



Il modello di Ising

Simulazione di Materia Condensata e Biosistemi

Filippo Negrini (Matricola: 47127A)



UNIVERSITÀ
DEGLI STUDI
DI MILANO



Table of Contents

1 Introduzione

- ▶ **Introduzione**
- ▶ Metodi numerici
- ▶ Simulazioni modello di Ising 1D
- ▶ Simulazioni modello di Ising 1D
- ▶ Conclusioni
- ▶ 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 $T_c \neq 0$

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

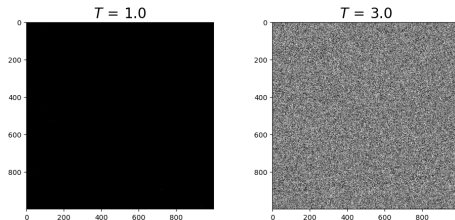
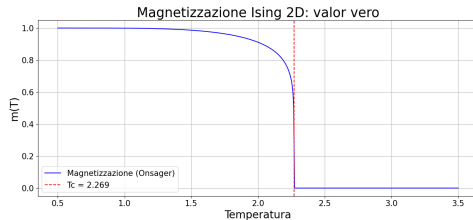




Table of Contents

2 Metodi numerici

- ▶ Introduzione
- ▶ **Metodi numerici**
- ▶ Simulazioni modello di Ising 1D
- ▶ Simulazioni modello di Ising 1D
- ▶ Conclusioni
- ▶ Backup modello di Ising 1D
- ▶ Backup modello di Ising 2D

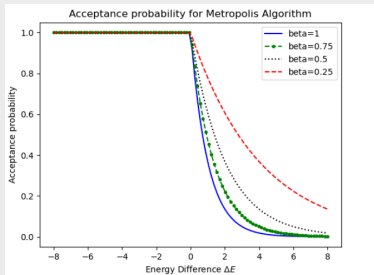


Metropolis vs Wolff

2 Metodi numerici

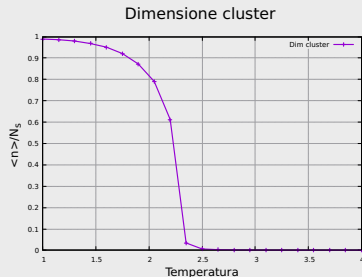
Metropolis

- ◇ 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 $T \simeq T_c$

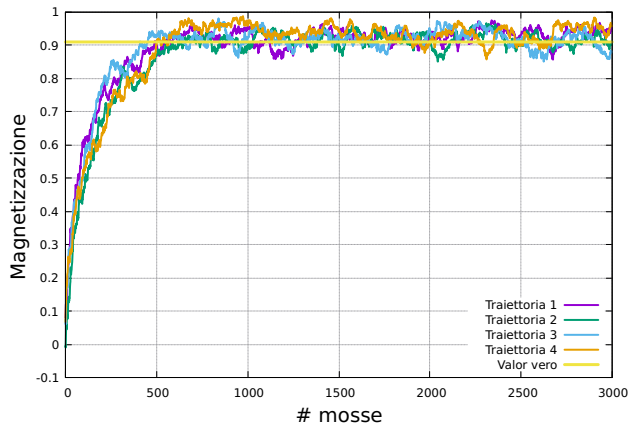




Termalizzazione

2 Metodi numerici

Termalizzazione: 3000 spin, $T = 0.5$



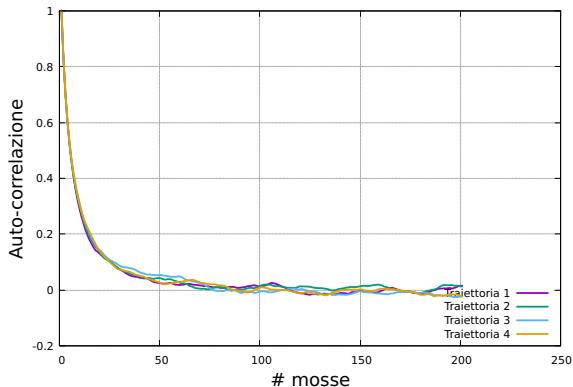
- ◇ Giungere all'equilibrio termodinamico
- ◇ Attenzione a stati metastabili
- ◇ Dipendenza dalla condizione iniziale



Auto-correlazione

2 Metodi numerici

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



Autocorrelazione per modello di Ising 2D.

Definizione

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

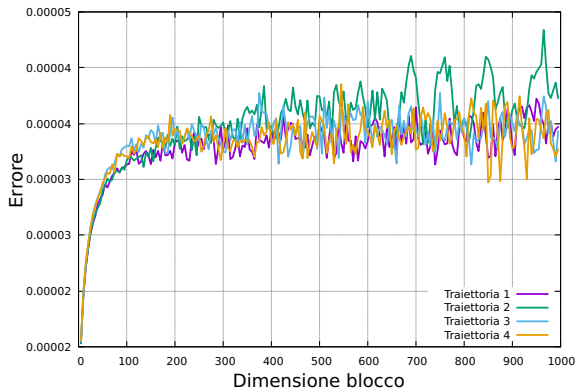
- ◇ $\chi(t) \propto e^{-t/t_c}$
- ◇ Indipendenza statistica fra configurazioni
- ◇ $n_{max} = \frac{t_{max}}{2t_c}$



