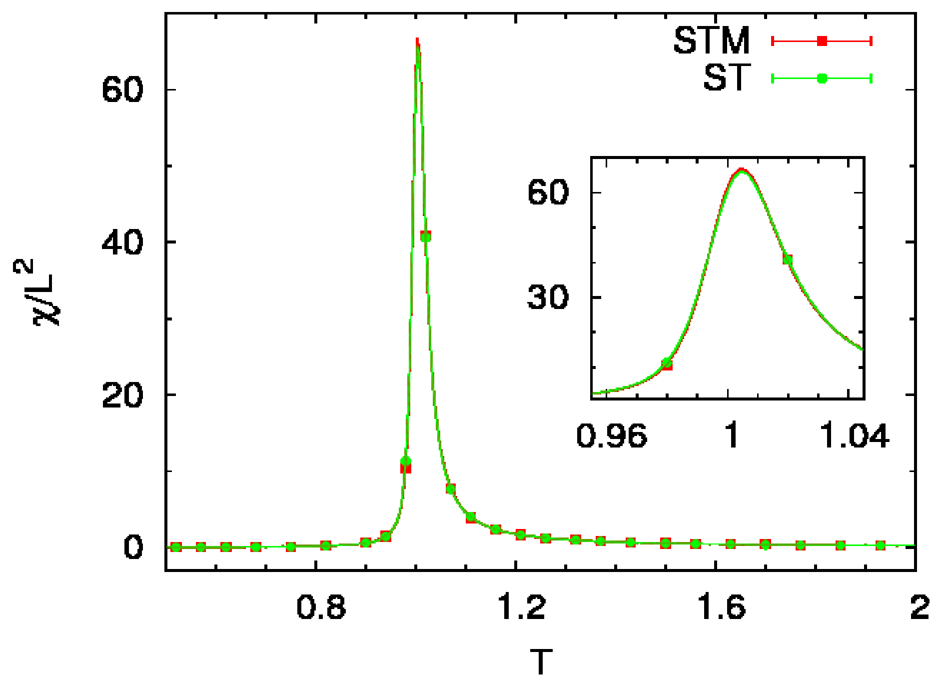


red: by STM
green: both
blue: by ST

It’s not relevant

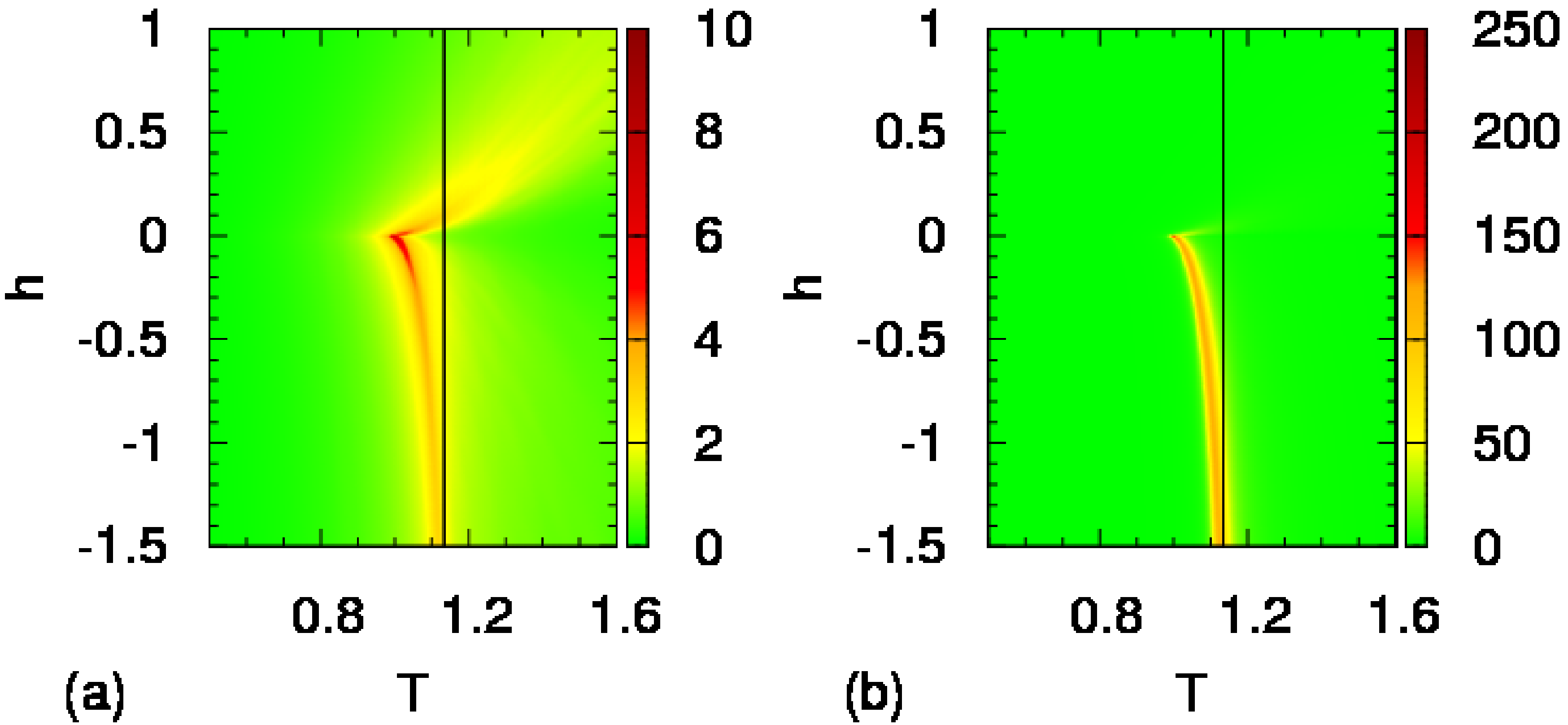
Reweighting results for $h = 0$ are shown. The reweighting techniques work properly!! Thus, those representative are sampled well with STM. The ST method draws more samples from the narrower area.



