MonteCarlo simulation of irreversible growth of magnetic thin films in the presence of external fields

Julian and Simona

Introduction

- Preparation and characterization of magnetic nanowires and films is of great interest for the development of advanced microelectronics devices.
  - Study of the behavior of magnetic materials in confined geometries
  - Theory: study of equilibrium properties of magnetic films (Ising)
  - This work: study of far-from-equilibrium properties of growing (thin) magnetic film (Magnetic Eden Models, MEM)
    - Archetypical growth model (MEM)

Magnetic Eden Models

- Eden growth starts from a single particle called the seed. One then proceeds to add a new particle on a randomly chosen unoccupied site in the immediate neighborhood (<u>the perimeter</u>) of the seed.
- The growth process continues by randomly adding new particles to the perimeter of the previously formed cluster
- MEM adds an additional degree of freedom to the Eden model: <u>the spin of the added particle</u>

$$E = -\frac{J}{2} \sum_{\langle ij, i'j' \rangle} S_{ij} S_{i'j'}$$

J = coupling const between NN spins

S_{ij} = ± 1(for spin 1/2 particles

MEM growth process consists in adding further spins to the growing cluster taking into account the corresponding interaction energies.

The orientation of the added spins depend on

1) <u>energetic interactions with already deposited spins</u>
2) <u>the temperature (Boltzmann factor)</u>

Ising Models and MEM

$$\mathcal{H} = -\frac{J}{2} \sum_{\langle ij, i'j' \rangle} S_{ij} S_{i'j'}$$

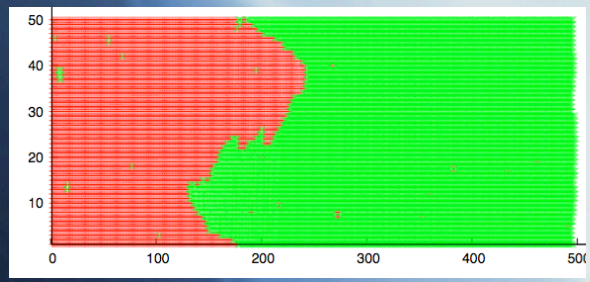
- Similarity between MEM and Ising?
- Ising describes magnetic systems under equilibrium conditions (phase transitions in equilibrium magnetic systems)
- MEM describes the irreversible growth of magnetic materials (far from equilibrium condition)

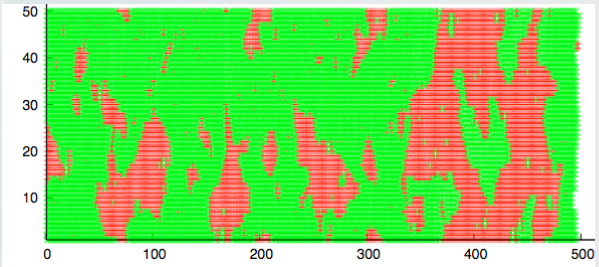
Monte Carlo simulation

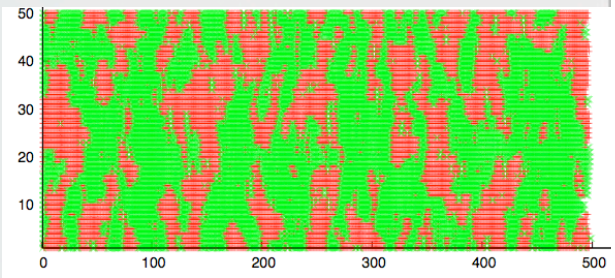
- Growth is simulated in confined (stripped) geometries;
- MEM in (1+1) dimensions is studied in the square lattice using a rectangular geometry: L x M with M>>L;
- Coordinates (i,j) : $1 \leq i \leq M$ and $1 \leq j \leq L$
- Starting seed for the growing cluster is a column of parallel oriented spins placed at i = 1;
- Procedure ……

Results

- Spontaneous magnetization reversal:
  - Finite dimension L
  - Sufficiently low T
- Long clusters are constituted by a sequence of well ordered magnetic domains of average length l_D >> L.







T = 0.4, L = 50

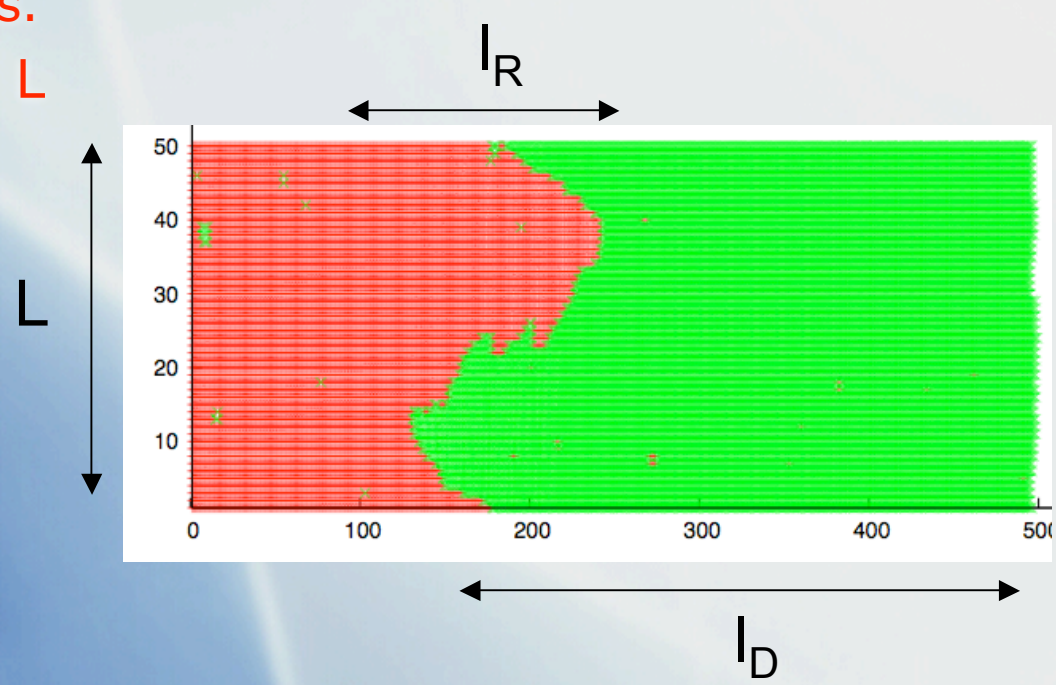
T = 0.6, L = 50

T = 0.8, L = 50

This phenomenon is not a magnetization reversal of thin films induced by a field .Here the reversal happens during the growth process and in the absence of any applied magnetic field.