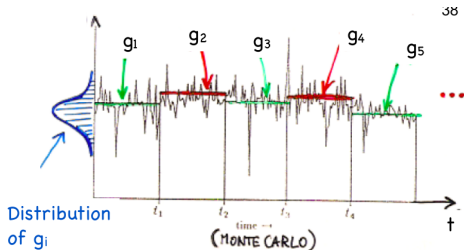
Data-blocking

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}



Table of Contents

3 Simulazioni modello di Ising 1D

- ▶ Introduzione
- ▶ Metodi numerici
- ▶ **Simulazioni modello di Ising 1D**
- ▶ Simulazioni modello di Ising 1D
- ▶ Conclusioni
- ▶ Backup modello di Ising 1D
- ▶ Backup modello di Ising 2D



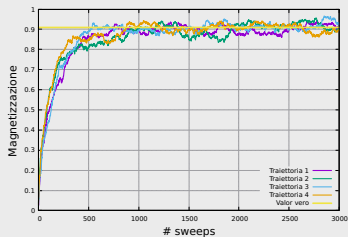
Caratterizzazione

3 Simulazioni modello di Ising 1D

Termalizzazione

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

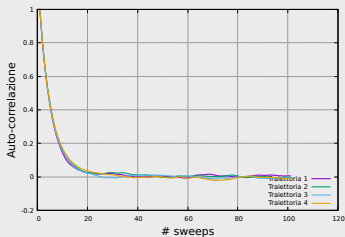
Termalizzazione: 10000 spin, $T = 0.5$



Auto-correlazione

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

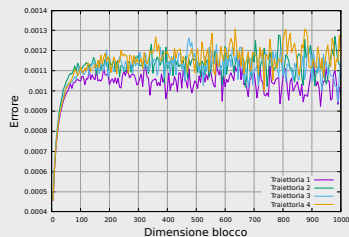
Autocorrelazione m: 1000 spin, $T = 1.5$



Blocchi

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

Dimensione blocco: 3000 spin, $T = 1.0$

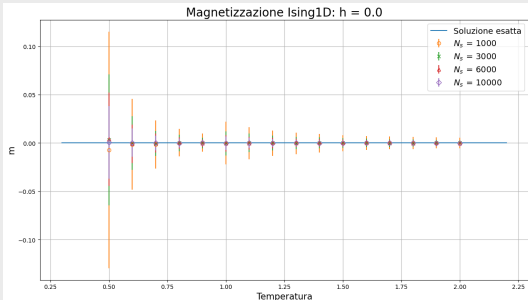




Magnetizzazione

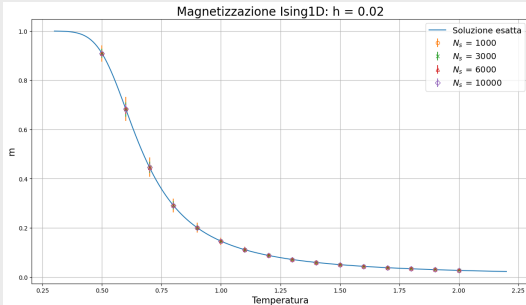
3 Simulazioni modello di Ising 1D

$$h = 0.0$$



◇ $m = 0$ per ogni $T \neq 0$

$$h = 0.02$$



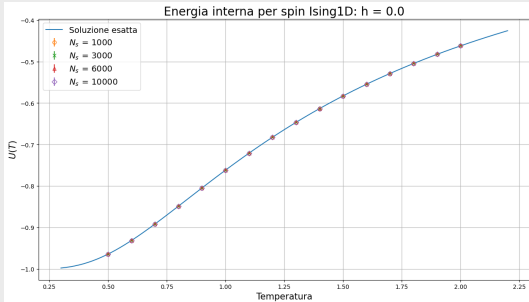
◇ campo magnetico impone ordine



Energia interna

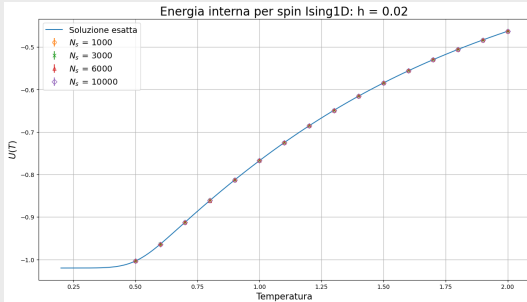
3 Simulazioni modello di Ising 1D

$h = 0.0$



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

$h = 0.02$



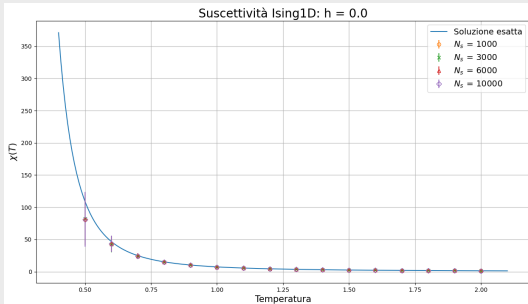
◇ per $T \rightarrow 0$ l'energia $U(T) \rightarrow -1.02$



