27/10/2021

Implementazione numerica

codice di diagonalizzazione esatta (ED)
exact diagonalization

Spazi di Hilbert $\mathcal{H}$ a dimensione FINITA

→ sistemi di spin-1/2 su reticolo unidimensionale

N siti ⇒ $\dim \mathcal{H} = 2^N$

- 1 sito $\quad \mathcal{H}^{(1)} = \mathrm{span}\{|\uparrow\rangle, |\downarrow\rangle\}$ rispetto all'asse z

spin-1/2 ↔ quantum bit (qubit)

$|\uparrow\rangle \equiv |0\rangle \qquad |\downarrow\rangle \equiv |1\rangle \qquad \dim \mathcal{H}^{(1)} = 2^1 = 2$

[base computazionale]

- 2 siti $\quad \mathcal{H}^{(2)} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(1)} = \mathrm{span}\{\underbrace{|\uparrow,\uparrow\rangle}_{|\uparrow\rangle_1 \otimes |\uparrow\rangle_2}, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow\downarrow\rangle\}$

$|\uparrow,\uparrow\rangle = |00\rangle \qquad |\uparrow,\downarrow\rangle = |01\rangle$

$|\downarrow,\uparrow\rangle = |10\rangle \qquad |\downarrow,\downarrow\rangle = |11\rangle$

$\dim \mathcal{H}^{(2)} = 2^2 = 4$

- N siti: $\quad \mathcal{H}^{(N)} = \underbrace{\mathcal{H}^{(1)} \otimes \mathcal{H}^{(1)} \otimes \dots \otimes \mathcal{H}^{(1)}}_{N \text{ volte}}$

$\dim \mathcal{H}^{(N)} = 2^N$

indice di sito $i = 1, \dots, 2^N$

i → converto in notazione binaria → base computazionale

- Operatori hanno una struttura tensoriale

$$\hat{H}_{Is} = -J \sum_j \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z - g \sum_j \hat{\sigma}_j^x - h \sum_j \hat{\sigma}_j^z$$

$$\hat{\sigma}_1^\alpha \equiv \underset{\text{I sito}}{\hat{\sigma}^\alpha} \otimes \underset{\text{II sito}}{\hat{\mathbb{1}}_2} \otimes \underset{\text{III sito}}{\hat{\mathbb{1}}_2} \otimes \dots \otimes \hat{\mathbb{1}}_2 \qquad (\alpha = x, y, z)$$

matrici 2x2 $\quad \hat{\mathbb{1}}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$$\hat{\sigma}_j^z \hat{\sigma}_{j+1}^z = \underset{\text{I sito}}{\hat{\mathbb{1}}_2} \otimes \dots \otimes \underset{(j-1)\text{ sito}}{\hat{\mathbb{1}}_2} \otimes \underset{j\text{-sito}}{\hat{\sigma}^z} \otimes \underset{(j+1)\text{ sito}}{\hat{\sigma}^z} \otimes \underset{(j+2)\text{ sito}}{\hat{\mathbb{1}}_2} \otimes \dots \otimes \underset{N\text{-sito}}{\hat{\mathbb{1}}_2}$$

prodotto tensore: $\hat{A} \otimes \hat{B} = \begin{pmatrix} a_{11}B & a_{12}B & a_{13}B & \cdots \\ a_{21}B & a_{22}B & a_{23}B & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}$

$\hat{A}$ matrice $n_A \times n_A$

$\hat{B}$ " $n_B \times n_B$

$\Rightarrow \hat{A} \otimes \hat{B}$ matrice $n_A n_B \times n_A n_B$

es. $\hat{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ $\hat{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$

$$\Rightarrow \hat{A} \times \hat{B} = \left(\begin{array}{cc|cc} a_{11} b_{11} & a_{11} b_{12} & a_{12} b_{11} & a_{12} b_{12} \\ a_{11} b_{21} & a_{11} b_{22} & a_{12} b_{21} & a_{12} b_{22} \\ \hline \multicolumn{2}{c|}{a_{21} \times B} & \multicolumn{2}{c}{a_{22} \times B} \end{array}\right)$$

se $\hat{A} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\rightarrow$ $\hat{\mathbb{1}} \otimes \hat{B} = \left(\begin{array}{c|c} \cdot\ \cdot & 0 \\ \cdot\ \cdot & \\ \hline & \cdot\ \cdot \\ 0 & \cdot\ \cdot \end{array}\right)$ blocchi di zeri

non nulli

le Hamiltoniane con cui abbiamo a che fare sono tipicamente SPARSE (ci sono tanti zeri)

$\rightarrow$ somme di termini a "uno" e a "due corpi"

