Thermodynamics of trajectories of the 1D-Ising model

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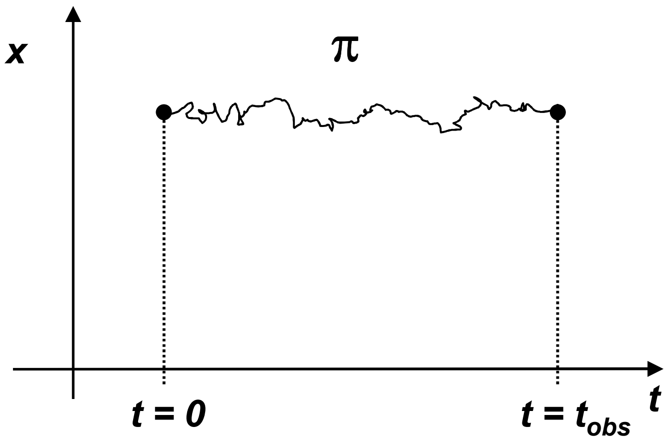
•s-Ensemble



{π} : Space of trajectories in thermal equilibrium from $0 \le t \le t_{obs}$

P[π] : Probability of the trajectory π in this space

Time extensive variables depending on π :

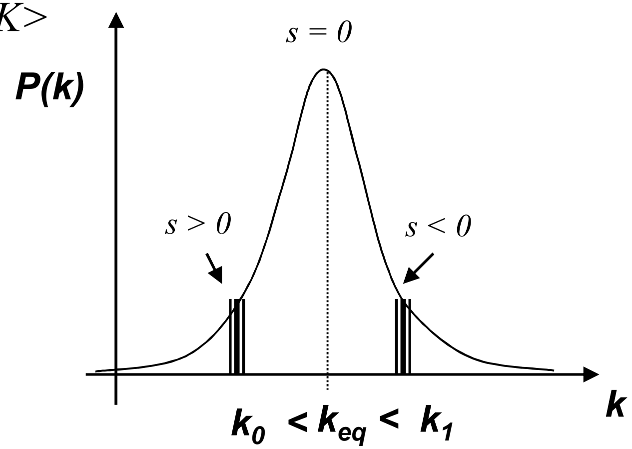
K : activitiy, number of changes of configuration in π

$$M_{tobs} = \int_0^{t_{obs}} m(t')dt' \qquad U_{t_{obs}} = \int_0^{t_{obs}} E(t')dt'$$

Field s: biasing P similar to the Boltzman factor we define the s-ensamble

$$P[\pi, s] = P[\pi] \cdot e^{-s \cdot K}$$

In this dynamical ensamble *s* adjusts <K>



Dynamical Partition Function :

$$Z(s, t_{obs}) = \sum_{\{\pi\}} P[\pi] \cdot e^{-s \cdot K}$$

Dynamical Free Energy :

$$\psi(s) = -\lim_{t_{obs} \to \infty} \left[\frac{\ln(Z(t_{obs}, s))}{t_{obs}} \right]$$

First order Transitions s=0 KCM ***J. P. Garrahan, et al Phys. Rev. Lett. 98, 195702 (2007).***

•1D-Ising Model with s-Ensemble

$$H = -\sum_{i=1}^{N} J \cdot s_i s_{i+1} - \sum_{i=1}^{N} h \cdot s_i$$

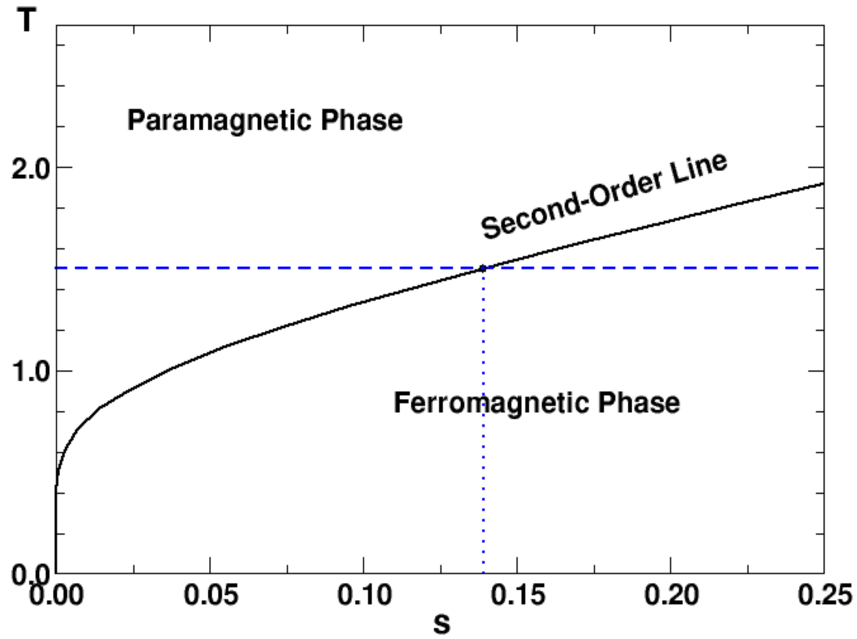
The model has a trivial singularity at *T=0, s=0*. The master equation using Glauber dynamics can be written with field s. The dymamical free energy is given by the largest eigenvalue of the evolution operator W **(Jack and Sollich, *Prog. Theor. Phys. Supp*.184, 304 (2010))**:

$$\psi(s,T) = -\max(w_i)$$

$\frac{\partial \psi(s,T)}{\partial s}$ ⟶ is continuous

$\frac{\partial^2 \psi(s,T)}{\partial s^2}$ ⟶ diverges to a line of dynamical critical points given by:

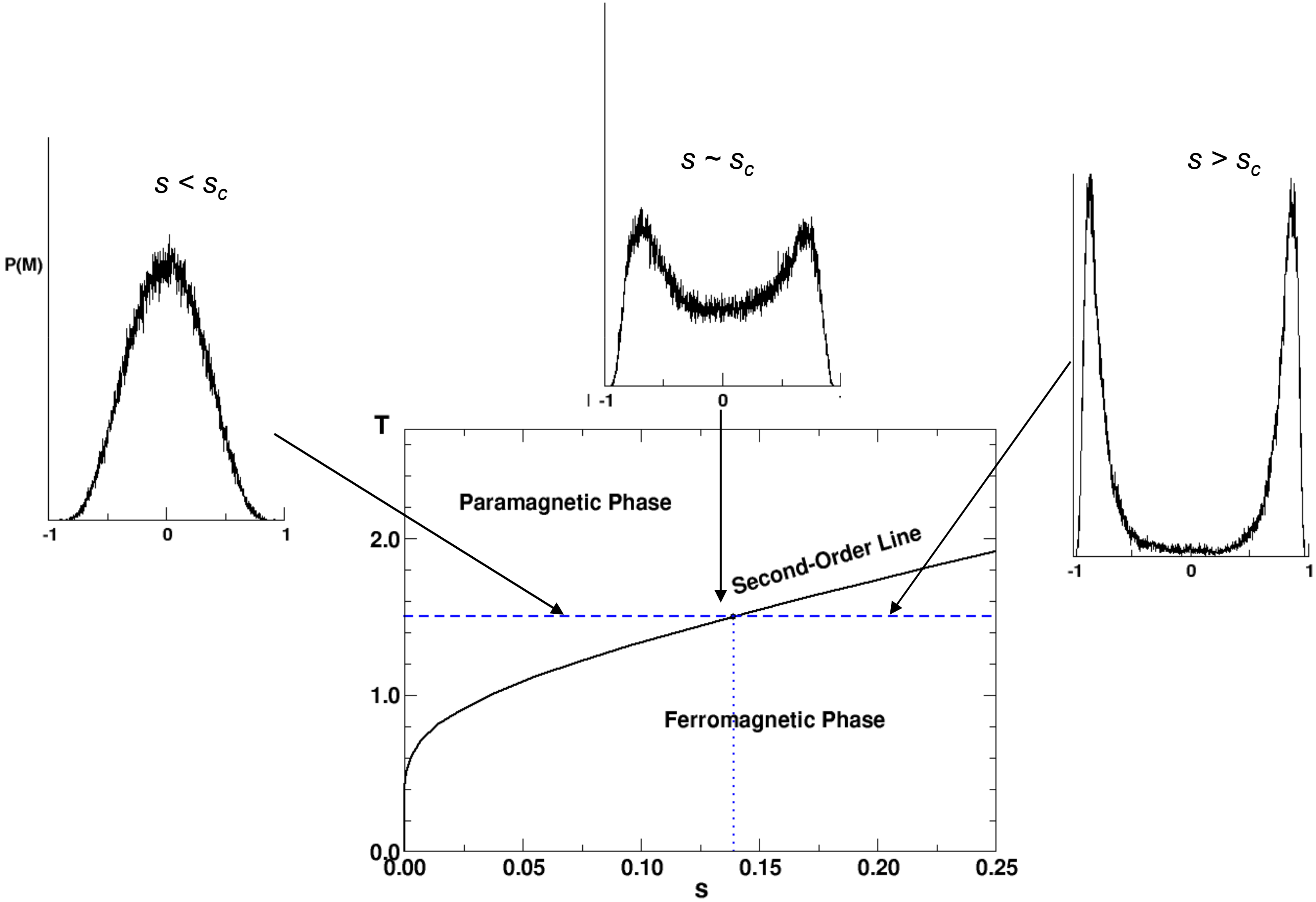
$$s_c = -\ln\left[\tanh\left(2J / k_B T\right)\right]$$