Suscettività magnetica

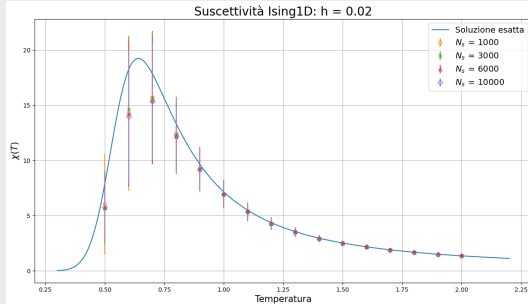
3 Simulazioni modello di Ising 1D

$$h = 0.0$$



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

$$h = 0.02$$



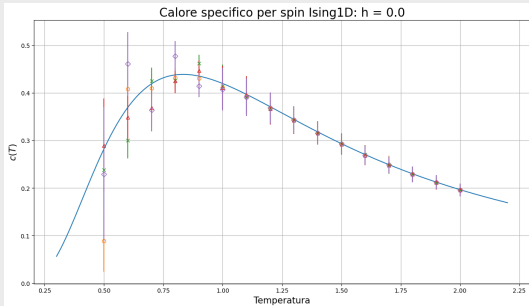
◇ picco a $T \neq 0$ dovuto ad h



Calore specifico

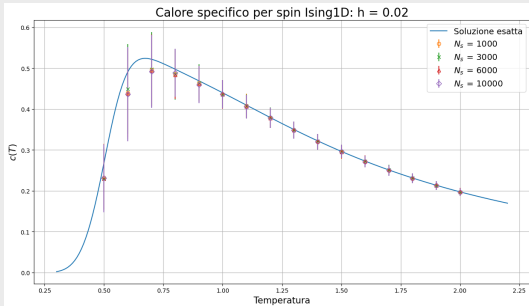
3 Simulazioni modello di Ising 1D

$$h = 0.0$$



◇ difficoltà a studiare il picco

$$h = 0.02$$



◇ campo magnetico semplifica lo studio



Table of Contents

4 Simulazioni modello di Ising 1D

- ▶ Introduzione
- ▶ Metodi numerici
- ▶ Simulazioni modello di Ising 1D
- ▶ **Simulazioni modello di Ising 1D**
- ▶ Conclusioni
- ▶ Backup modello di Ising 1D
- ▶ Backup modello di Ising 2D



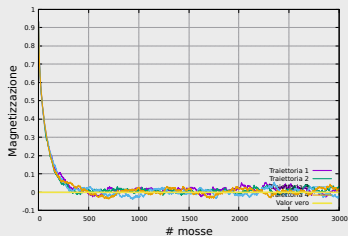
Caratterizzazione con metropolis

4 Simulazioni modello di Ising 1D

Termalizzazione

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

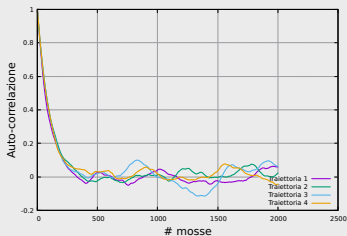
Termalizzazione: $N = 500$ spin, $T = 2.5$



Auto-correlazione

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

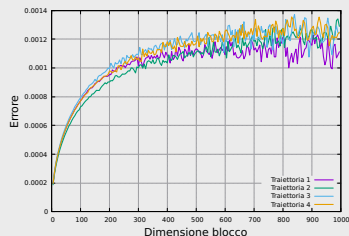
Autocorrelazione m: $N = 100$, $T = 2.5$



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

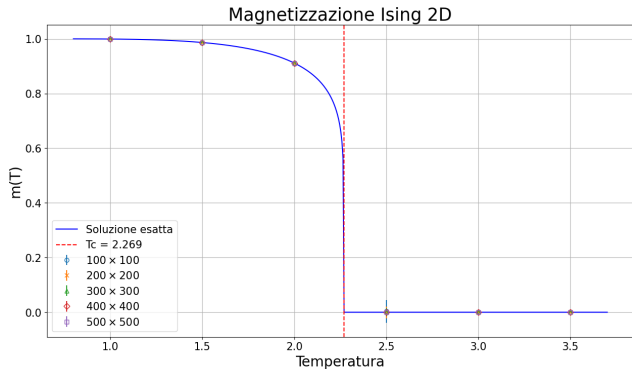
Auto-correlazione

Blocchi



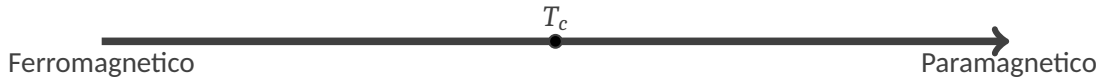
Magnetizzazione

4 Simulazioni modello di Ising 1D



◇ Magnetizzazione spontanea per $T < T_c$

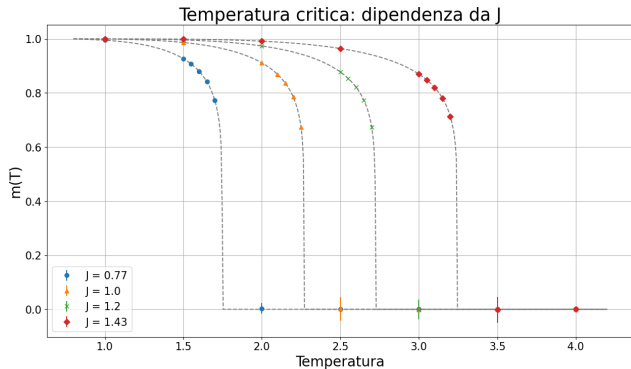
◇ Transizione di fase a T_c





Dipendenza da J

4 Simulazioni modello di Ising 1D



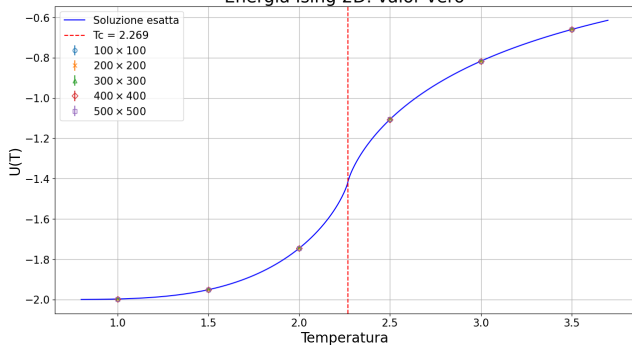
- ◇ Aumenta J , aumenta T_c
- ◇ Presenza o meno di ordine dipende dall'intensità dell'interazione