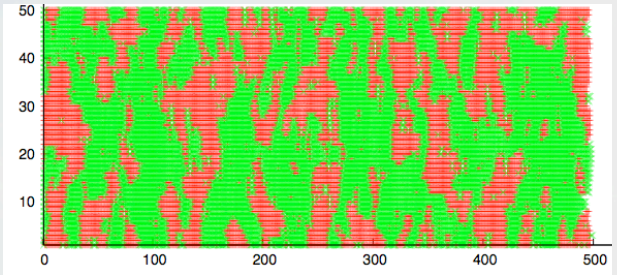
Results II

- The phenomenon is essentially due to the small size of the thin film and it becomes <u>irrelevant in the thermodynamic limit</u> (finite size effect) ;
- Characteristic length scale of the phenomenon are two:
  - l_D , the domain length
  - l_R, the length of the region where spontaneous reversal happens.
- $l_D >> l_R \sim L$



Results III

- Increasingly long domains tend to show up at lower temperatures
  - High temperatures means transitioning to a disordered state, which will favor fluctuations over ordered domain



T = 0.8, L = 50

- The average domain length diverges as the we increase the lattice size toward the thermodynamic limit. (effect irrelevant)

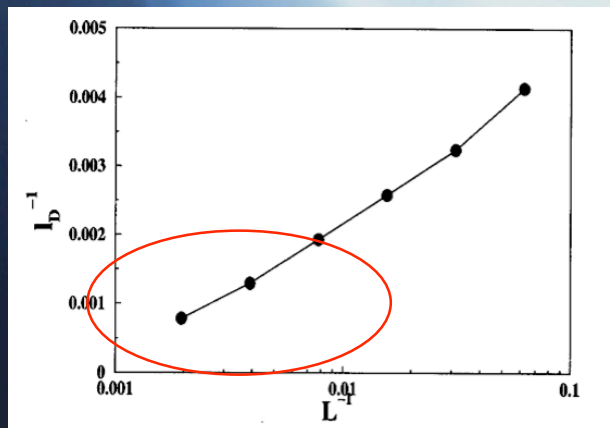
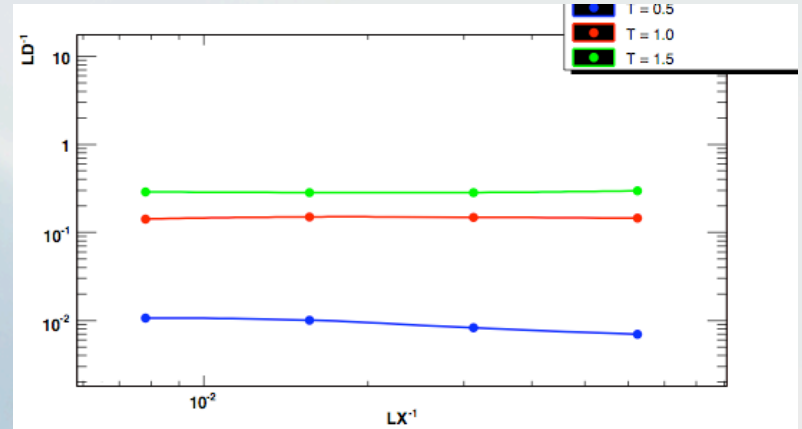


FIG. 3. Log–linear plot of l_D^{-1} vs L^{-1} for the temperature $T=0.5$ and lattice sizes in the range $16 \leqslant L \leqslant 512$. The line is a guide to the eye, showing that the characteristic domain length diverges in the thermodynamic limit ($L \to \infty$).



Comparison with Ising models

- Study of the interplay between finite size-effects and broken symmetry at thermal phase transitions.
- T_C is the critical temperature at which, in a thermally driven phase transition, the system changes from a spontaneously ordered state (below T_C) to a disordered state (> T_C temperatures);

In the absence of an externally applied magnetic field (H= 0) the low temperature ordered phase is a state with non-vanishing spontaneous magnetization (M= ± 1). This spontaneous symmetry breaking is only possible in the thermodynamic limit.
The magnetization of a finite system, averaged over a sufficiently large observation time, vanishes at every positive temperature, irrespective of the finite size of the sample

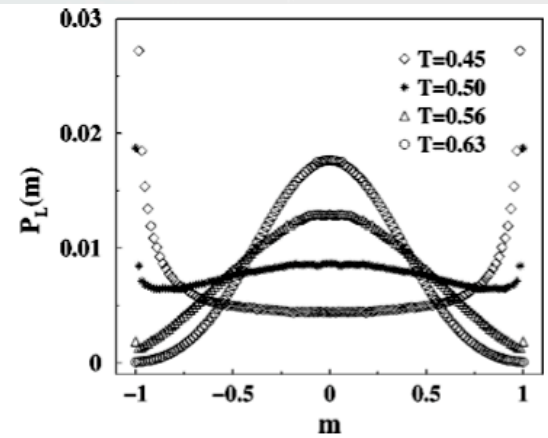


FIG. 1. Plots of the probability distribution of the mean column magnetization $P_L(m)$ versus m for the fixed lattice width $L=128$ and different temperatures. The sharp peaks at $m=\pm 1$ for $T=0.45$ have been truncated in order to allow a detailed observation of the plots corresponding to higher temperatures. This behavior resembles that of the one-dimensional Ising model. More details in the text.

Comparison with Ising Models (II)

- In the MEM, the spontaneous magnetization reversal causes the magnetization of the whole film to vanish at every non zero temperature (sifficiently low), provided that the film length l_F (which plays the role of the observation time) is much larger than l_D (which plays the role of the ergodic time, or the time necessary to observe the system to pass from one state of magnetization to another);
- In the thermodynamic limit (lattice size going to infinite) the ergodic time diverges, so <u>there is broken symmetry. It is not possible anymore to observe the passage from a magnetization status to another.</u>
- A way to verify the similar behaviour of MEM and Ising is to plot the probability distribution of the mean column magnetization ($P_L(m)$)

Comparison with Ising Model (III)

At high temperatures the distribution is Gaussian (disordered state).
With lower temps the distribution broadens and two peaks show, for m = ± 1.
The behavior is the same of the order parameter probability of the 1-d Ising model.

