



# Il modello di Ising

Simulazione di Materia Condensata e Biosistemi

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UNIVERSITÀ  
DEGLI STUDI  
DI MILANO



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- ▶ Backup modello di Ising 1D
- ▶ Backup modello di Ising 2D



# Hamiltoniana

## 1 Introduzione

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$

- ◇ Interazione fra primi vicini
- ◇ Accoppiamento con un campo esterno



Modello di Ising 1D con condizioni periodiche.



# Modello di Ising 1D

## 1 Introduzione

- ◇ Teoria di campo medio
- ◇ Sistema presenta una transizione di fase a  $T_c \neq 0$

$$m = \tanh [\beta (h + Jn_{nn}m)]$$

- ◇ Soluzione analitica
- ◇ Sistema disordinato per ogni  $T \neq 0$  a campo esterno nullo

$$m = \frac{\sinh(\beta h)}{\sqrt{e^{-4\beta J} + \sinh^2(\beta h)}}$$

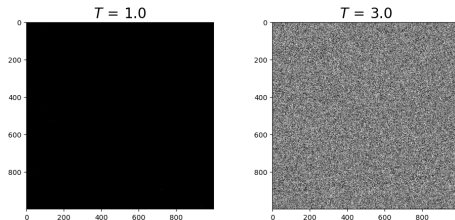
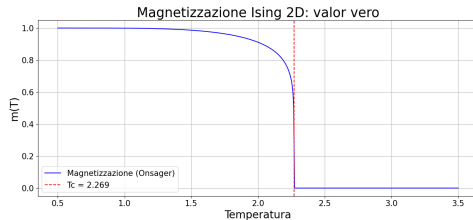


# Modello di Ising 2D

## 1 Introduzione

- ◇ Soluzione analitica per  $h = 0$
- ◇ Sistema presenta una transizione di fase a  $T_c \neq 0$

$$m(\beta, h = 0) = \begin{cases} \left[ 1 - \frac{1}{\sinh^4(2\beta J)} \right]^{\frac{1}{8}} & T < T_c \\ 0 & T > T_c \end{cases}$$





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## 2 Metodi numerici

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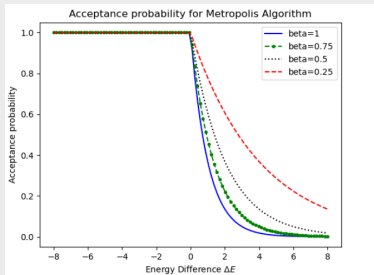


# Metropolis vs Wolff

## 2 Metodi numerici

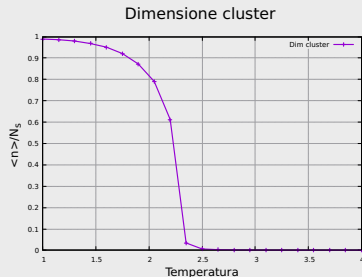
### Metropolis

- ◇ Tentata inversione di un singolo spin
- ◇  $A(\nu | \mu) = \min [1, e^{-\beta(E_\nu - E_\mu)}]$
- ◇ Ottimo per  $T \ll T_c$  oppure  $T \gg T_c$



### Wolff

- ◇ Algoritmo di clustering
- ◇  $P_{add} = 1 - \exp(-2\beta J)$
- ◇ Ottimo per  $T \simeq T_c$

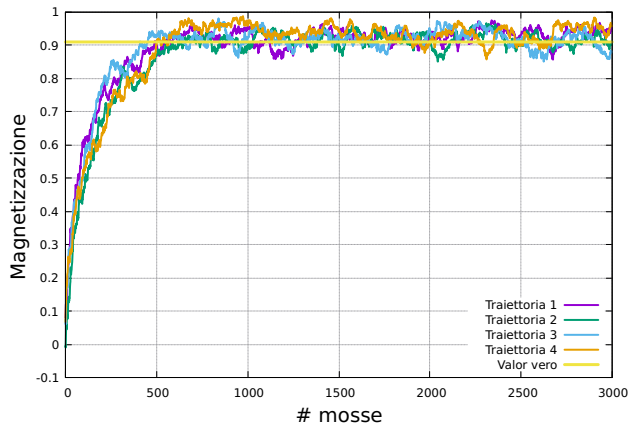




# Termalizzazione

## 2 Metodi numerici

Termalizzazione: 3000 spin,  $T = 0.5$



- ◇ Giungere all'equilibrio termodinamico
- ◇ Attenzione a stati metastabili
- ◇ Dipendenza dalla condizione iniziale

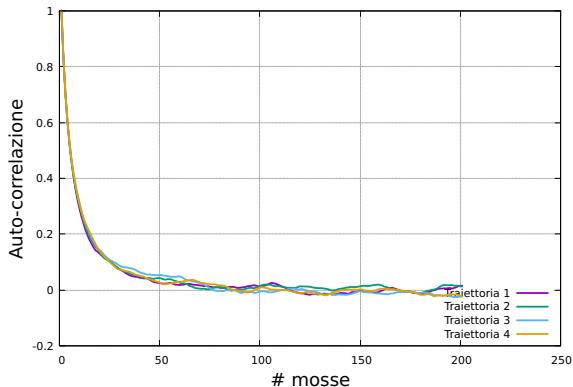




# Auto-correlazione

## 2 Metodi numerici

Autocorrelazione m:  $N = 500$ ,  $T = 2.0$



Autocorrelazione per modello di Ising 2D.