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

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



Calore specifico

4 Simulazioni modello di Ising 1D



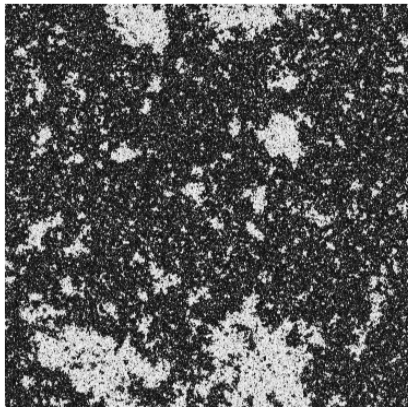
Suscettività

4 Simulazioni modello di Ising 1D

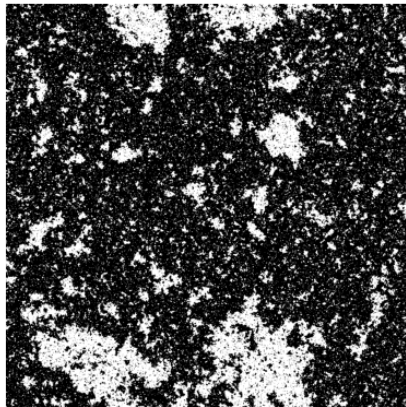


Coarse graining

4 Simulazioni modello di Ising 1D



CG
→

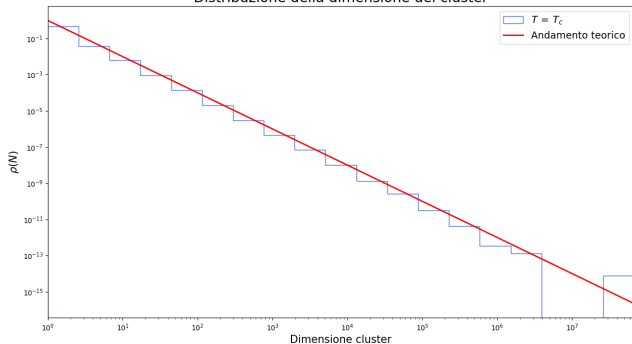




Dimensioni cluster

4 Simulazioni modello di Ising 1D

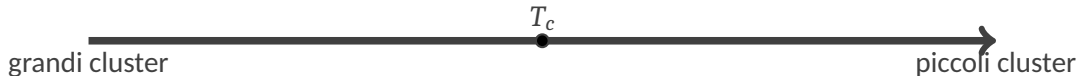
Distribuzione della dimensione dei cluster



$$\diamond P(s) \propto s^{-\alpha}$$

$$\diamond \alpha \simeq 2$$

\diamond perdita di un parametro di scala





Esponenti critici

4 Simulazioni modello di Ising 1D



Table of Contents

5 Conclusioni

- ▶ Introduzione
- ▶ Metodi numerici
- ▶ Simulazioni modello di Ising 1D
- ▶ Simulazioni modello di Ising 1D
- ▶ **Conclusioni**
- ▶ Backup modello di Ising 1D
- ▶ Backup modello di Ising 2D



Fine

5 Conclusioni

Grazie per l'attenzione



Table of Contents

6 Backup modello di Ising 1D

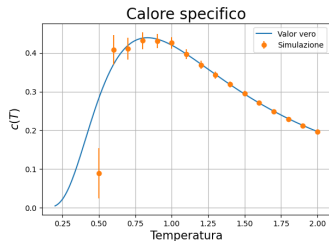
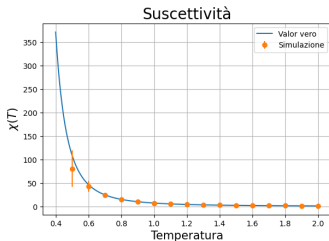
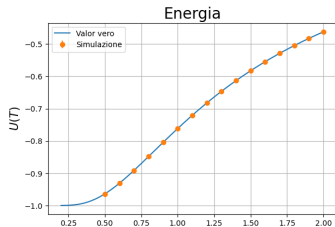
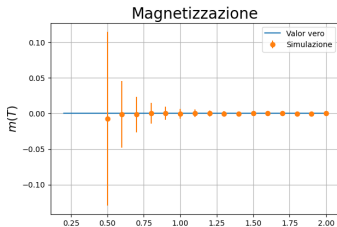
- ▶ Introduzione
- ▶ Metodi numerici
- ▶ Simulazioni modello di Ising 1D
- ▶ Simulazioni modello di Ising 1D
- ▶ Conclusioni
- ▶ **Backup modello di Ising 1D**
- ▶ Backup modello di Ising 2D