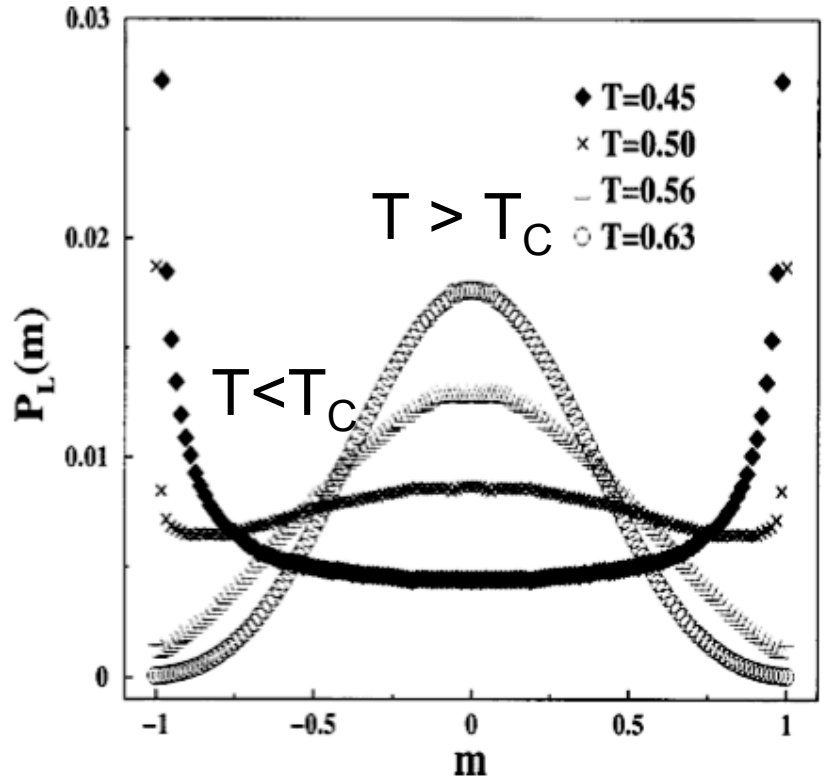
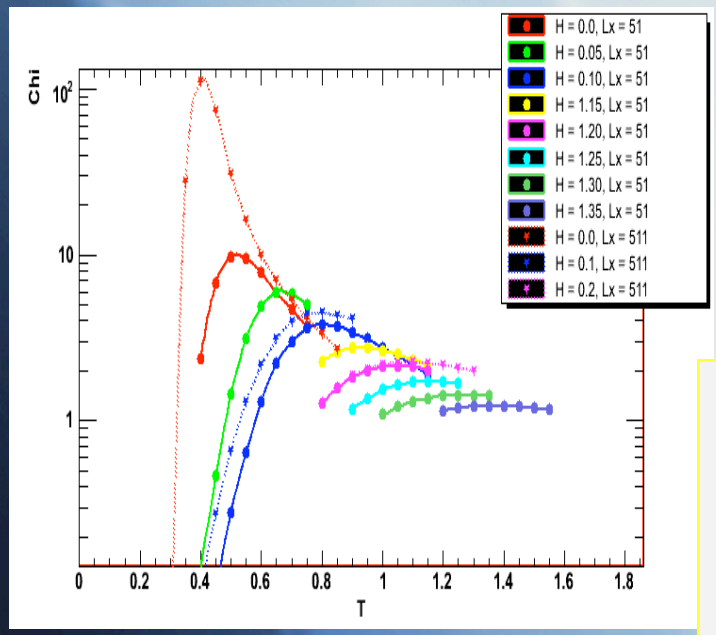


FIG. 4. Data corresponding to the $(1+1)$-dimensional MEM: plots of the probability distribution of the mean column magnetization $P_L(m)$ vs m for the fixed lattice width $L=128$ and different temperatures, as indicated in the figure. The sharp peaks at $m=\pm 1$ for $T=0.45$ have been truncated, in order to allow a detailed observation of the plots corresponding to higher temperatures. This behavior resembles that of the one-dimensional Ising model.

A pseudo phase transition to a disordered state occurs for a critical temperature which is dependent on the film width L .
However in the thermodynamic limit ($L \to \infty$) the (1+1) dimensional MEM is not critical (the transition takes place at T = 0) while a second order phase transition is expected to occur a finite temperature for (2+1)-MEM.

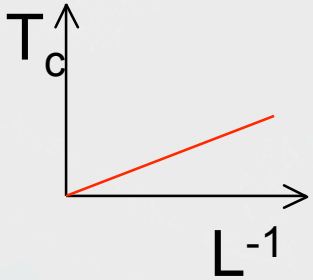
Effect of adding a bulk field H

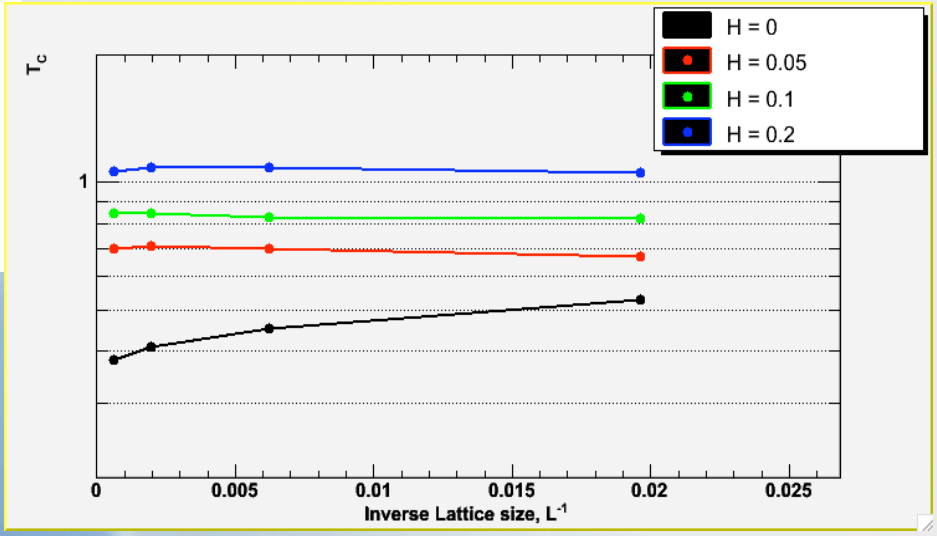
Adding a bulk magnetic field H, will introduce a competing effect with the temperature in terms of ordering the spins and controlling the spontaneous magnetization reversal



The plot of susceptibility (χ) vs temperature gives the T_C of a system, as the maximum of the curve