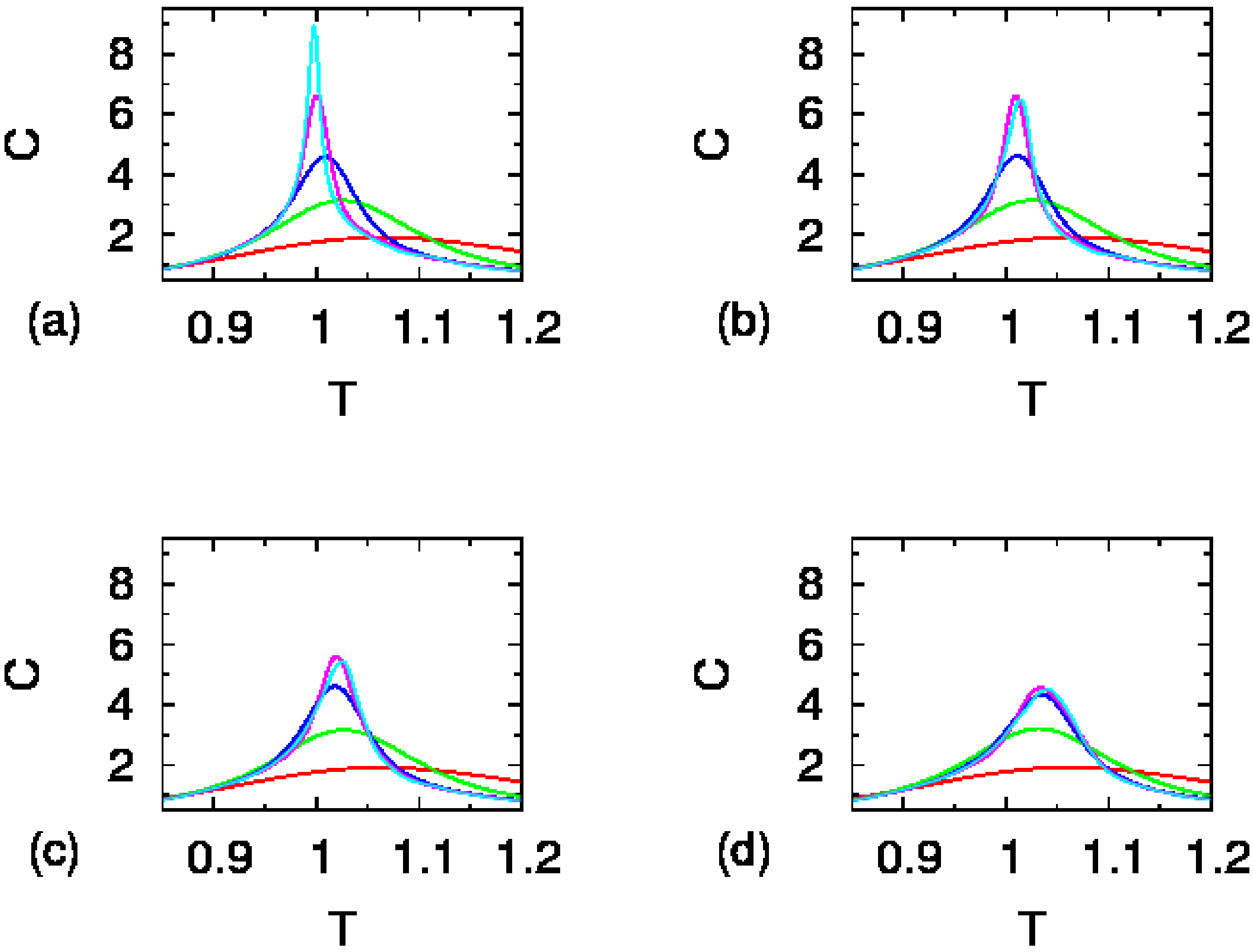


Reweighting around wide area

- Reweighting in a wide area is possible.
- Specific heat and susceptibility. (L=80)