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

6 Backup modello di Ising 1D

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

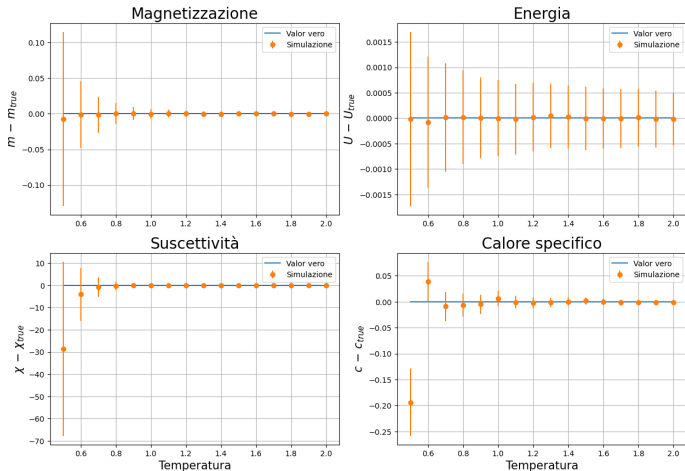




Differenza dal valor vero per $N_s = 1000$, $h = 0.0$

6 Backup modello di Ising 1D

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

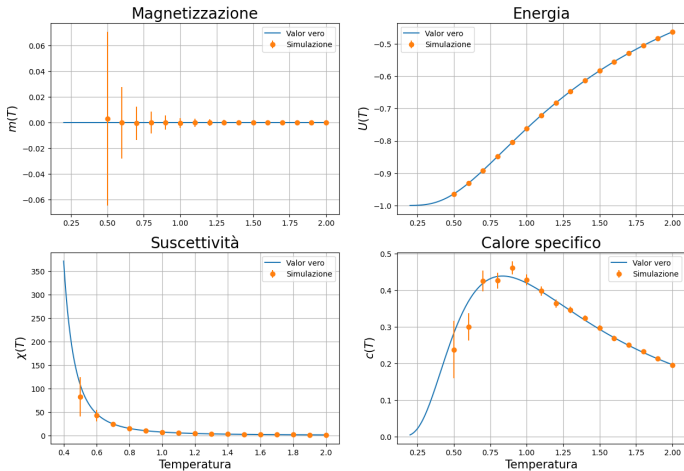




Osservabili per $N_s = 3000$, $h = 0.0$

6 Backup modello di Ising 1D

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

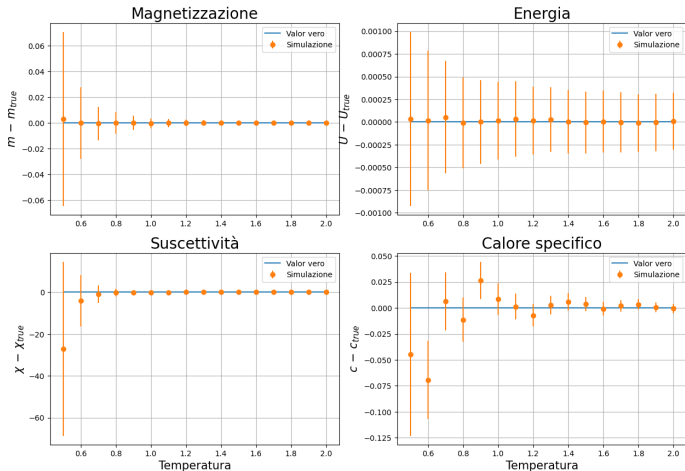




Differenza dal valor vero per $N_s = 3000$, $h = 0.0$

6 Backup modello di Ising 1D

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

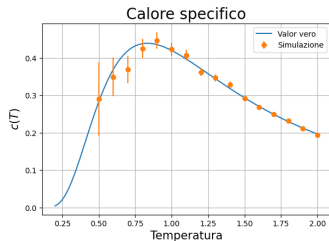
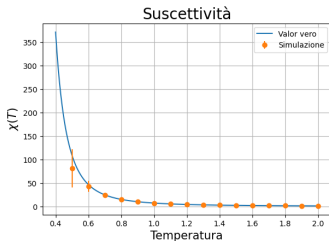
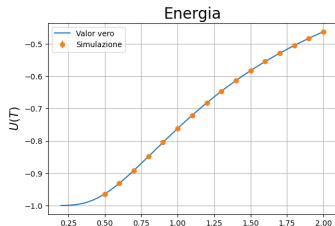
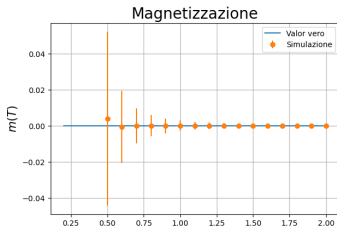




Osservabili per $N_s = 6000$, $h = 0.0$

6 Backup modello di Ising 1D

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

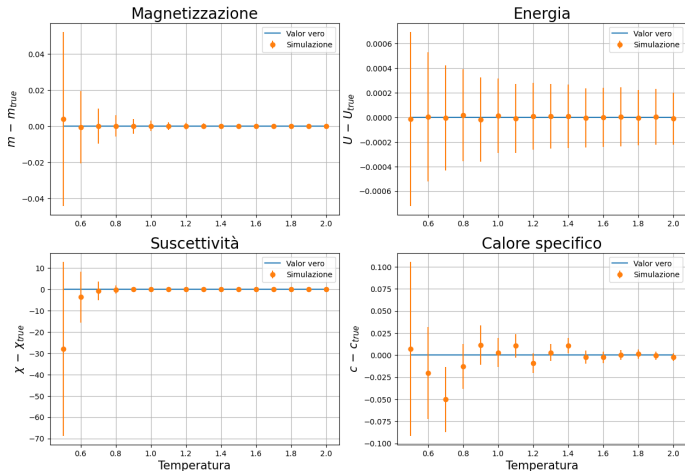




Differenza dal valor vero per $N_s = 6000$, $h = 0.0$

6 Backup modello di Ising 1D

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

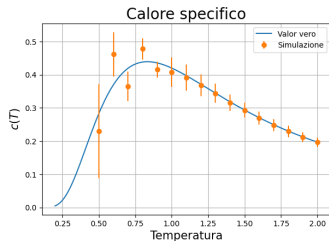
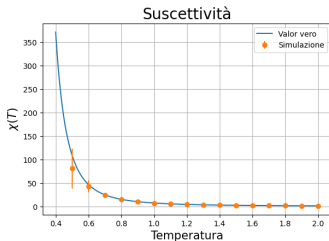
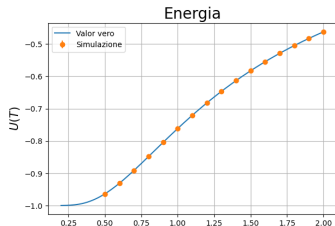
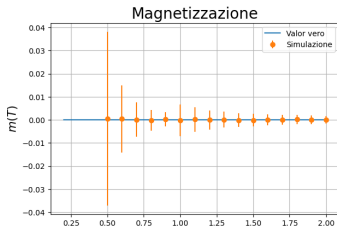