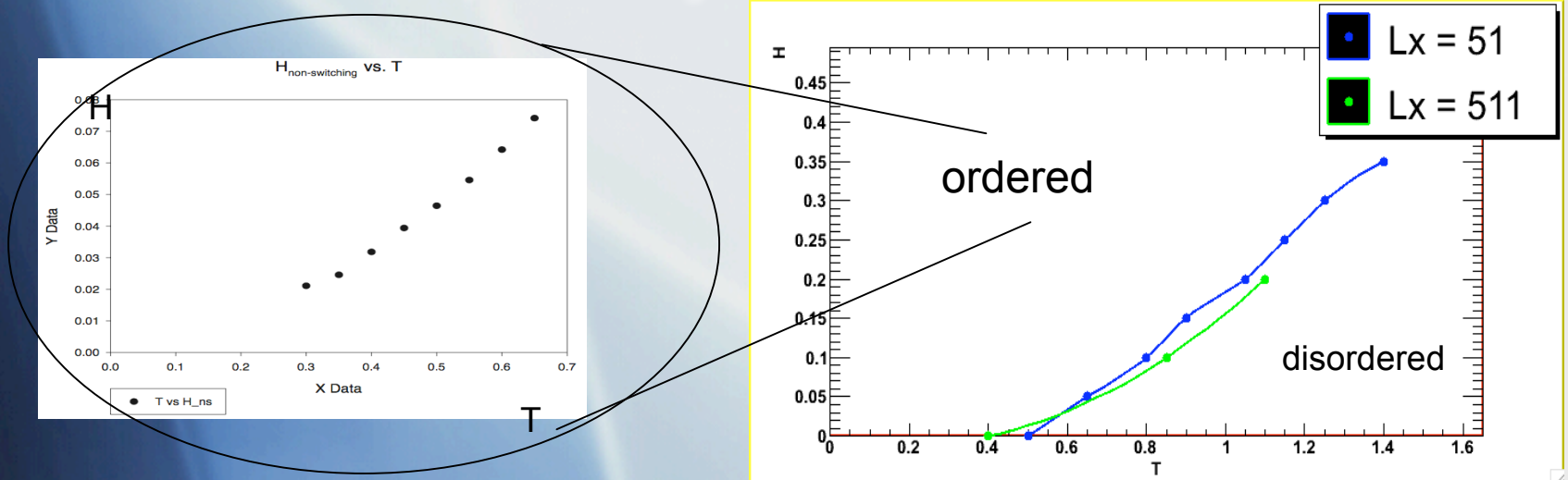
For H = 0, $T_c \rightarrow 0$ in the thermodynamic limit;
For H $\neq 0$, T_C will not be zero also for large enough lattice size, since the field will be always able to break the symmetry and force the spins to align.





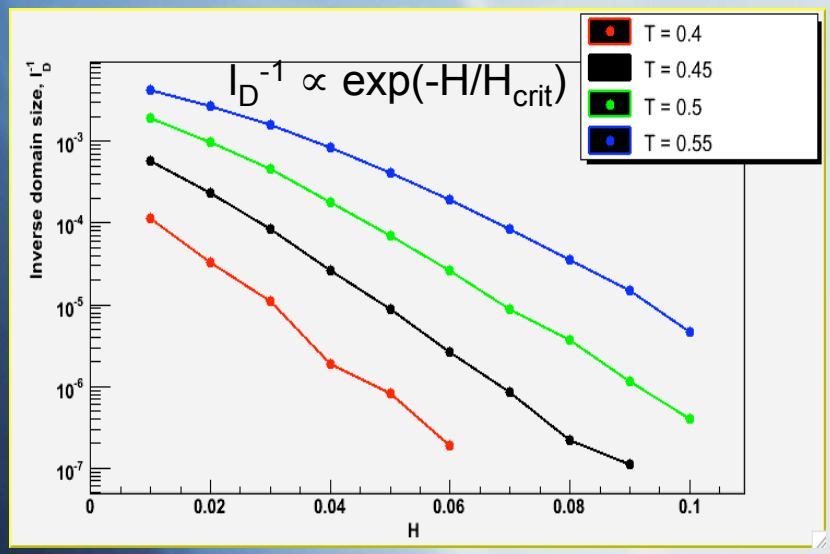
Adding a bulk field (II)

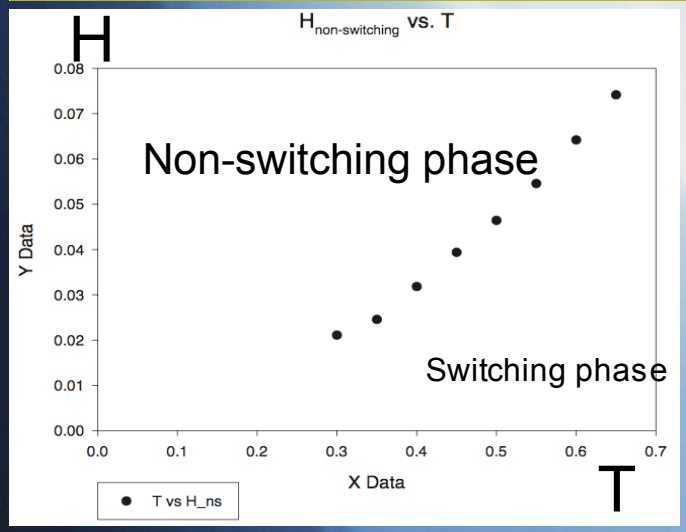
- In the plane H vs T there will be three regions:
  - 1) a disordered region (above a critical temperature, where even the effect of the field is not enough to order the system)
  - 2) a ordered region where spontaneous magnetization reversal can occur
  - 3) a ordered region where spontaneous magnetization will not occur anymore because of the influence of the field which will force the spins to align in one way or another.

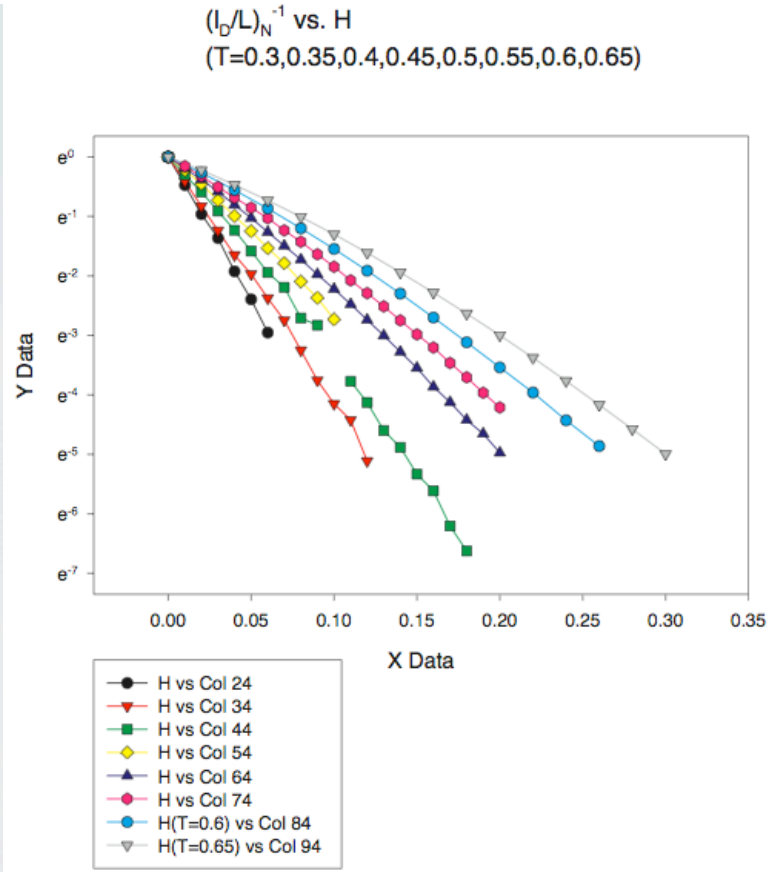


Adding a bulk field (III)