### Definizione

$$\chi(t) = \frac{\langle m(t')m(t' + t) \rangle_{t'} - \langle m \rangle^2}{\sigma_m^2}$$

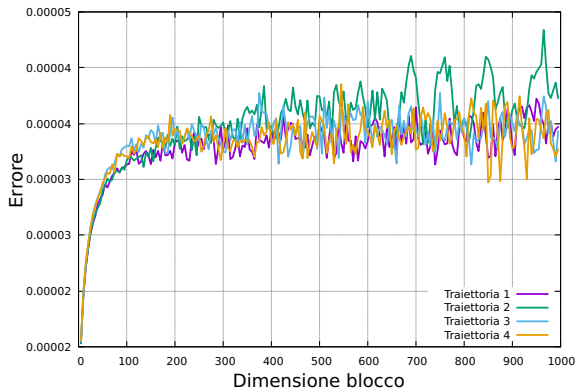
- ◇  $\chi(t) \propto e^{-t/t_c}$
- ◇ Indipendenza statistica fra configurazioni
- ◇  $n_{max} = \frac{t_{max}}{2t_c}$



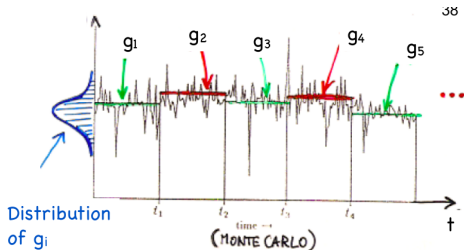
# Data-blocking

## 2 Metodi numerici

Dimensione blocco:  $N = 500$ ,  $T = 2.0$



Analisi per dimensione blocchi nel caso di un modello di Ising 2D.



- ◇ Dati raggruppati in blocchi
- ◇ Errore satura quando raggiunta  $l_{lim}$



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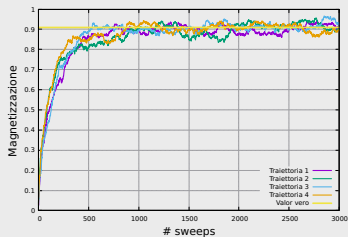
# Caratterizzazione

## 3 Simulazioni modello di Ising 1D

### Termalizzazione

- ◇ Maggiore  $T$ , minore  $t_{ter}$
- ◇  $t_{ter}^{max} \simeq 600$  sweeps

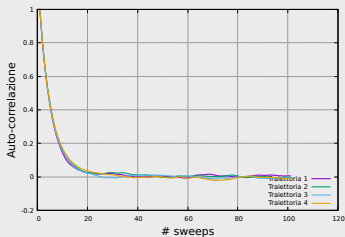
Termalizzazione: 10000 spin,  $T = 0.5$



### Auto-correlazione

- ◇ Maggiore  $T$ , minore  $t_c$
- ◇  $t_c^{max} \simeq 500$  sweeps

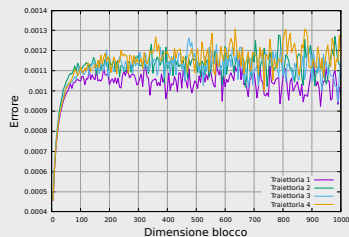
Autocorrelazione m: 1000 spin,  $T = 1.5$