Reweighting around wide area 2



L=5, 10, 20, 40, and 80

(a) h=0

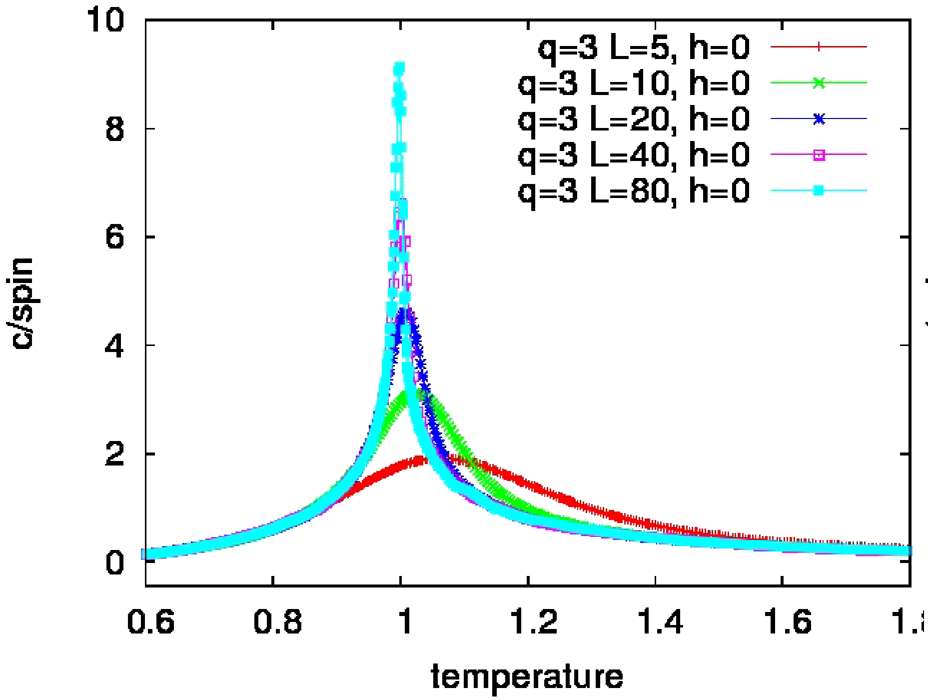
(b) h=0.005

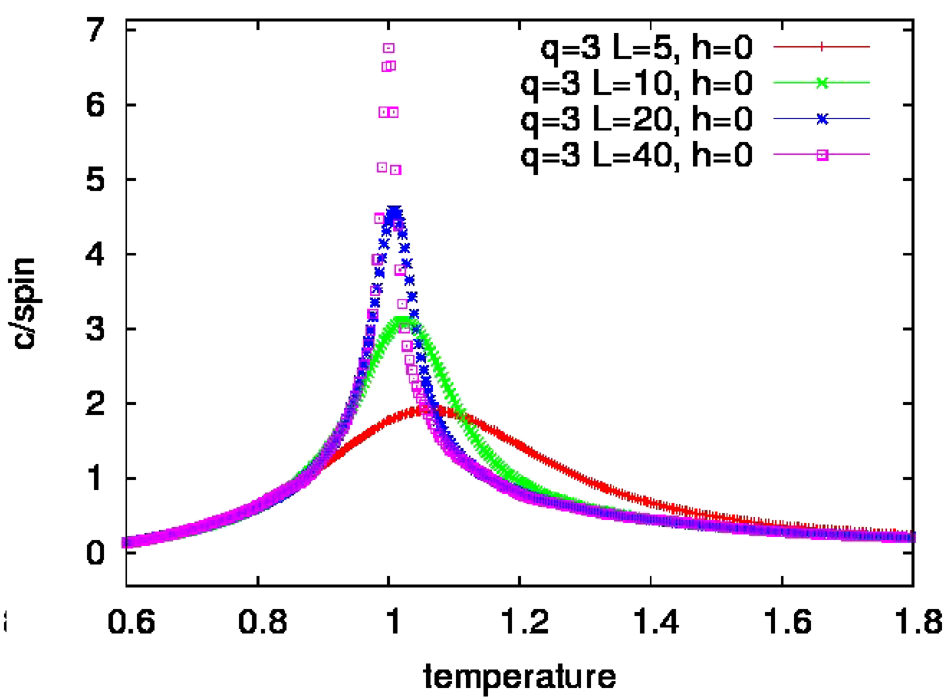
(c) h=0.01

(d) h=0.02

Specific heat C converges at smaller L as h increases.