R. Jack and P. Sollich, *Prog. Theor. Phys. Supp.*<u>184</u>, 304 (2010).

• **Monte Carlo Simulations**

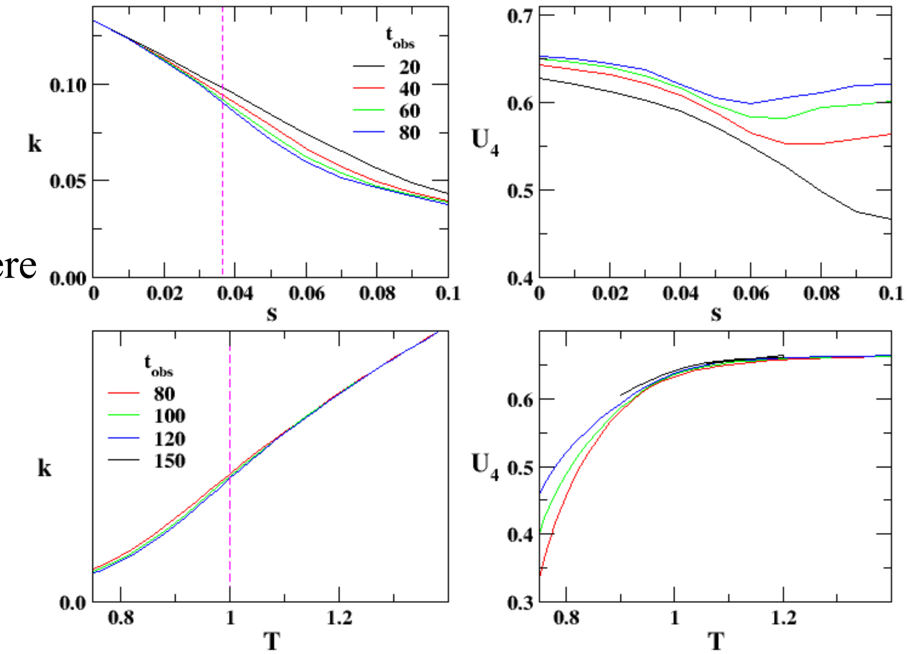
Trajectories: Standard Glauber dynamics at Temperature T=1.5
s-Ensamble: Transition Path Sampling with different *s*