### Blocchi

- ◇ Maggiore  $T$ , minore  $l_{blk}$
- ◇  $l_{blk}^{max} \simeq 1000$  sweeps

Dimensione blocco: 3000 spin,  $T = 1.0$

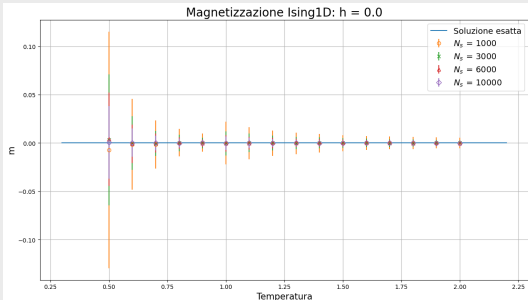




# Magnetizzazione

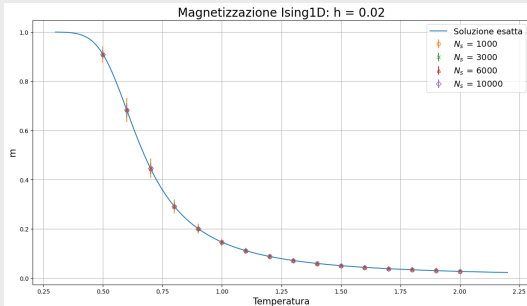
## 3 Simulazioni modello di Ising 1D

$$h = 0.0$$



◇  $m = 0$  per ogni  $T \neq 0$

$$h = 0.02$$



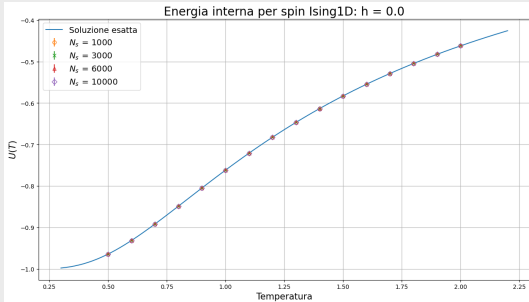
◇ campo magnetico impone ordine



# Energia interna

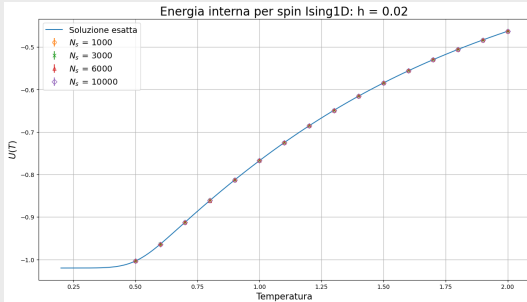
## 3 Simulazioni modello di Ising 1D

$h = 0.0$



◇ per  $T \rightarrow 0$  l'energia  $U(T) \rightarrow -1$

$h = 0.02$



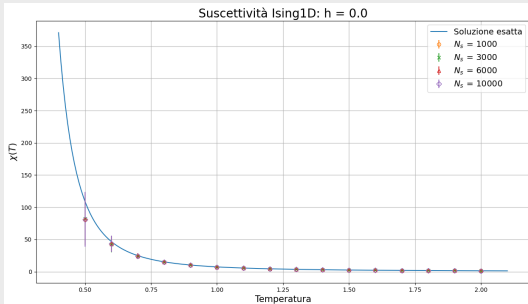
◇ per  $T \rightarrow 0$  l'energia  $U(T) \rightarrow -1.02$



# Suscettività magnetica

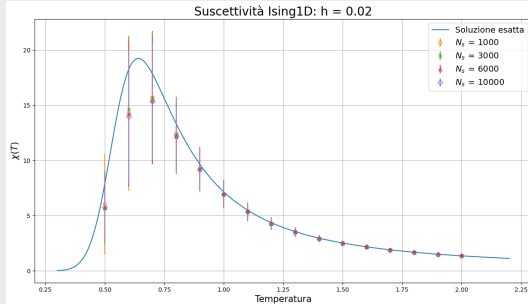
## 3 Simulazioni modello di Ising 1D

$$h = 0.0$$



◇ aumento per  $T \rightarrow 0$  perchè  $T_c = 0$

$$h = 0.02$$



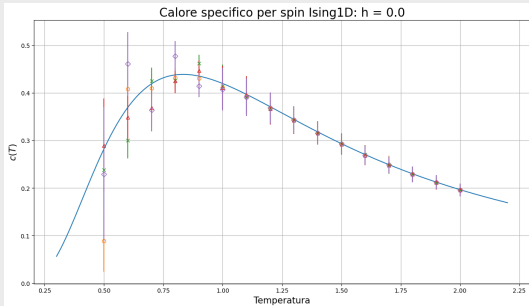
◇ picco a  $T \neq 0$  dovuto ad  $h$



# Calore specifico

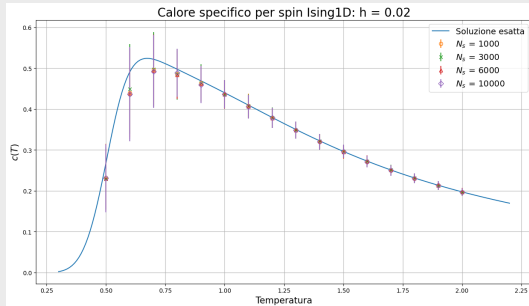
## 3 Simulazioni modello di Ising 1D

$h = 0.0$



◇ difficoltà a studiare il picco

$h = 0.02$



◇ campo magnetico semplifica lo studio





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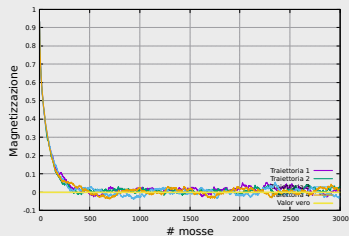
# Caratterizzazione con metropolis

## 4 Simulazioni modello di Ising 1D

### Termalizzazione

- ◇  $t_{ter}$  maggiori per  $T \simeq T_c$
- ◇  $t_{ter}^{max} \simeq 500$  sweeps

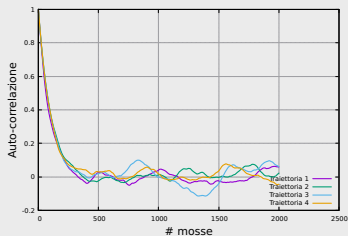
Termalizzazione:  $N = 500$  spin,  $T = 2.5$