→ Costruzione della matrice $\hat{H}$ sulla base computazionale

III campo longitudinale: $\boxed{-h \sum_{j=1}^{N} \hat{\sigma}_j^z}$ matrice DIAGONALE

$$\hat{\sigma}_j^z \,|\ldots\ldots 1_j \ldots\rangle = -|\ldots\ldots 1_j \ldots\ldots\rangle$$

$$\hat{\sigma}_j^z \,|\ldots\ldots 0_j \ldots\rangle = +|\ldots\ldots 0_j \ldots\ldots\rangle$$

es: $N=3$ $i = 1,2,3,\ldots, \overset{8}{2^3} = |000\rangle, |001\rangle, |010\rangle, \ldots, |111\rangle$

$$\hat{\sigma}_1^z = \hat{\sigma}^z \otimes \hat{\mathbb{1}} \otimes \hat{\mathbb{1}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 &&& \\ & 1 && \\ && 1 & \\ &&& 1 \end{pmatrix} =$$

$$= \begin{pmatrix} 1 &&&&&&& \\ & 1 &&&&&& \\ && 1 &&&&& \\ &&& 1 &&&& \\ &&&& -1 &&& \\ &&&&& -1 && \\ &&&&&& -1 & \\ &&&&&&& -1 \end{pmatrix}$$

$\hat{\sigma}_2^z = \begin{pmatrix} 1 & \\ & \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & \end{pmatrix} \ldots \begin{pmatrix} 1 & \\ & \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} = \begin{pmatrix} 1 && \\ & 1 & \\ && -1 \end{pmatrix}$

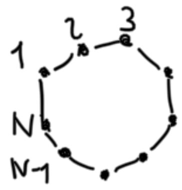
$$\hat\sigma_2^z = \begin{pmatrix}1&\\&1\end{pmatrix}\otimes\begin{pmatrix}1&\\&-1\end{pmatrix}\otimes\begin{pmatrix}1&\\&1\end{pmatrix} = \begin{pmatrix}1&\\&1\end{pmatrix}\otimes\begin{pmatrix}1&&&\\&1&&\\&&-1&\\&&&-1\end{pmatrix} = \begin{pmatrix}1&&&&&&&\\&1&&&&&&\\&&-1&&&&&\\&&&-1&&&&\\&&&&1&&&\\&&&&&1&&\\&&&&&&-1&\\&&&&&&&-1\end{pmatrix}$$

Ⓘ Interazione : $-J\sum_j \hat\sigma_j^z\hat\sigma_{j+1}^z$ diagonale

gli estremi della sommatoria dipendono dalle condizioni al contorno

aperte $\quad$ 1 — 2 — 3 — - - - - - N $\quad\Rightarrow j = 1,\dots,N-1$

chiuse



$\Rightarrow j = 1,\dots,N \qquad \hat\sigma_{N+1}^z \equiv \hat\sigma_1^z$

$$\hat\sigma_1^z\otimes\hat\sigma_2^z\otimes\hat{\mathbb{1}} = \begin{pmatrix}1&\\&-1\end{pmatrix}\otimes\begin{pmatrix}1&\\&-1\end{pmatrix}\otimes\begin{pmatrix}1&\\&1\end{pmatrix} = \begin{pmatrix}1&&&\\&-1&&\\&&-1&\\&&&1\end{pmatrix}\otimes\begin{pmatrix}1&\\&1\end{pmatrix} =$$

$$= \begin{pmatrix}1&&&&&&&\\&1&&&&&&\\&&-1&&&&&\\&&&-1&&&&\\&&&&-1&&&\\&&&&&-1&&\\&&&&&&1&\\&&&&&&&1\end{pmatrix}$$

$$\{|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle\}$$ base computazionale su 3 siti

$$\hat\sigma_j^z\otimes\hat\sigma_{j+1}^z|\dots 0_j\, 0_{j+1}\dots\rangle = +|\dots 0_j\, 0_{j+1}\dots\rangle$$

$$\hat\sigma_j^z\otimes\hat\sigma_{j+1}^z|\dots 1_j\, 1_{j+1}\dots\rangle = +|\dots 1_j\, 1_{j+1}\dots\rangle$$

$$\hat\sigma_j^z\otimes\hat\sigma_{j+1}^z|\dots 0_j\, 1_{j+1}\dots\rangle = -|\dots 0_j\, 1_{j+1}\dots\rangle$$

$$\hat\sigma_j^z\otimes\hat\sigma_{j+1}^z|\dots 1_j\, 0_{j+1}\dots\rangle = -|\dots 1_j\, 0_{j+1}\dots\rangle$$

Ⓘⓘ campo trasverso: $-g\sum_{j=1}^N \hat\sigma_j^x$ NON diagonale

$$\hat\sigma_j^x|\dots 0_j\dots\rangle = |\dots 1_j\dots\rangle$$

$$\hat\sigma_j^x|\dots 1_j\dots\rangle = |\dots 0_j\dots\rangle$$

$$\hat\sigma_1^x \equiv \hat\sigma^x\otimes\hat{\mathbb{1}}_2\otimes\hat{\mathbb{1}}_2 = \begin{pmatrix}0&1\\1&0\end{pmatrix}\otimes\begin{pmatrix}1&\\&1\end{pmatrix}\otimes\begin{pmatrix}1&\\&1\end{pmatrix} = \begin{pmatrix}0&1\\1&0\end{pmatrix}\otimes\begin{pmatrix}1&&&\\&1&&\\&&1&\\&&&1\end{pmatrix} =$$