l_D length will depend on the H intensity



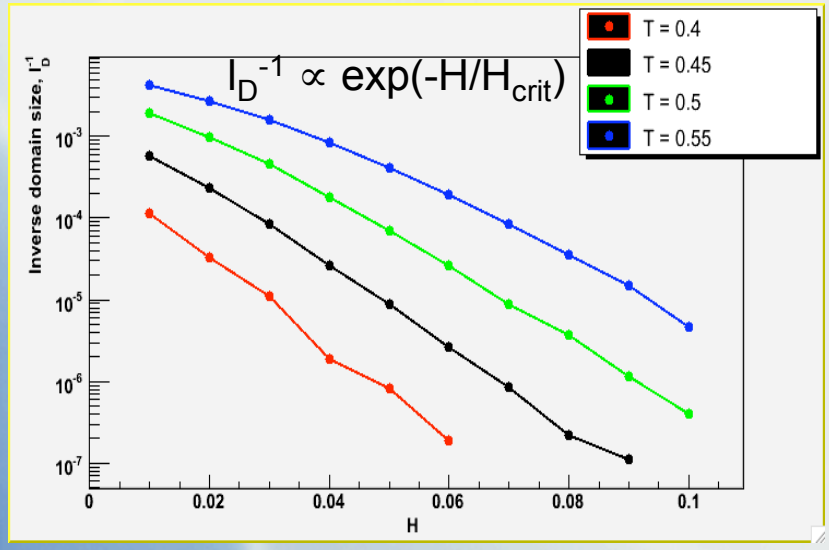




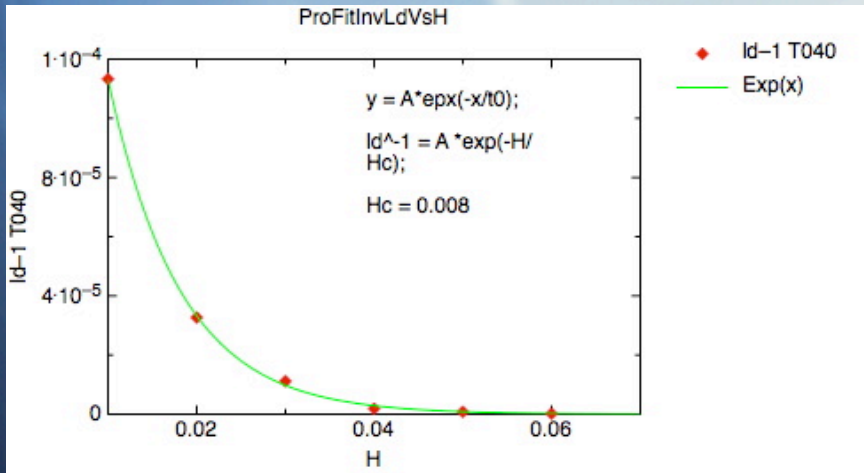
- There will be, for each temperature a value of the field H_{crit} for which there won't be a spontaneous magnetization reversal anymore

Finding H_c

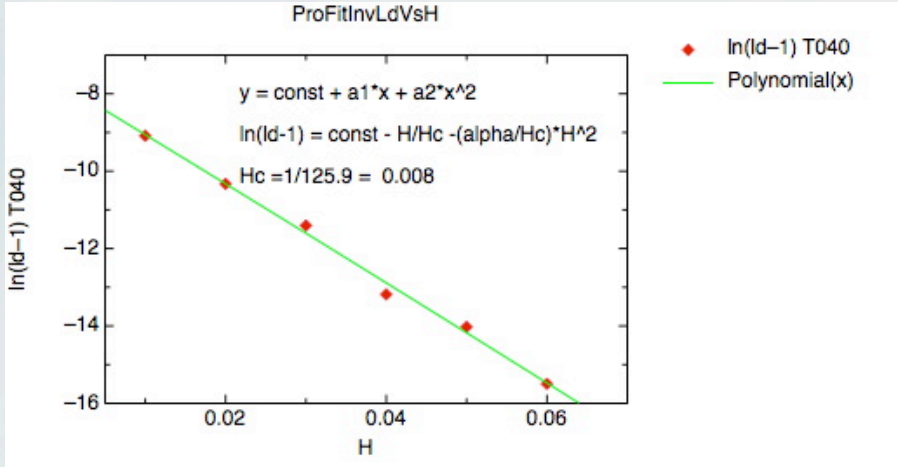
- To find H_c we assumed that the relation between L_D^{-1} and H is exponential. Two hypothesis have been tested:
  - $L_D^{-1} \propto A \times \exp(-H/H_c)$
  - $\ln(L_D^{-1}) \propto \ln(A) + (-H/H_c) + (\alpha/H_c)*H^2$
- Infact some of the curves are not completely straight, indicating a possible quadratic effect.



Finding H_c

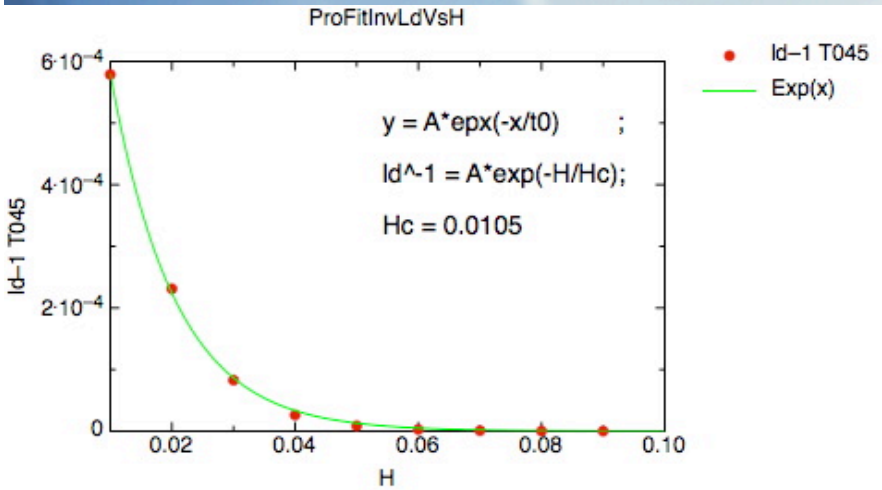



```
==========================================
Fit Algorithm: Levenberg-Marquardt

Function  :    Exp
 Descr 1  :    y = A * exp(-(x-x0)/t0)  + const
 Descr 2  :    exponential function

Data      :    ProFitInvLdVsH

output    :    y
 y  column:    ld-1 T040
 Δy value :    0.0
 Δy distr.:    Gaussian

input     :    x
 x  column:    H
 Δx value :    0.0
 Δx distr.:    Gaussian


Iterations:    6
------------------------------------------
Chi squared    =    3.2055e-12
Fitted parameters:            Standard
deviations:
A    =    3.8564e-4      ΔA   =    1.0350e-5
t0   =    8.1588e-3      Δt0  =    1.5665e-4
```