### Auto-correlazione

- ◇  $t_c$  maggiori per  $T \simeq T_c$
- ◇  $t_c^{max} \simeq 400$  sweeps

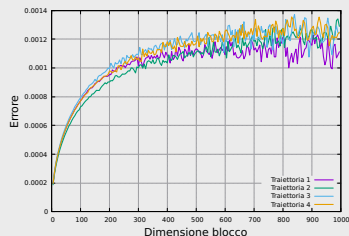
Autocorrelazione m:  $N = 100$ ,  $T = 2.5$



### Blocchi

- ◇  $l_{blk}$  maggiori per  $T \simeq T_c$
- ◇  $l_{blk}^{max} \simeq 1000$  sweeps

Dimensione blocco:  $N = 400$ ,  $T = 2.5$





# Caratterizzazione con Wolff

4 Simulazioni modello di Ising 1D

**Termalizzazione**

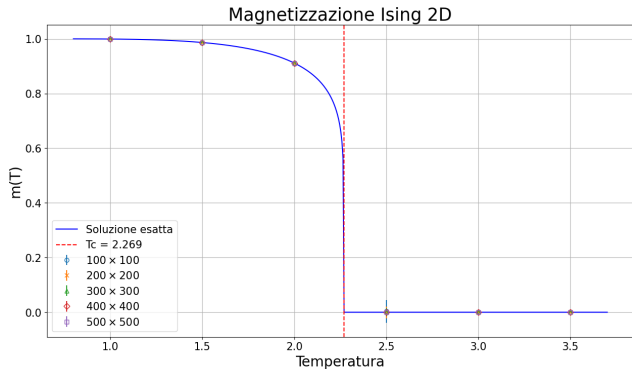
**Auto-correlazione**

**Blocchi**



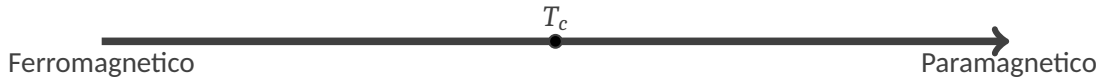
# Magnetizzazione

## 4 Simulazioni modello di Ising 1D



◇ Magnetizzazione spontanea  
per  $T < T_c$

◇ Transizione di fase a  $T_c$

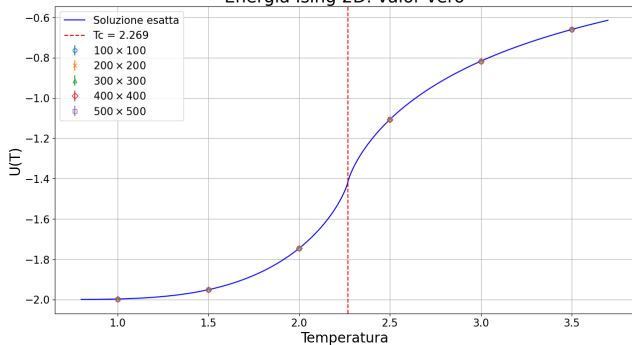




# Energia

## 4 Simulazioni modello di Ising 1D

Energia Ising 2D: valor vero



- ◇ copro tutto il reticolo con due legami per spin
- ◇ picco del calore specifico a  $T_c$

$$U = -NJ \coth(2\beta J) \left\{ 1 + \frac{2}{\pi} [2 \tanh^2(2\beta J) - 1] \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - k^2 \sin^2(\phi)}} \right\}$$



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# Fine

5 Conclusioni

Grazie per l'attenzione



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- ▶ **Backup modello di Ising 1D**
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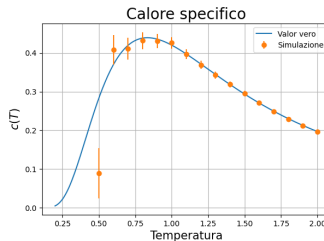
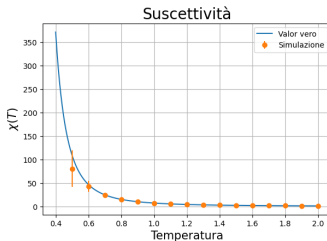
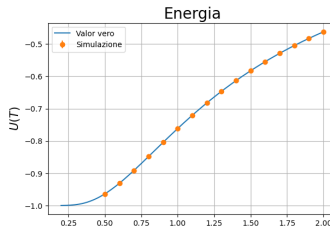
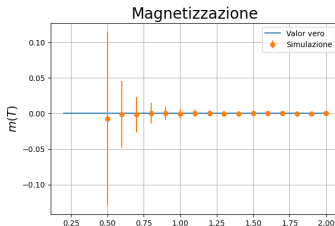