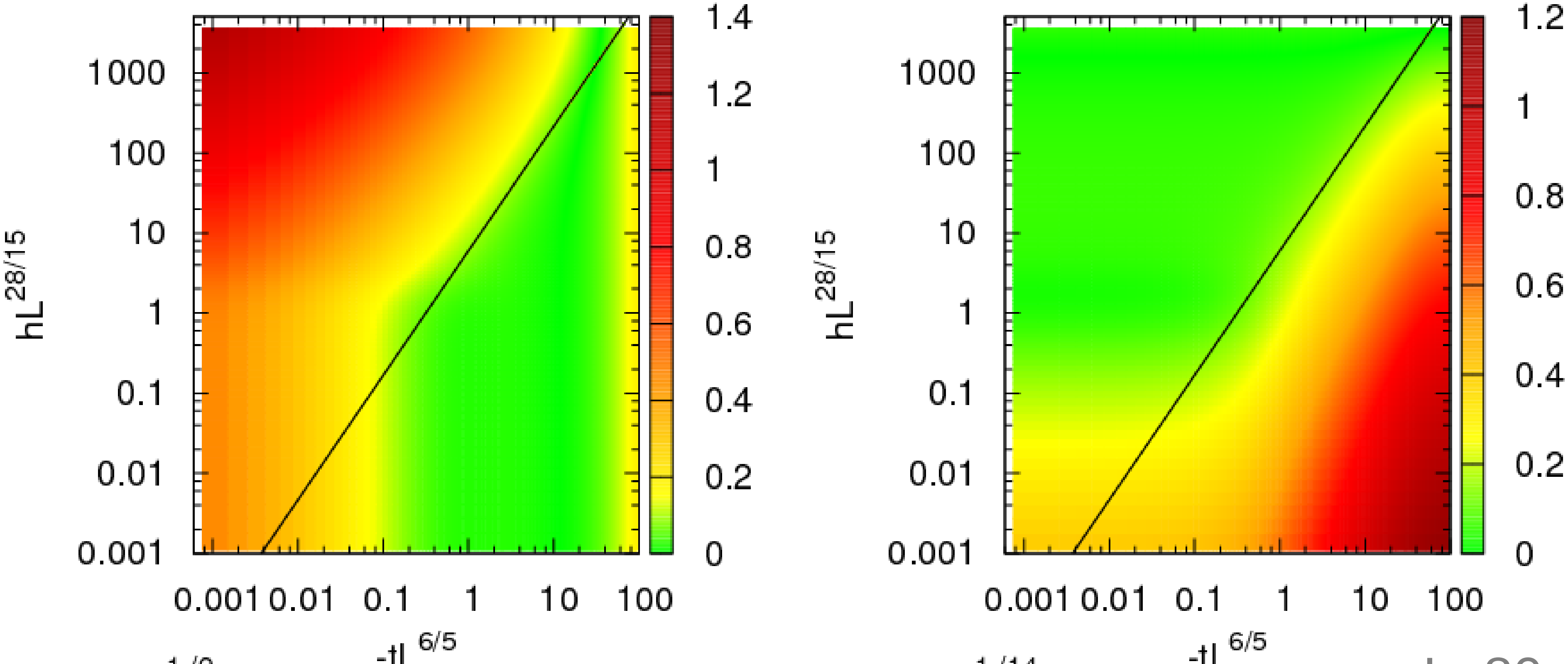
As an animation





Crossover with respect to *h* and *t*

$\propto m - t^{1/9}$ $\quad\quad$ $\propto m - h^{1/14}$



(a) m-$t^{1./9}$