$$= \left(\begin{array}{cccc|cccc}&&&&1&&&\\&&&&&1&&\\&&&&&&1&\\&&&&&&&1\\\hline 1&&&&&&&\\&1&&&&&&\end{array}\right)$$

$$\begin{pmatrix} & 1 & 1 \\ & 1 & 1 \end{pmatrix}$$

→ **Osservabili:** $A = \langle\psi|\hat{A}|\psi\rangle$

$$= \sum_{\substack{i_1 \dots i_N \\ j_1 \dots j_N}} C^*_{j_1 \dots j_N} C_{i_1 \dots i_N} \underbrace{\langle j_1 \dots j_N|\hat{A}|i_1 \dots i_N\rangle}_{\text{tipicamente } \hat{A} \text{ è una matrice sparsa}}$$

$|\psi\rangle = \sum_n C_n|n\rangle \rightarrow$ converto in in binario

$$= \sum_{i_1, \dots i_N = 0}^{1} C_{i_1, i_2, \dots i_N} |i_1, i_2, \dots, i_N\rangle$$

⇒ NON occorre calcolare tutti i $(2^N)^2$ valori di aspettazione, ma solo quelli non nulli.

28/10/2021

Lanczos (Arnoldi, Davidson)

principio di funzionamento ~1950 (utile per matrici $\hat{H}$ sparse)

→ tecnica variazionale per trovare il ground state. $|\psi_{g.s.}\rangle$, $E_{g.s.}$

1) • prendo uno stato $|\psi_0\rangle$ (a priori arbitrario)

2) • costruisco un secondo stato $|\tilde{\psi}_1\rangle$ a partire da $|\psi_0\rangle$

$$|\tilde{\psi}_1\rangle = \hat{K}|\psi_0\rangle \qquad \hat{K} \text{ è "generico"}$$

3) • orto-normalizzo $|\tilde{\psi}_1\rangle$ rispetto a $|\psi_0\rangle$

$$|\psi_1\rangle = \frac{\hat{K} - \langle\psi_0|\hat{K}|\psi_0\rangle}{\sqrt{\langle\psi_0|\hat{K}^\dagger\hat{K}|\psi_0\rangle - |\langle\psi_0|\hat{K}|\psi_0\rangle|^2}}|\psi_0\rangle \qquad \left(\begin{array}{l} \langle\psi_1|\psi_0\rangle = 0 \\ |\langle\psi_1|\psi_1\rangle|^2 = 1 \end{array} \right)$$

4) • costruisco $\mathcal{H}_1 = \text{span}\{|\psi_0\rangle, |\psi_1\rangle\}$

e diagonalizzo $\hat{H}$ su questo spazio:

$$\hat{H}_{ridotta} = \begin{pmatrix} \langle\psi_0|\hat{H}|\psi_0\rangle & \langle\psi_1|\hat{H}|\psi_0\rangle \\ \langle\psi_0|\hat{H}|\psi_1\rangle & \langle\psi_1|\hat{H}|\psi_1\rangle \end{pmatrix}$$

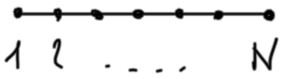
[NOTA: occorre solo saper applicare $\hat{H}$ ad un generico stato $|\psi\rangle$
$|\psi\rangle \to \hat{H}|\psi\rangle$]

5) • ↳ stato a energia minima: $|\psi_0^{(1)}\rangle = \alpha|\psi_0\rangle + \beta|\psi_1\rangle$ $\quad |\alpha|^2 + |\beta|^2 = 1$

6) • Itero la procedura $|\psi_0\rangle \mapsto |\psi_0^{(1)}\rangle$

→ Test: Ising 1D in campo trasverso $\hat{H} = -\sum_j \hat{\sigma}^z_j \hat{\sigma}^z_{j+1} - g \sum_j \hat{\sigma}^x_j$

OBC $\quad E_{g.s.}(N, g=1) = 1 - \left[\sin\left(\frac{\pi}{2(2N+1)}\right)\right]^{-1}$



(Pfeuty, Ann. Phys. 57, 79 (1970))

• $N \to +\infty \qquad M^x = \frac{1}{\pi}\int_0^{\pi} \frac{dq}{\omega(q, g^{-1})} + \frac{1}{g}\cdot\frac{1}{\pi}\int_0^{\pi} \frac{\cos q \, dq}{\omega(q, g^{-1})}$

Se $g=1$: $\qquad$ con $\omega(q,g) = \sqrt{1+g^2+2g\cos q}$

$$\begin{cases} M^x = \frac{2}{\pi} \\ \langle \hat{\sigma}^x_j \hat{\sigma}^x_{j+r} \rangle - (M^x)^2 = \frac{4}{\pi^2}\cdot\frac{1}{4r^2-1} \end{cases}$$

MAGNETIZZAZIONE TRASVERSA