# Osservabili per $N_s = 1000$ , $h = 0.0$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 1000$ ,  $h = 0.0$

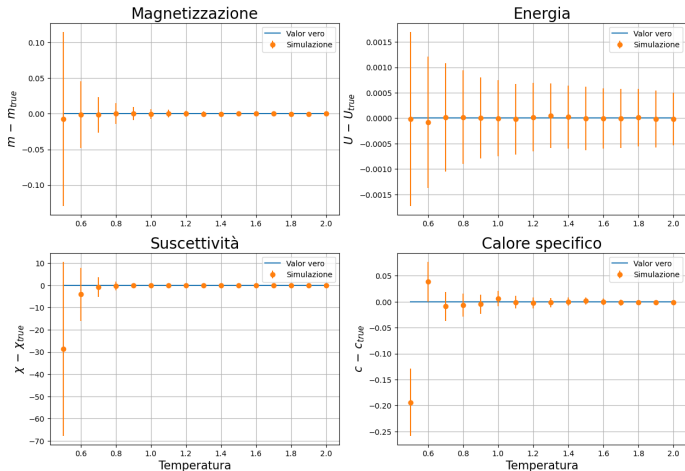




# Differenza dal valor vero per $N_s = 1000$ , $h = 0.0$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 1000$ ,  $h = 0.0$

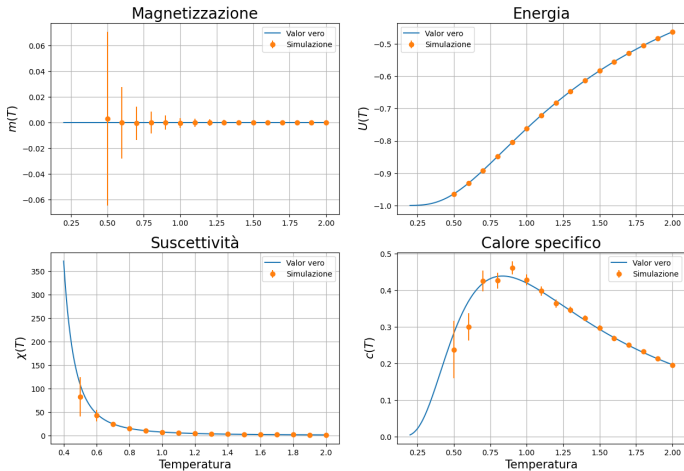




# Osservabili per $N_s = 3000$ , $h = 0.0$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 3000$ ,  $h = 0.0$

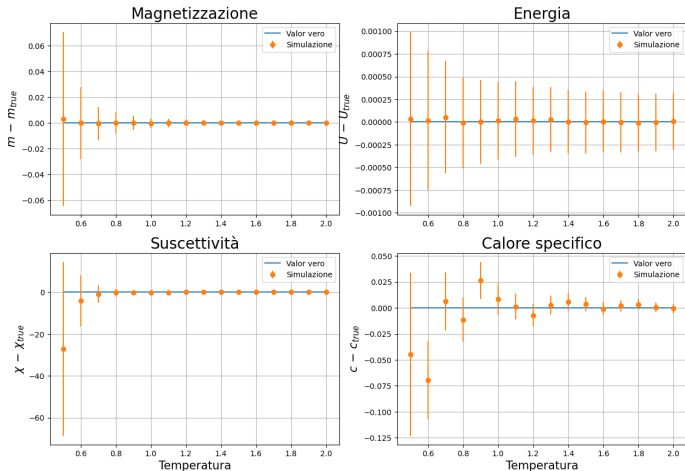




# Differenza dal valor vero per $N_s = 3000$ , $h = 0.0$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 3000$ ,  $h = 0.0$

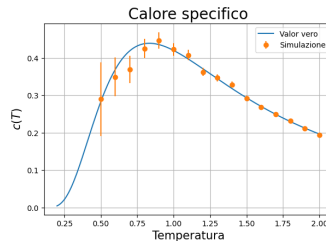
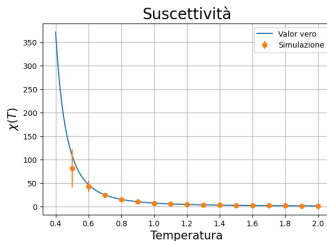
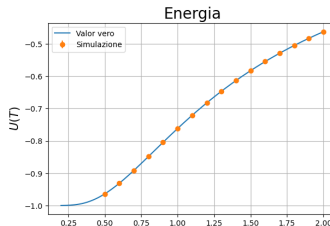
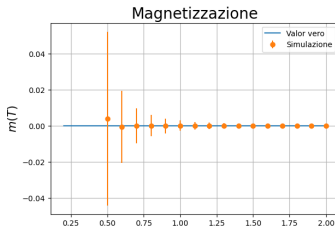




# Osservabili per $N_s = 6000$ , $h = 0.0$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 6000$ ,  $h = 0.0$

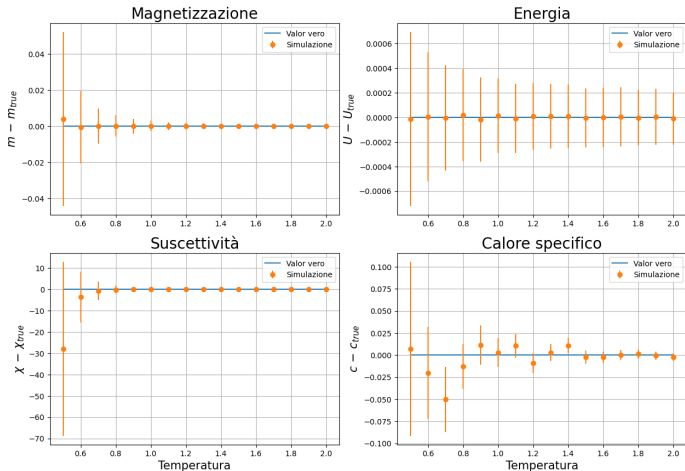




# Differenza dal valor vero per $N_s = 6000$ , $h = 0.0$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 6000$ ,  $h = 0.0$