(b) m-$h^{1./14}$

L=80

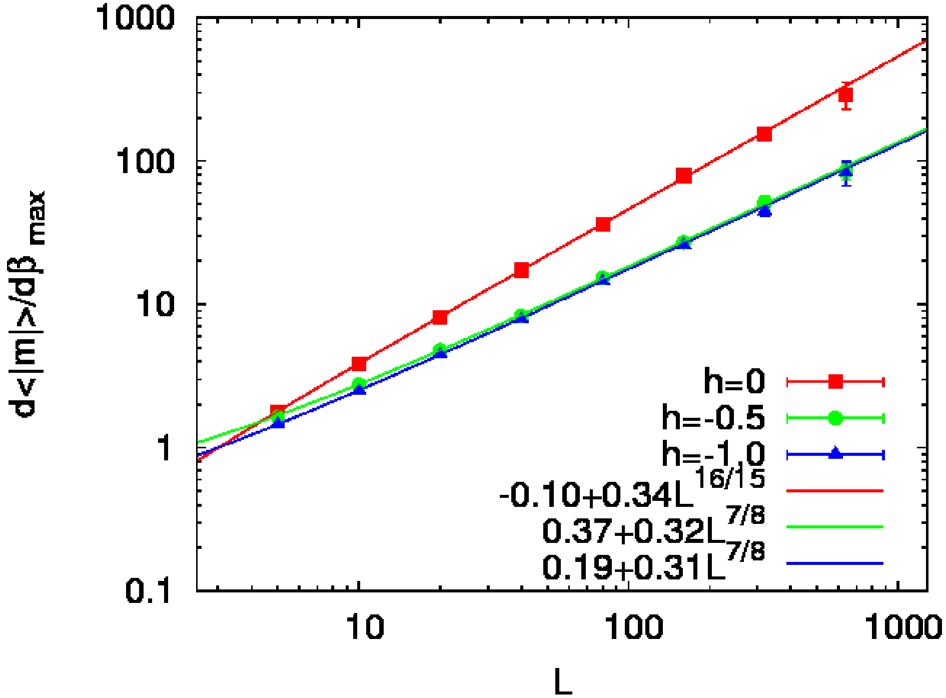
$$t = |T - T_c|/T_c$$

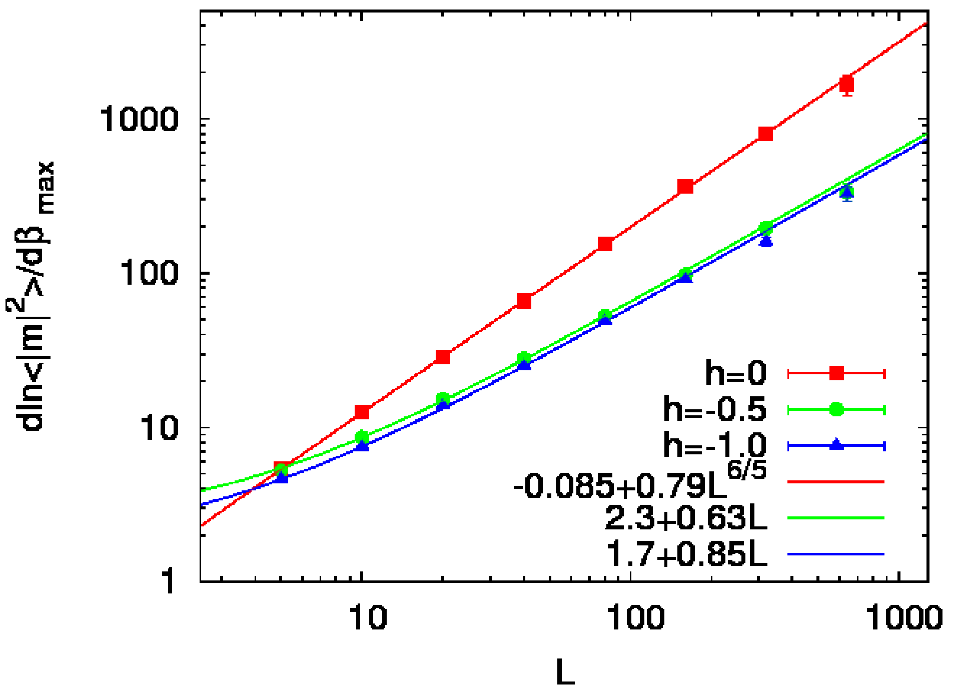
$$L^{2/15} m = \psi(tL^{6/5}, hL^{28/15})$$