Osservabili per $N_s = 10000$, $h = 0.0$

6 Backup modello di Ising 1D

Ising 1D: $N_s = 10000$, $h = 0.0$

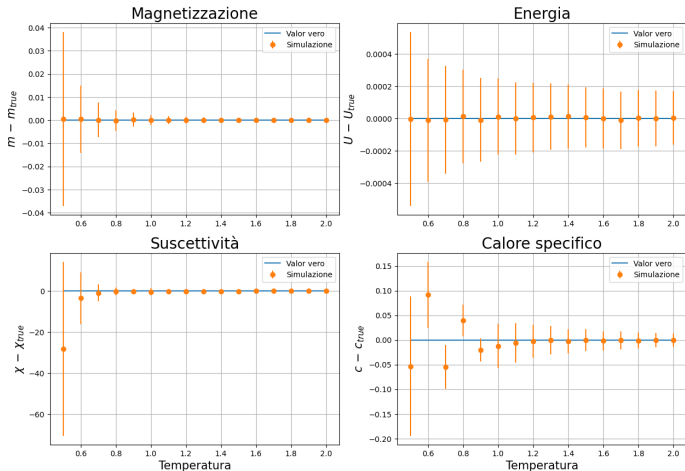




Differenza dal valor vero per $N_s = 10000$, $h = 0.0$

6 Backup modello di Ising 1D

Ising 1D: $N_s = 10000$, $h = 0.0$

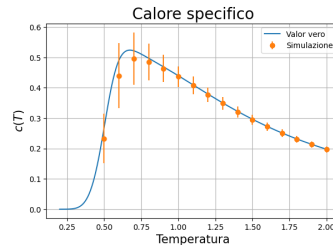
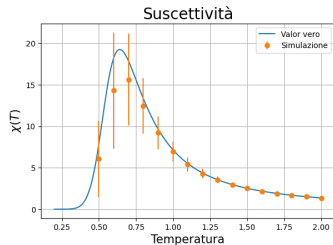
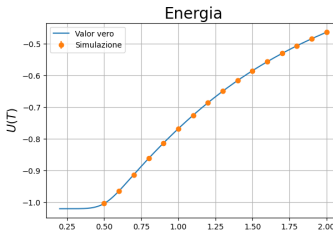
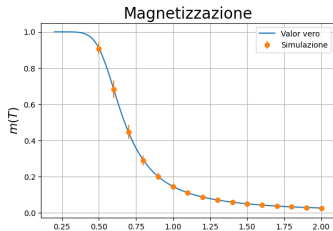




Osservabili per $N_s = 1000$, $h = 0.02$

6 Backup modello di Ising 1D

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

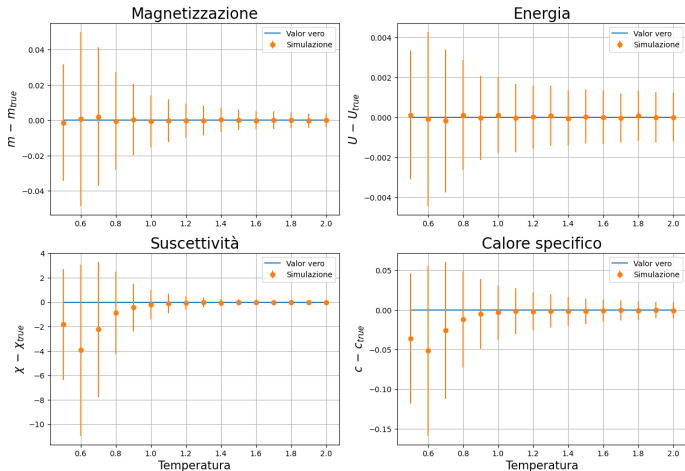




Differenza dal valor vero per $N_s = 1000$, $h = 0.02$

6 Backup modello di Ising 1D

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

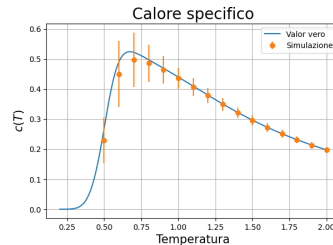
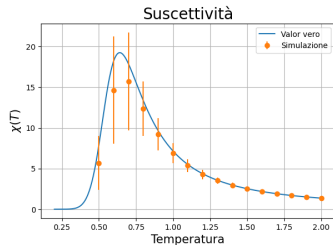
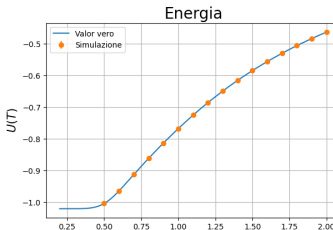
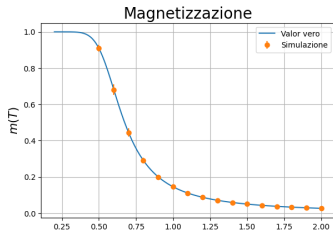