- **Observables**

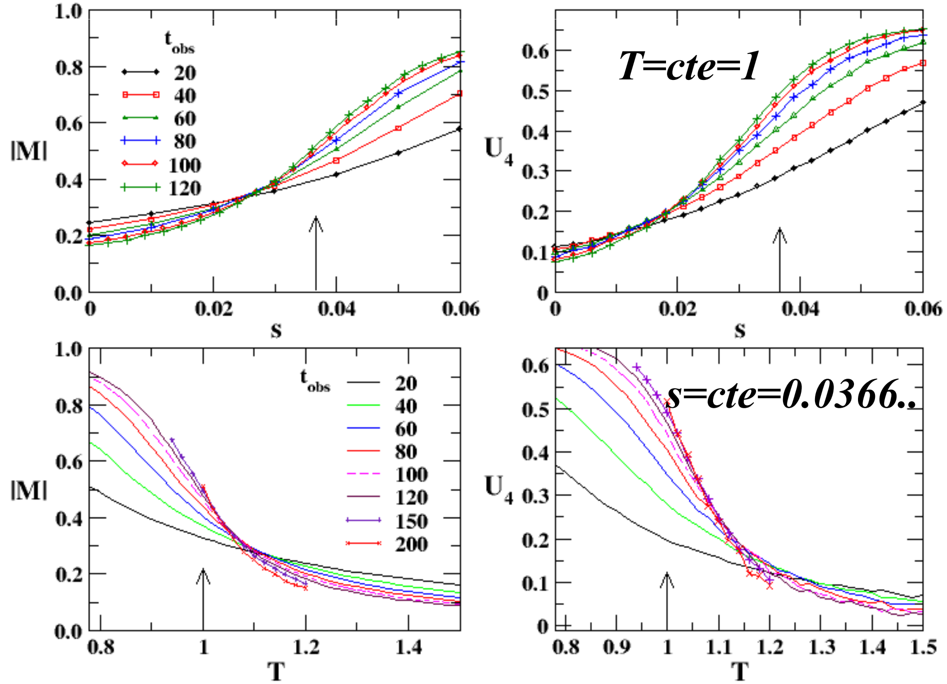
$$k = \frac{K}{N t_{obs}}$$

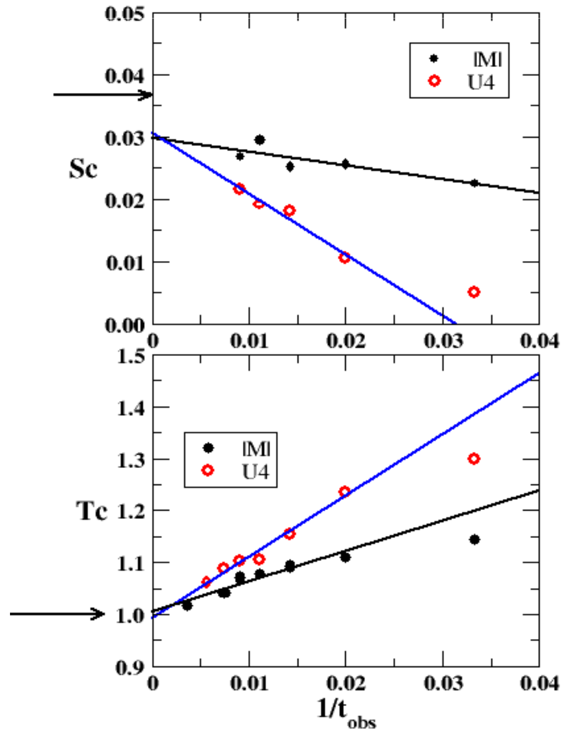
Usually the activity is the order parameter but NOT here



But, we can use the integrated magnetization

$$M = \frac{\int_0^{t_{obs}} m(t')dt'}{N t_{obs}}$$

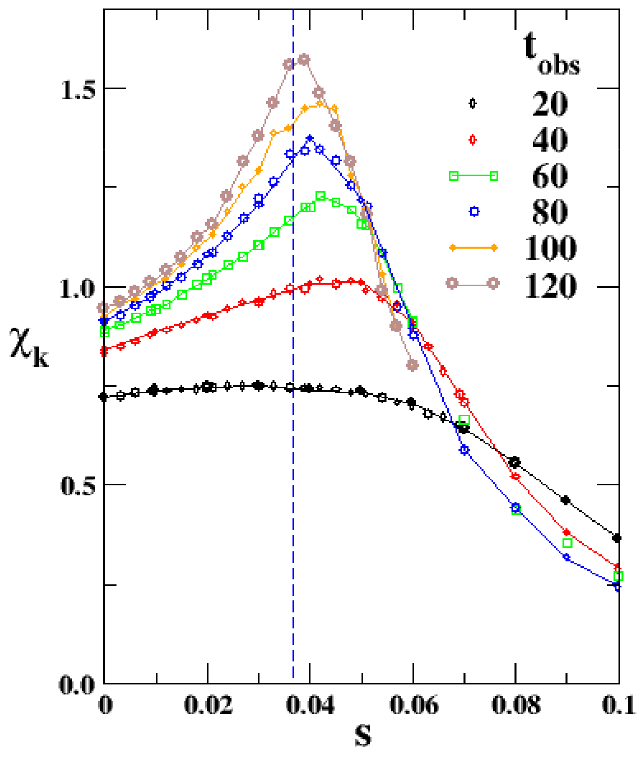


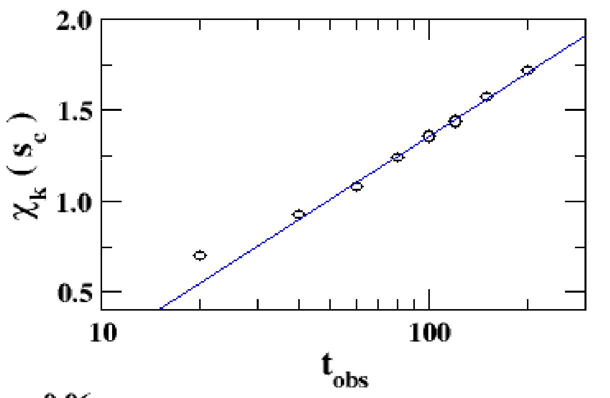


•Finite Size Scaling I (k↔s)