$t^{-14/9} h \ll 1$: $m \sim t^{1/9}$

$t^{-14/9} h \gg 1$: $m \sim h^{1/14}$

Crossover 2-1

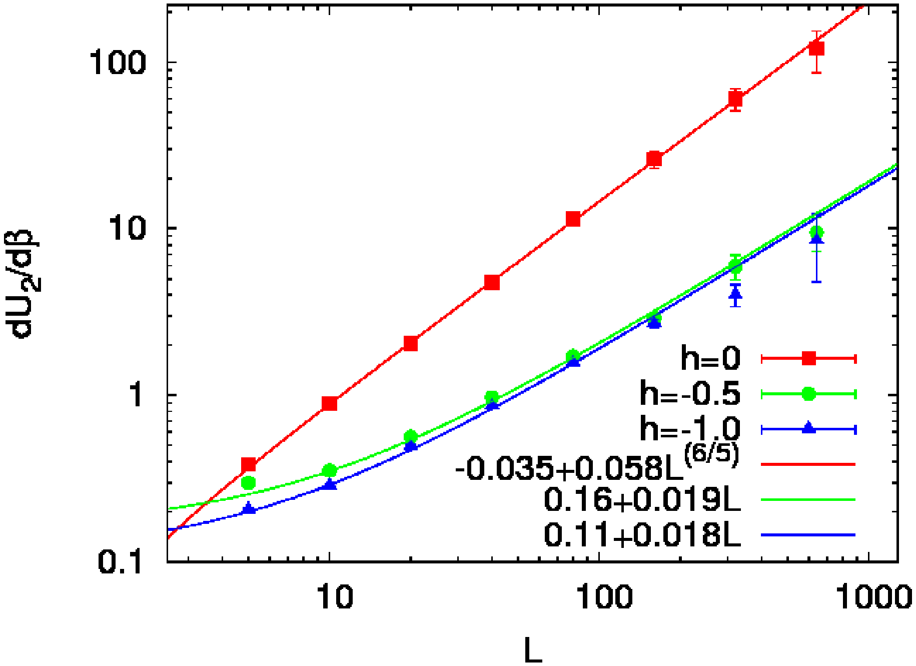


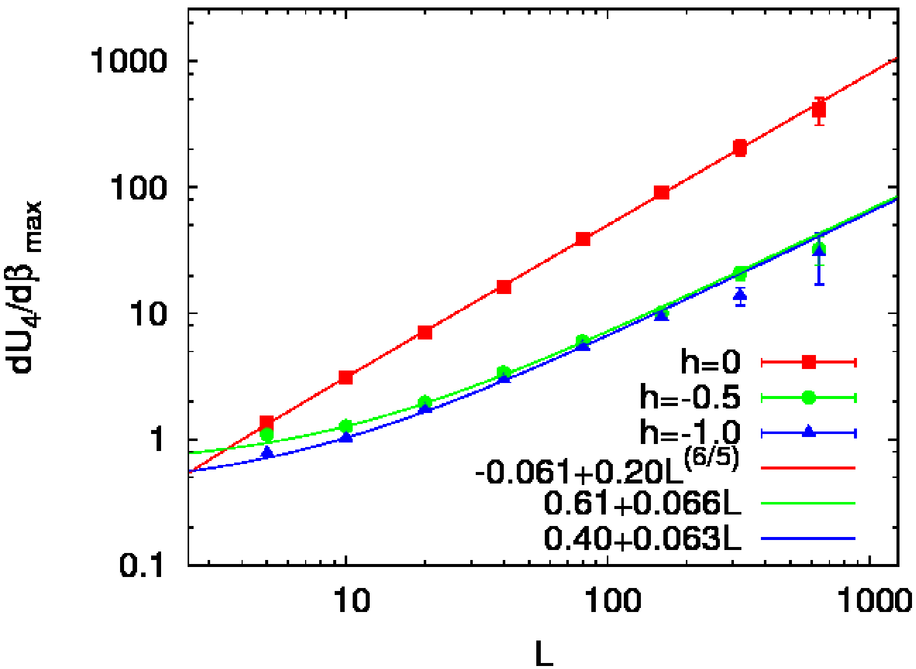


How O_{max} changes is different between Ising and Potts. With negative h and large L, the system behave as two-dimensional Ising model.

$\sim L^{(1-\beta)/\nu}$ $\sim L^{1/\nu}$

Crossover 2-2





How O_{max} changes is different between Ising and Potts.
With negative h and large L, the system behave as two-dimensional Ising model.

$\sim L^{1/\nu}$

$\sim L^{1/\nu}$

Conclusions

We applied STM method to the two-dimensional Potts model (up to L=160).

The tradeoff between sample density and sampling area was not relevant, and we succeeded in reweighting at various conditions.

We also depicted the crossover behaviors.