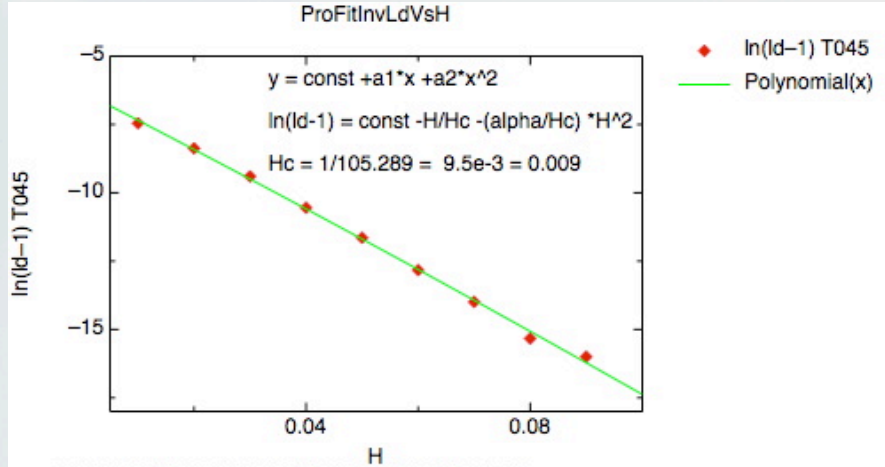



```
it Algorithm:  Polynomial

Function  :    Polynomial
 Descr 1  :    f(x) = const + a1*x + a2*x^2
 Descr 2  :    deg: degree of the polynomial

Data      :    ProFitInvLdVsH

output    :    y
 y  column:    ln(ld-1) T040
 Δy value :    0.0
 Δy distr.:    Gaussian

input     :    x
 x  column:    H
 Δx value :    0.0
 Δx distr.:    Gaussian


Iterations:    1
------------------------------------------
Chi squared    =    0.1527
Fitted parameters:            Standard deviations:
const    =    -7.7946        Δconst   =    0.4036
a1       =    -125.9177      Δa1      =    26.4030
a2       =    -34.5176       Δa2      =    369.2340
```

Finding H_c

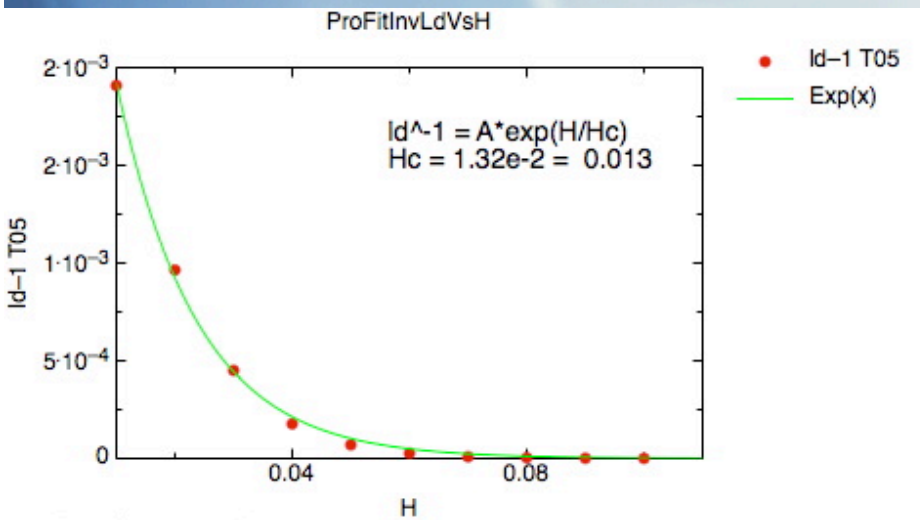



```
Function  :    Exp
 Descr 1  :    y = A * exp(-(x-x0)/t0)  + const
 Descr 2  :    exponential function

Data      :    ProFitInvLdVsH

output    :    y
 y  column:    ld-1 T045
 Δy value :    0.0
 Δy distr.:    Gaussian

input     :    x
 x  column:    H
 Δx value :    0.0
 Δx distr.:    Gaussian


Iterations:    8
-----------------------------------------
Chi squared    =    1.4039e-10
Fitted parameters:            Standard
deviations:
A    =    1.5047e-3      ΔA   =    2.9764e-5
t0   =    1.0497e-2      Δt0  =    1.7311e-4
```

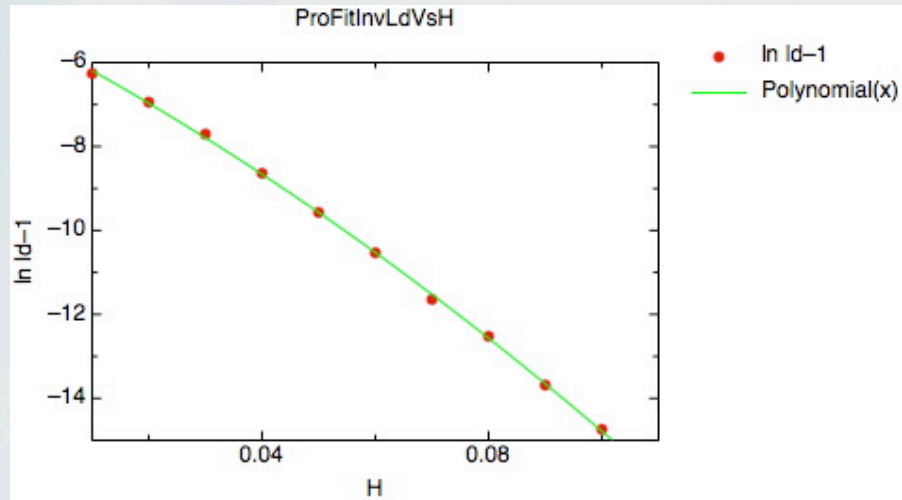



```
=========================================
Fit Algorithm: Polynomial

Function  :    Polynomial
 Descr 1  :    f(x) = const + a1*x + a2*x^2
 Descr 2  :    deg: degree of the polynomial

Data      :    ProFitInvLdVsH

output    :    y
 y  column:    ln(ld-1) T045
 Δy value :    0.0
 Δy distr.:    Gaussian

input     :    x
 x  column:    H
 Δx value :    0.0
 Δx distr.:    Gaussian


Iterations:    1
-----------------------------------------
Chi squared    =    0.1466
Fitted parameters:            Standard deviations:
const     =    -6.2892       Δconst    =    0.1989
a1        =    -105.2894     Δa1       =    9.1317
a2        =    -55.9507      Δa2       =    89.0597
```