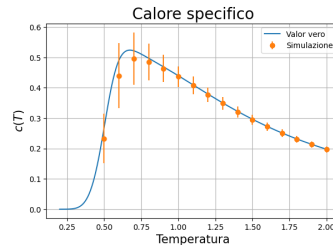
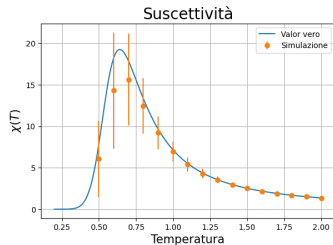
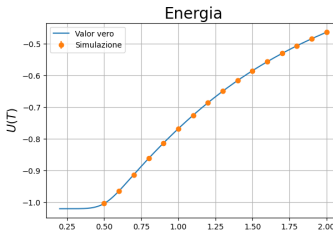
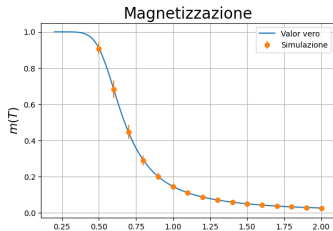




# Osservabili per $N_s = 1000$ , $h = 0.02$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 1000$ ,  $h = 0.02$

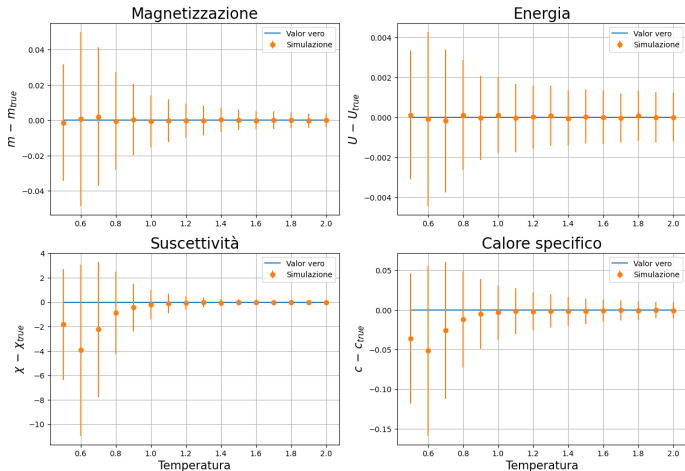




# Differenza dal valor vero per $N_s = 1000$ , $h = 0.02$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 1000$ ,  $h = 0.02$



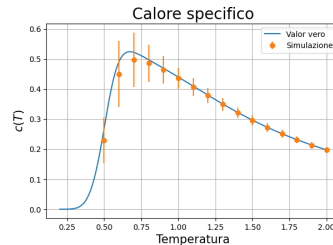
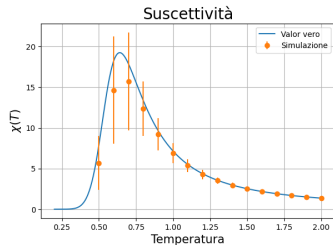
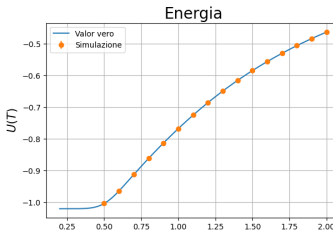
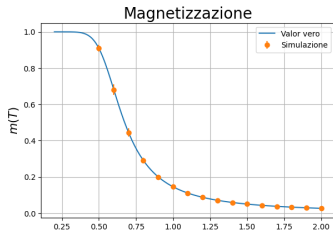




# Osservabili per $N_s = 3000$ , $h = 0.02$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 3000$ ,  $h = 0.02$

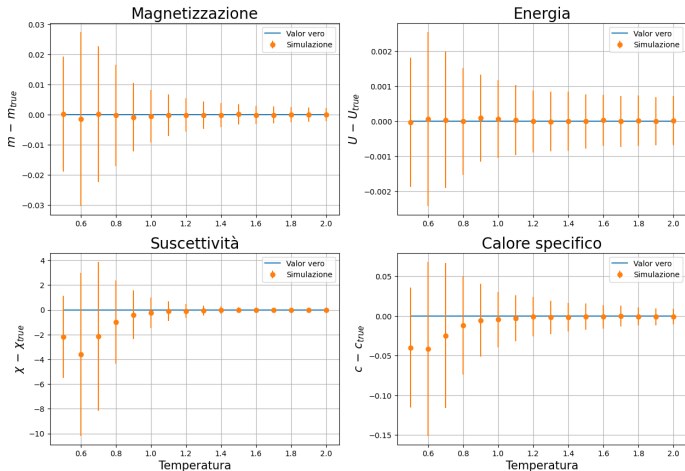




# Differenza dal valor vero per $N_s = 3000$ , $h = 0.02$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 3000$ ,  $h = 0.02$