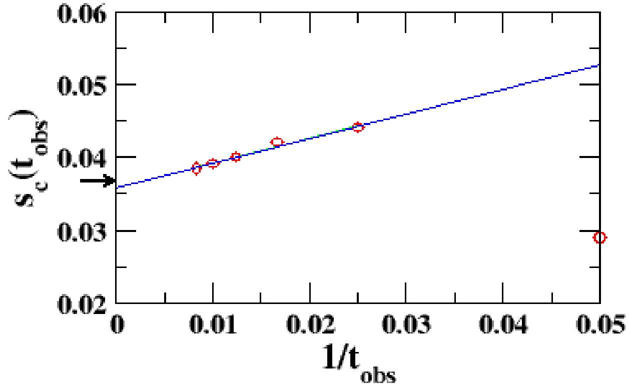
We need use the finite size scaling. ψ(s) is similar to the free energy of the Ising 2D f(T). So we expect the following finite size scaling for the activity k using now t_{obs} as the system size L

$$s_c = s_c(t_{obs}) + A t_{obs}^{-1/\upsilon} \qquad \chi_k = \frac{\langle K^2 \rangle - \langle K \rangle^2}{N t_{obs}} \propto \ln(t_{obs})$$





α ≈ 0

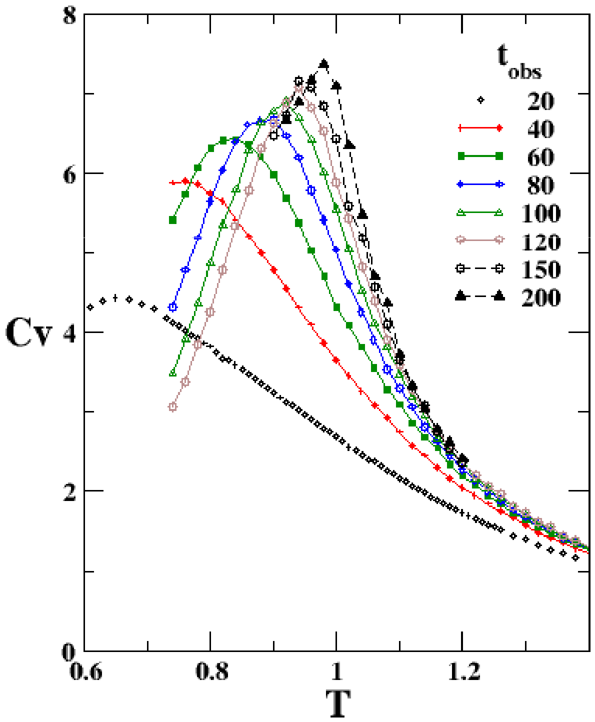


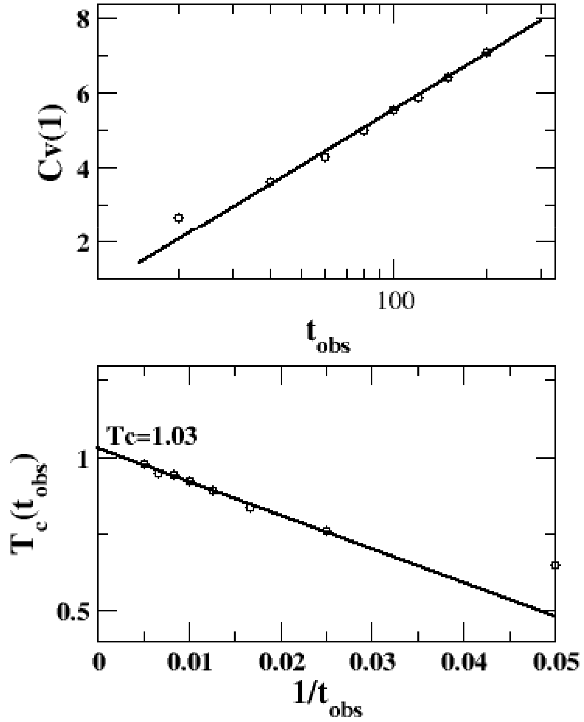
υ ≈ 1

•Finite Size Scaling II (U↔T)

If the *s* field is a temperature like variable we can use the same scaling for *T* and *U*:

$$T_c = T_c(t_{obs}) + A t_{obs}^{-1/\upsilon} \qquad Cv = \frac{\langle U_{t_{obs}}^{\ 2}\rangle - \langle U_{t_{obs}}\rangle^2}{N t_{obs}} \propto \ln(t_{obs})$$