Finding H_c




```
Function  :   Exp
 Descr 1  :   y = A * exp(-(x-x0)/t0)  + const
 Descr 2  :   exponential function

Data      :   ProFitInvLdVsH

output    :   y
 y  column:   ld-1 T05
 Δy value :   0.0
 Δy distr.:   Gaussian

input     :   x
 x  column:   H
 Δx value :   0.0
 Δx distr.:   Gaussian


Iterations:   8
-----------------------------------------
Chi squared    =    5.0701e-9
Fitted parameters:          Standard
deviations:
A    =    4.0065e-3      ΔA   =    1.0631e-4
t0   =    1.3626e-2      Δt0  =    3.4180e-4
```

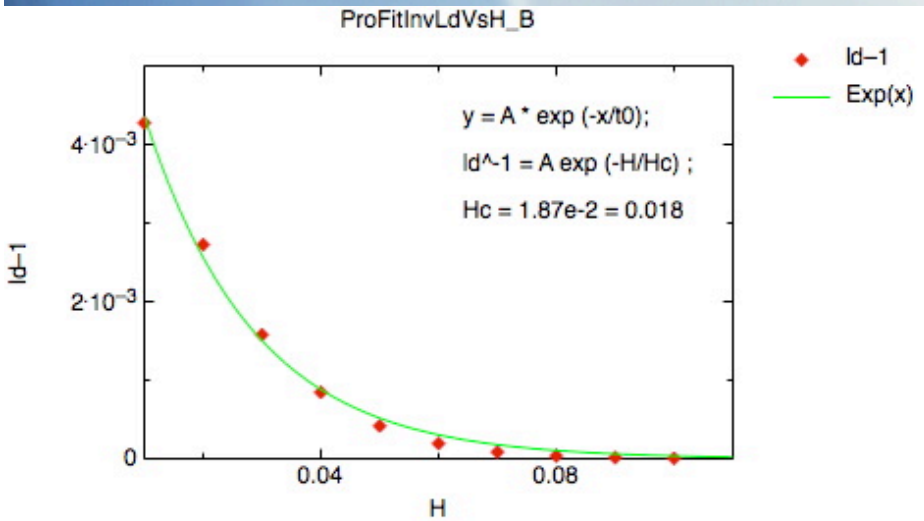


Polynomial(x)
x = const + a1*x + a2*x^2
x = const -H/Hc -const/Hc * H^2

```
Chi squared    =    3.2960e-2
Fitted parameters:          Standard deviations:
const    =    -5.4540       Δconst   =    8.0706e-2
a1       =    -71.4097      Δa1      =    3.3706
a2       =    -218.8791     Δa2      =    29.8626
```

const = -5.45
a1 = -71.4097 => Hc = -1/71.4097 = 0.014
a2 = -218.879 => alpha = -218/71 = 3.05

Finding H_c

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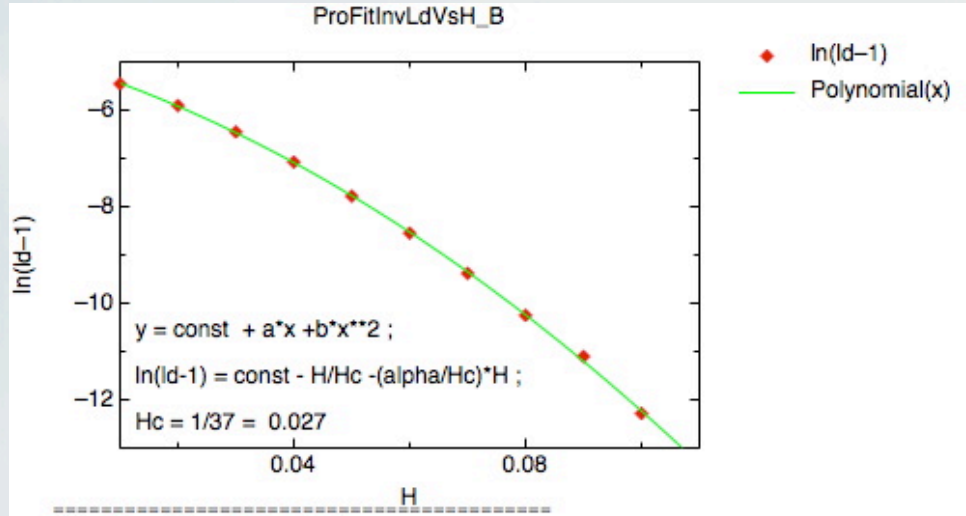
 Descr 2  :    exponential function