Osservabili per $N_s = 3000$, $h = 0.02$

6 Backup modello di Ising 1D

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

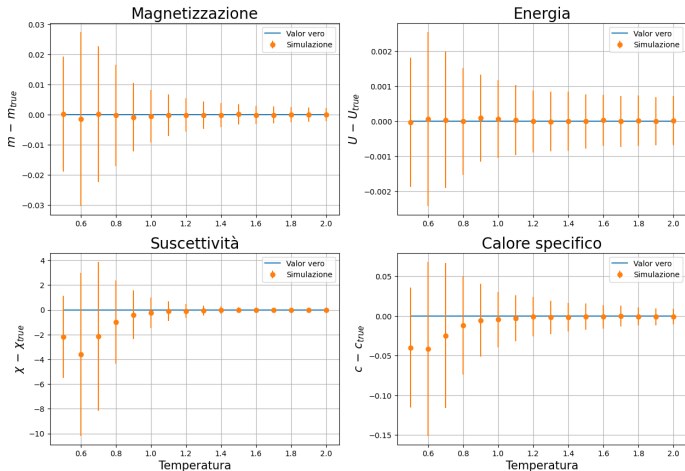




Differenza dal valor vero per $N_s = 3000$, $h = 0.02$

6 Backup modello di Ising 1D

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

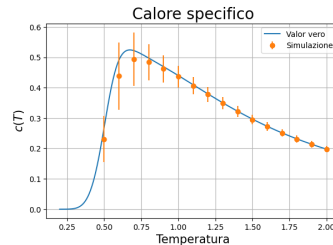
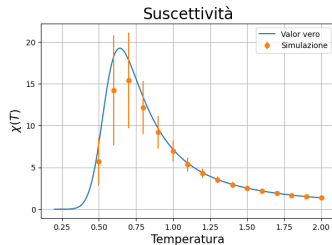
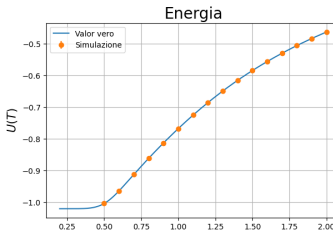
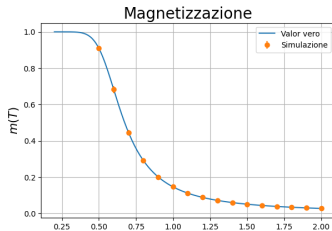




Osservabili per $N_s = 6000$, $h = 0.02$

6 Backup modello di Ising 1D

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

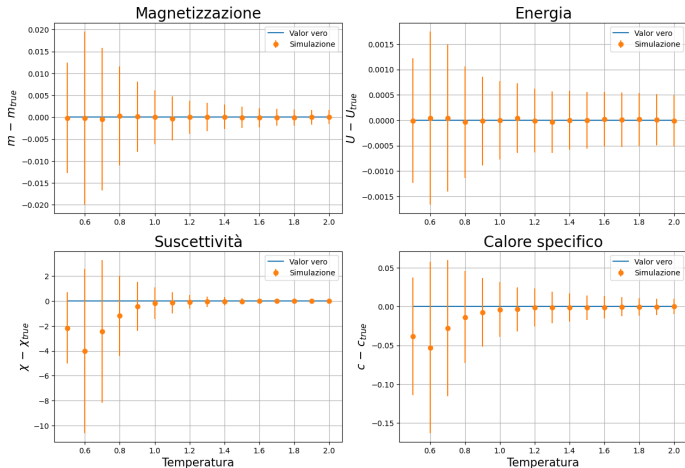




Differenza dal valor vero per $N_s = 6000$, $h = 0.02$

6 Backup modello di Ising 1D

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

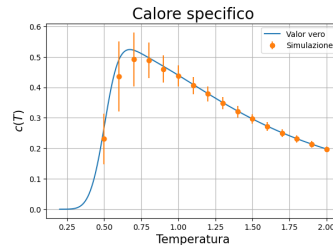
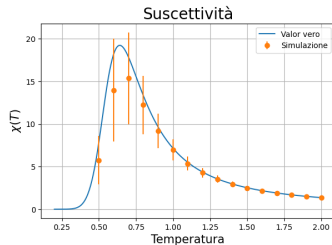
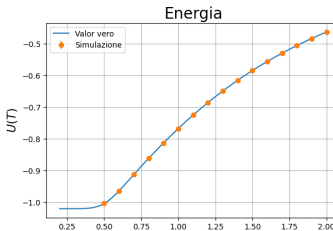
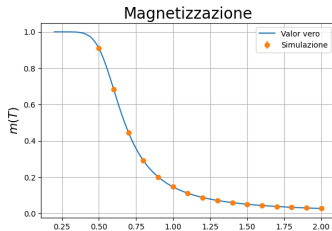