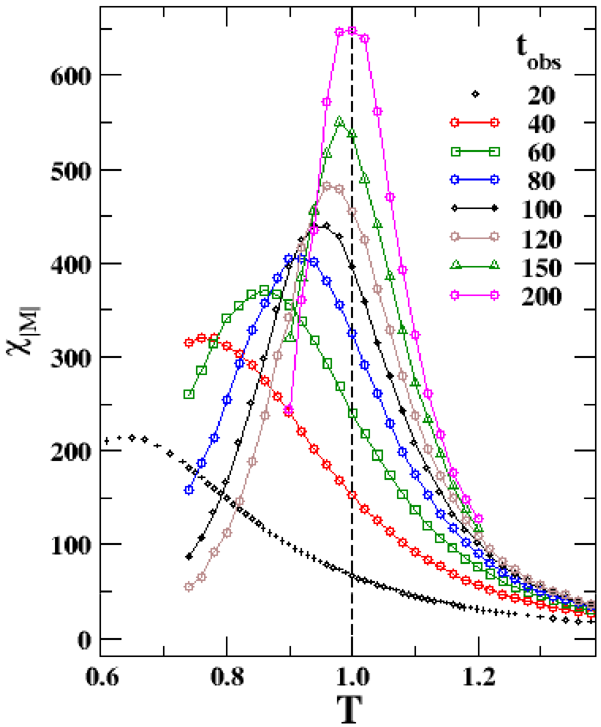


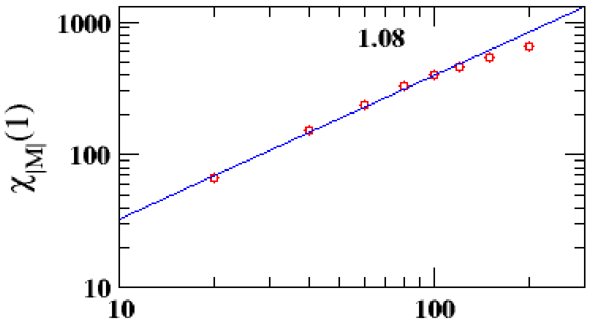
$\alpha \approx 0$

$\upsilon \approx 1$

The same is valid for **(U↔s) (k↔T)**

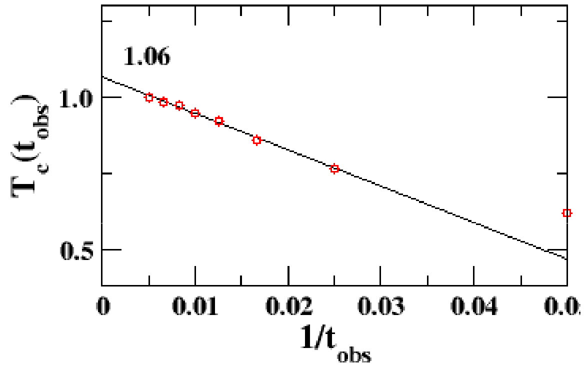
• Magnetic Susceptibility





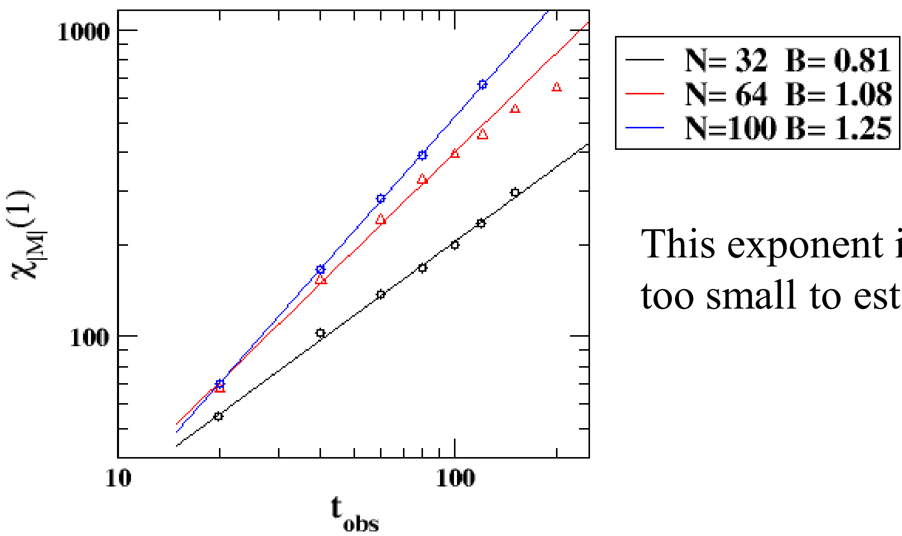
$$\chi_M \propto A t_{obs}^{\;B}$$

B= γ/υ = 1.75



$$T_c = T_c(t_{obs}) + A t_{obs}^{\;-1/\upsilon}$$