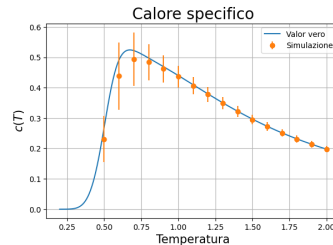
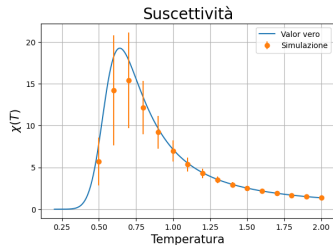
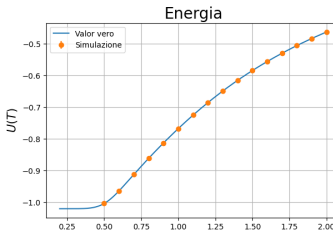
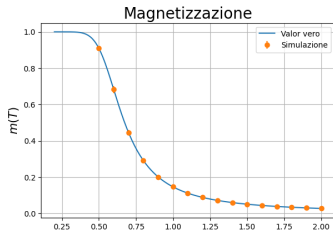




# Osservabili per $N_s = 6000$ , $h = 0.02$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 6000$ ,  $h = 0.02$

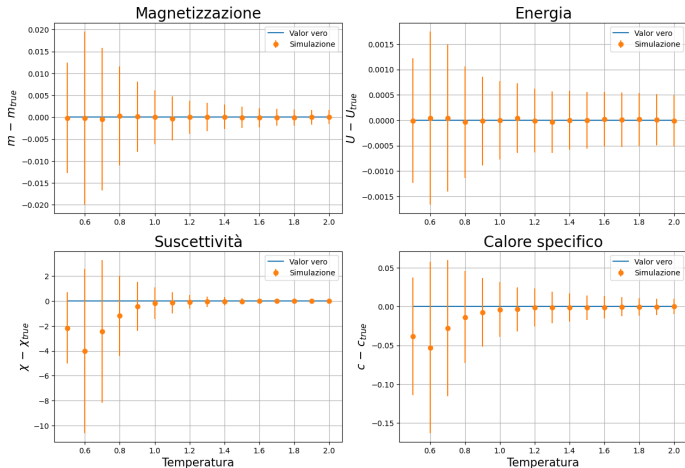




# Differenza dal valor vero per $N_s = 6000$ , $h = 0.02$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 6000$ ,  $h = 0.02$

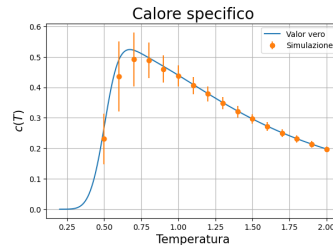
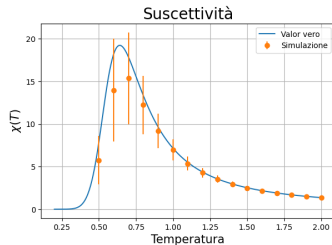
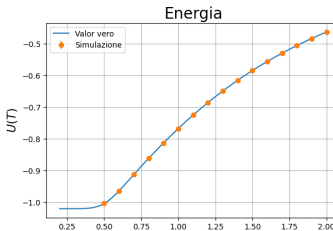
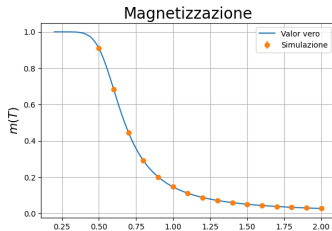




# Osservabili per $N_s = 10000$ , $h = 0.02$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 10000$ ,  $h = 0.02$

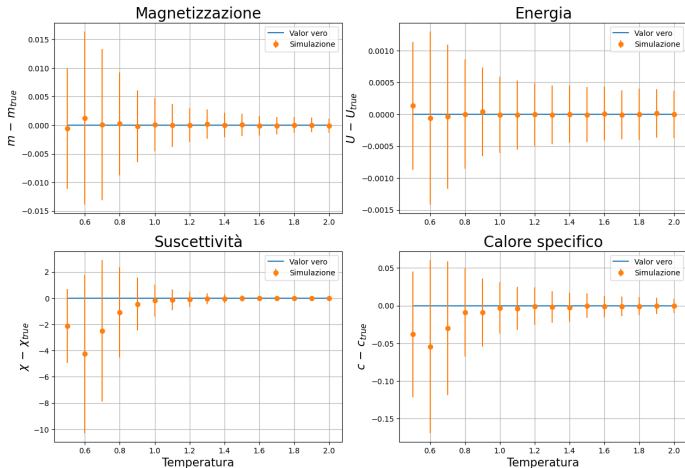




# Differenza dal valor vero per $N_s = 10000$ , $h = 0.02$

## 6 Backup modello di Ising 1D

Ising 1D:  $N_s = 10000$ ,  $h = 0.02$





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## 7 Backup modello di Ising 2D