Osservabili per $N_s = 10000$, $h = 0.02$

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: $N_s = 10000$, $h = 0.02$

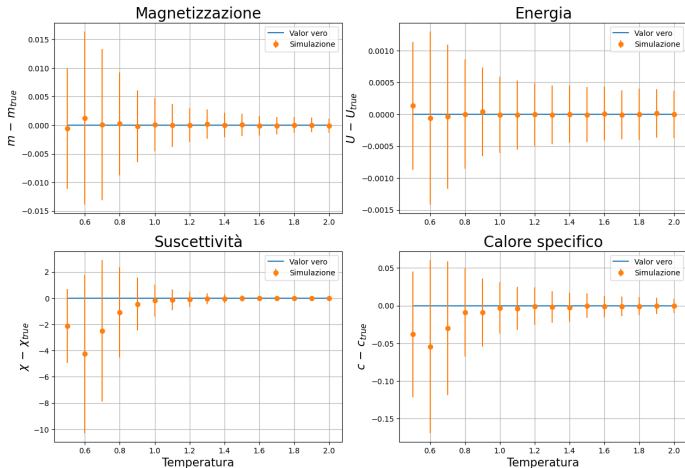




Table of Contents

7 Backup modello di Ising 2D

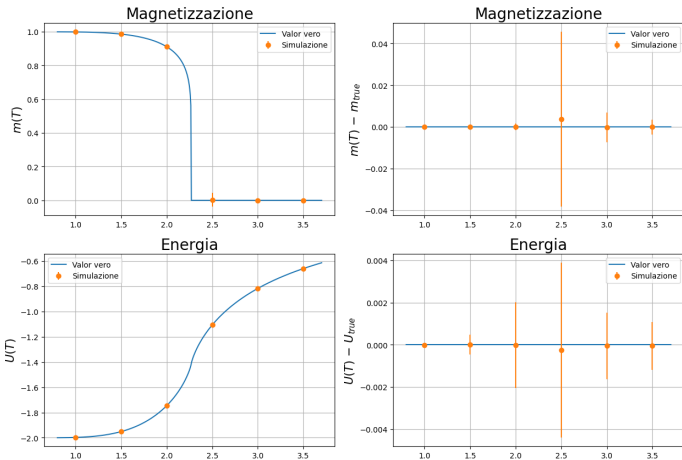
- ▶ Introduzione
- ▶ Metodi numerici
- ▶ Simulazioni modello di Ising 1D
- ▶ Simulazioni modello di Ising 1D
- ▶ Conclusioni
- ▶ Backup modello di Ising 1D
- ▶ Backup modello di Ising 2D



Osservabili per reticolo 100×100

7 Backup modello di Ising 2D

Ising 2D: reticolo 100×100

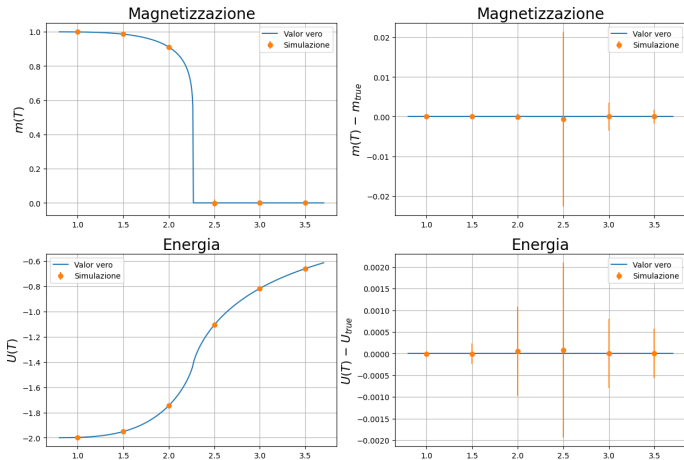




Osservabili per reticolo 200×200

7 Backup modello di Ising 2D

Ising 2D: reticolo 200×200

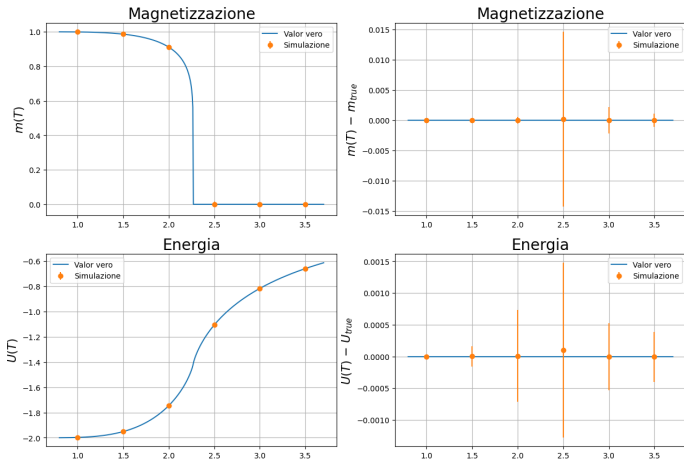




Osservabili per reticolo 300×300

7 Backup modello di Ising 2D

Ising 2D: reticolo 300×300

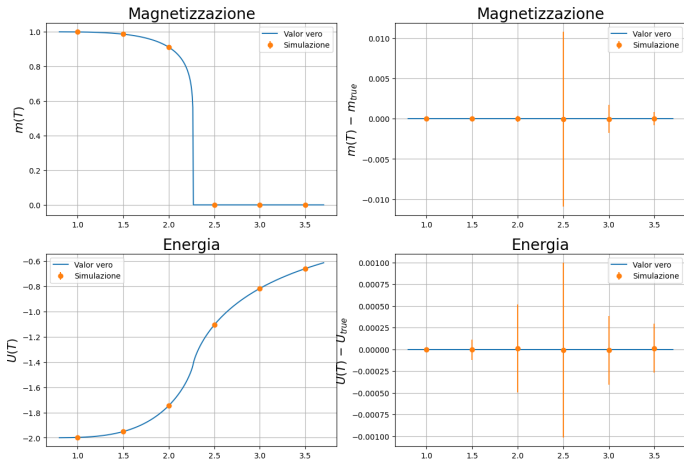




Osservabili per reticolo 400×400

7 Backup modello di Ising 2D

Ising 2D: reticolo 400×400





Osservabili per reticolo 500×500

7 Backup modello di Ising 2D

Ising 2D: reticolo 500×500