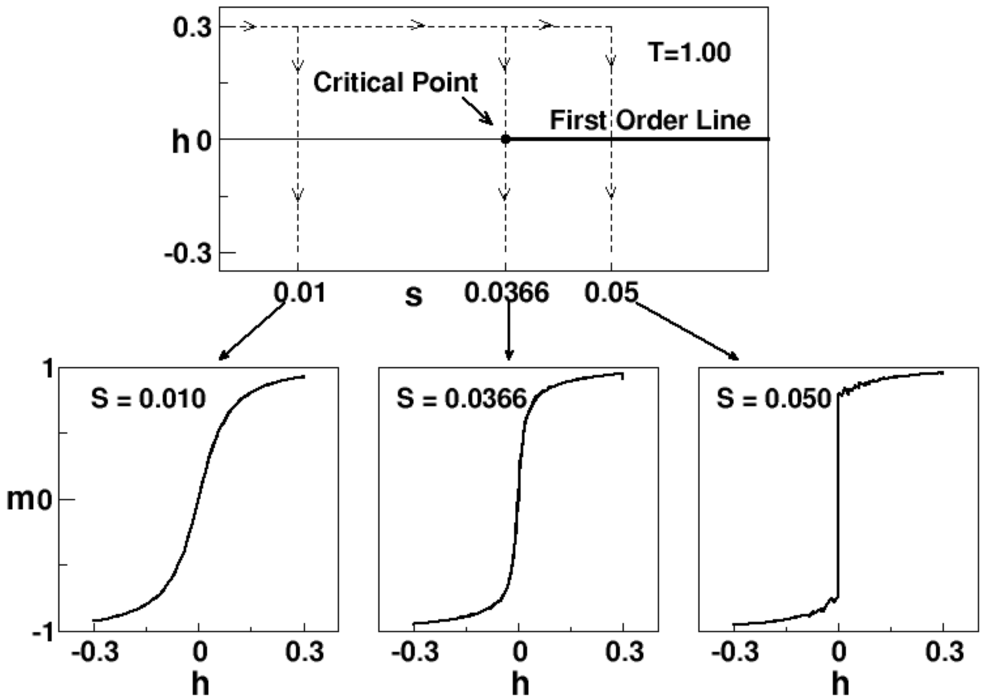
$\upsilon \approx 1$



This exponent is very sensitive to N. The present sizes are too small to estimate it with a reasonable precision.

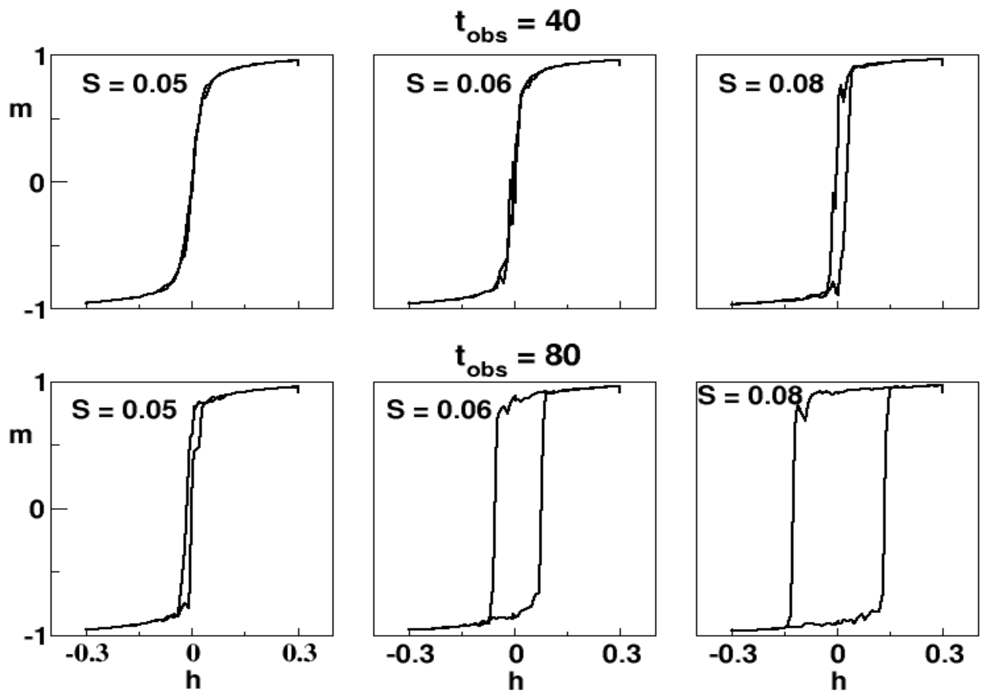
- **Magnetic Field (First Order)**

We can explore the phase diagram by using a magnetic field *h* (plane *h,s*)at constant Temperature