Data      :    ProFitInvLdVsH_B

output    :    y
 y  column:    ld-1
 Δy value :    0.0
 Δy distr.:    Gaussian

input     :    x
 x  column:    H
 Δx value :    0.0
 Δx distr.:    Gaussian


Iterations:    8
------------------------------------------
Chi squared    =    8.0831e-8
Fitted parameters:            Standard
deviations:
A     =    7.4376e-3      ΔA    =    2.7449e-4
t0    =    1.8751e-2      Δt0   =    7.3435e-4
```

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 Descr 2  :    deg: degree of the polynomial

Data      :    ProFitInvLdVsH_B

output    :    y
 y  column:    ln(ld-1)
 Δy value :    0.0
 Δy distr.:    Gaussian

input     :    x
 x  column:    H
 Δx value :    0.0
 Δx distr.:    Gaussian


Iterations:    1
------------------------------------------
Chi squared    =    1.5118e-2
Fitted parameters:            Standard deviations:
const     =    -5.0276        Δconst    =
     5.4659e-2
a1        =    -37.7437       Δa1       =    2.2828
a2        =    -342.9861      Δa2       =    20.2245
```
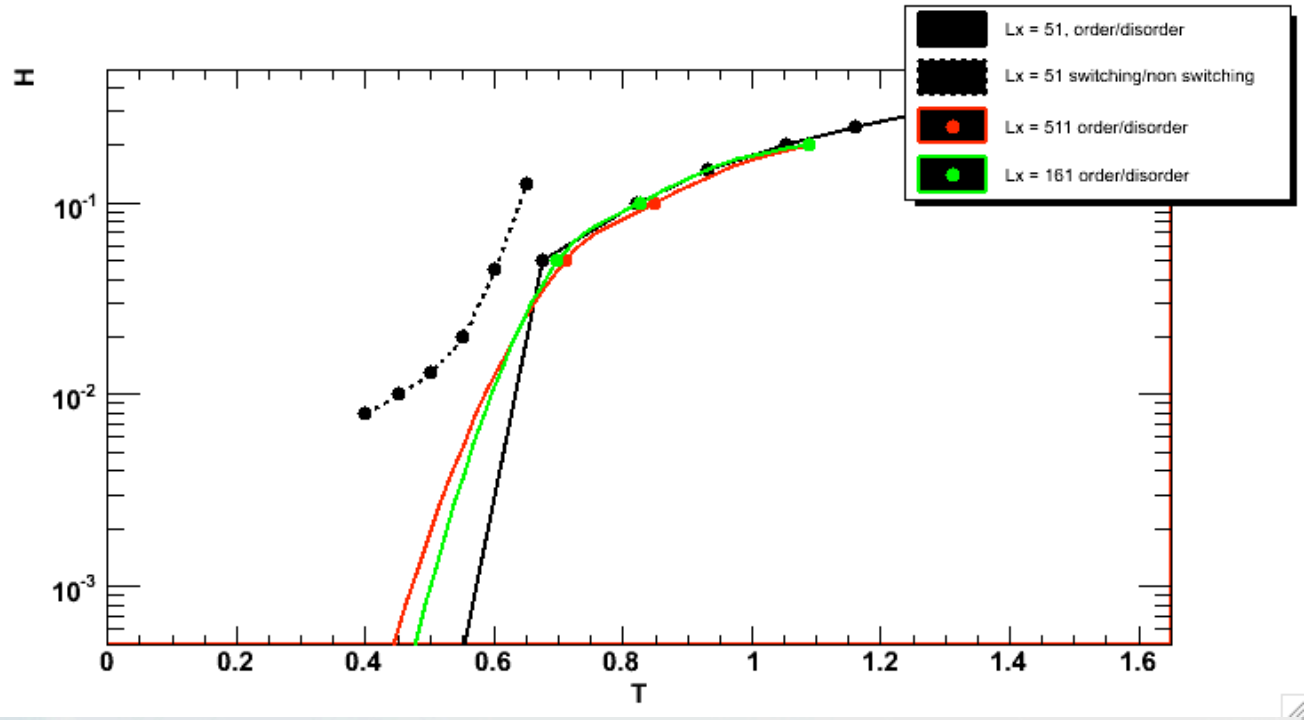
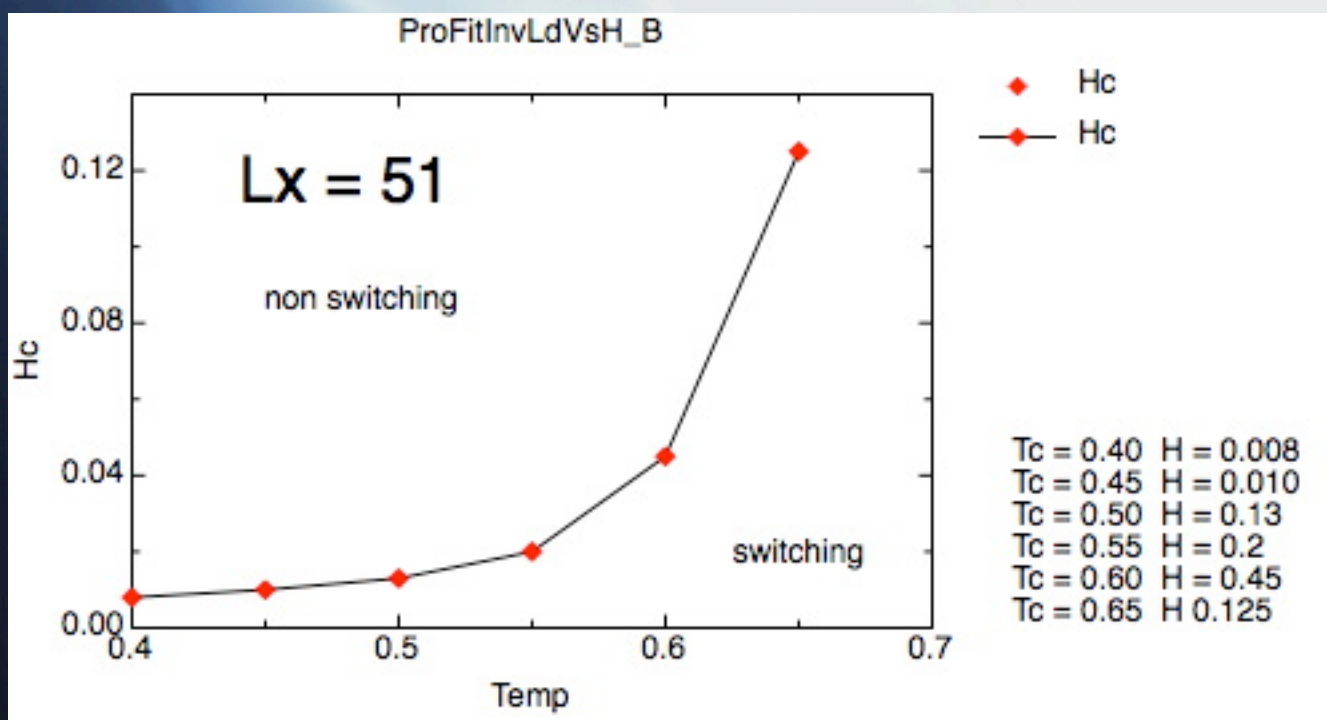

H_c


Lx = 51, order/disorder
Lx = 51 switching/non switching
Lx = 511 order/disorder
Lx = 161 order/disorder
H
T
10^{-1}
10^{-2}
10^{-3}
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6


ProFitInvLdVsH_B
Lx = 51
non switching
switching
Hc
Temp
0.00
0.04
0.08
0.12
0.4
0.5
0.6
0.7
Hc
Hc
Tc = 0.40 H = 0.008
Tc = 0.45 H = 0.010
Tc = 0.50 H = 0.13
Tc = 0.55 H = 0.2
Tc = 0.60 H = 0.45
Tc = 0.65 H 0.125