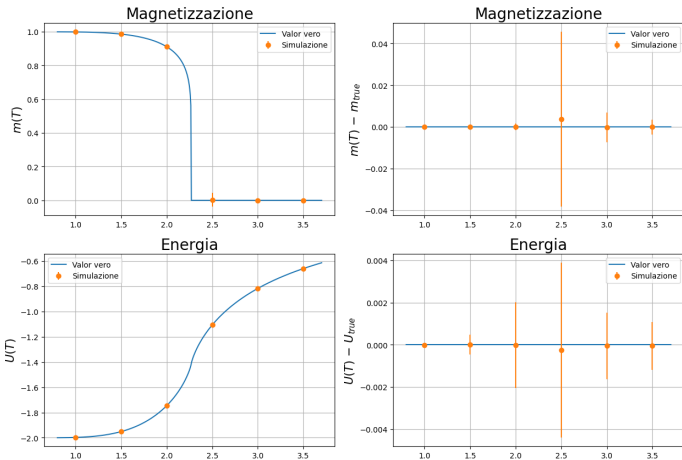
- ▶ Introduzione
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# Osservabili per reticolo $100 \times 100$

7 Backup modello di Ising 2D

Ising 2D: reticolo  $100 \times 100$



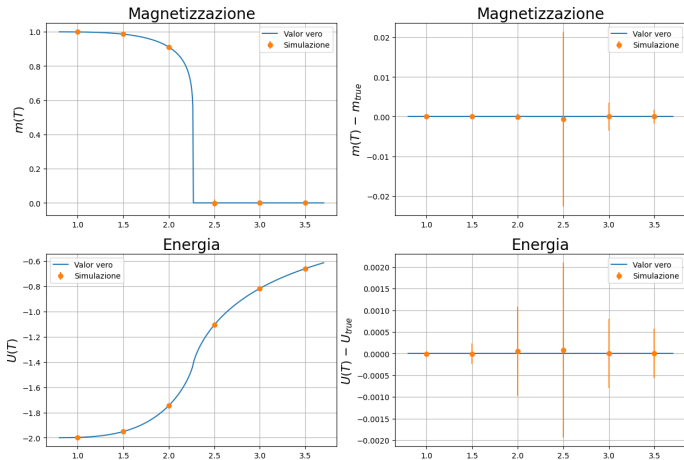




# Osservabili per reticolo $200 \times 200$

7 Backup modello di Ising 2D

Ising 2D: reticolo  $200 \times 200$

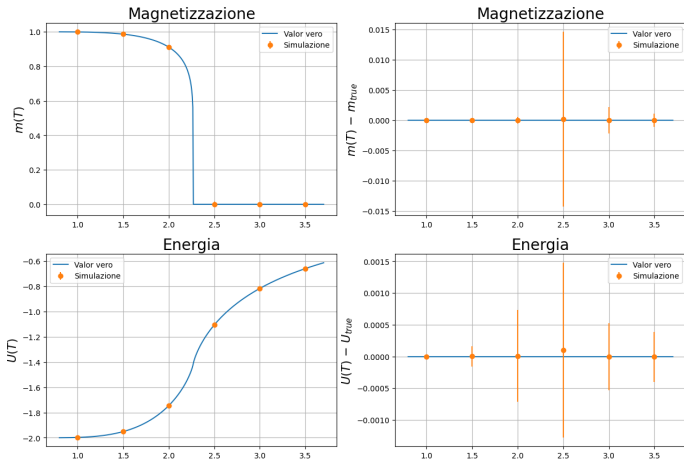




# Osservabili per reticolo $300 \times 300$

7 Backup modello di Ising 2D

Ising 2D: reticolo  $300 \times 300$

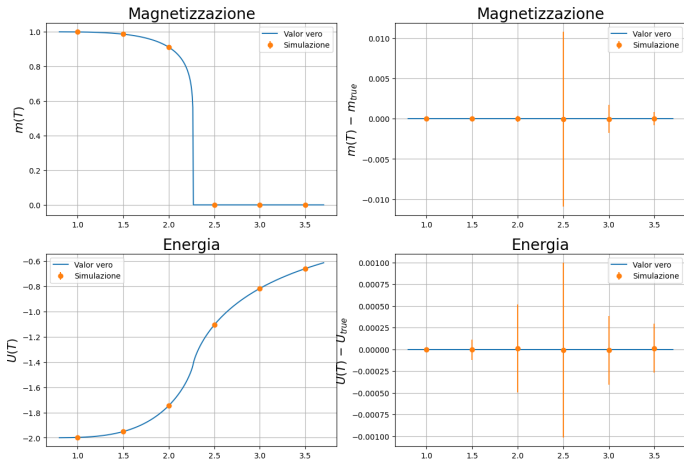




# Osservabili per reticolo $400 \times 400$

7 Backup modello di Ising 2D

Ising 2D: reticolo  $400 \times 400$





# Osservabili per reticolo $500 \times 500$

## 7 Backup modello di Ising 2D

Ising 2D: reticolo  $500 \times 500$