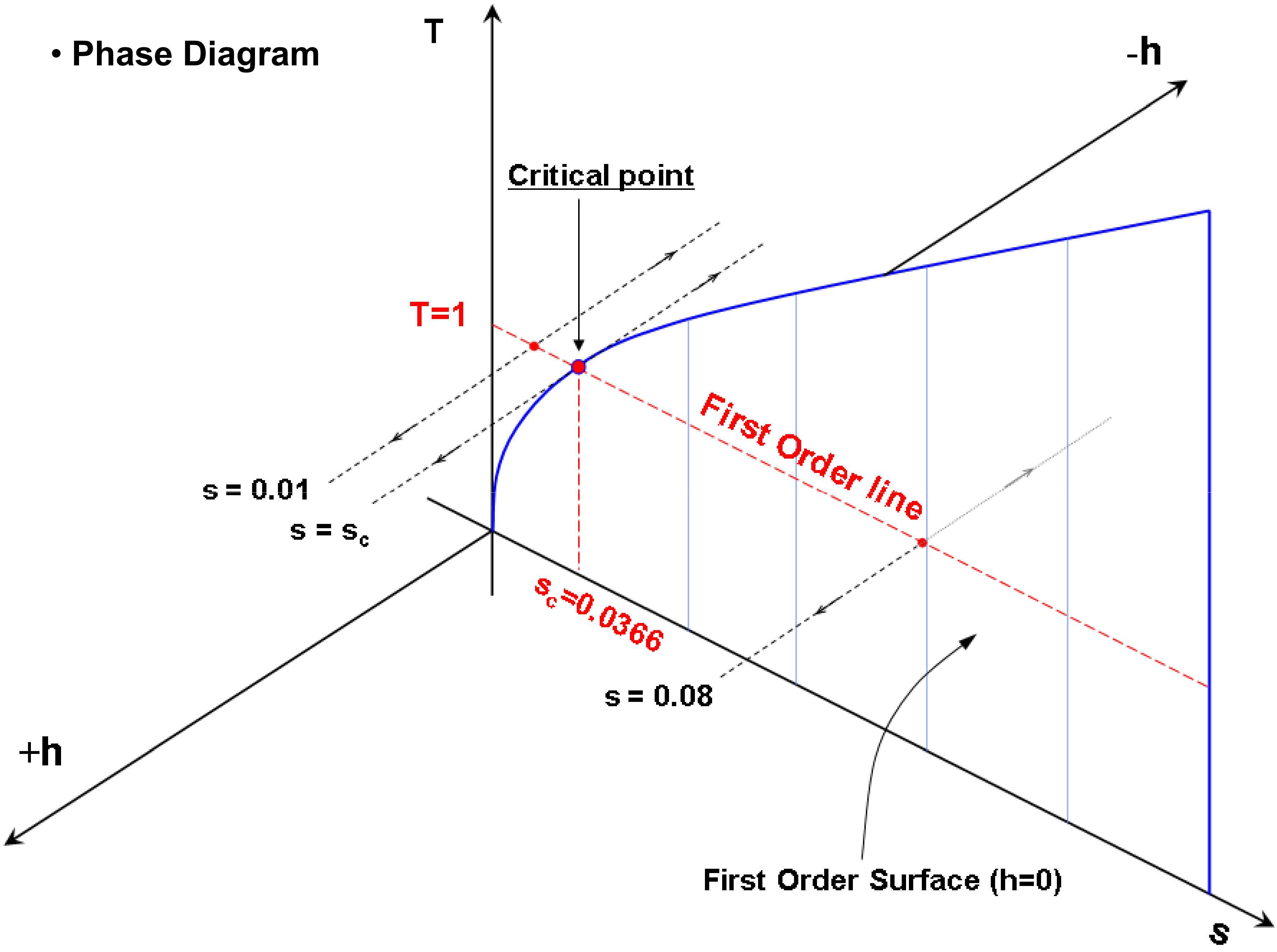


- **Hysteresis**

Histeresis loops are generated by driven the magnetic field around the line of the first order trransition. Its area increases (as expected) with *s* and with the size of the system (t_{obs})



• **Phase Diagram**



•Conclusions

- s and T are symetric variables with same finite size scaling law
- To determine more precisely the exponents we need use other technique (for example short time dynamics)
- With magnetic field we show that a plane of first order transition appears (it has not derived from the theoretical solution)