IMPLEMENTAZIONE NUMERICA

22/10/2020

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

- base computazionale

$\mathcal{H} = \mathbb{C}^{2N}$

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

$i = 1, 2, 3, \ldots, 2^N$

$\downarrow$ codificare in binario $(i-1)$

0 e 1

($\uparrow$) ($\downarrow$)

orientazione degli spin lungo z

$\hat{\sigma}^z |\uparrow\rangle = +|\uparrow\rangle$

$\hat{\sigma}^z |\downarrow\rangle = -|\downarrow\rangle$

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

		3° spin	2° spin	1° spin
$i=1$	$\to 0$	0	0	0
$i=2$	$\to 1$	0	0	1
$i=3$	$\to 10$	0	1	0
$i=4$	$\to 11$	0	1	1
$i=5$	$\to 100$	1	0	0
$i=6$	$\to 101$	1	0	1
$i=7$	$\to 110$	1	1	0
$i=8$	$\to 111$	1	1	1

$|i=1\rangle \equiv |\uparrow, \uparrow, \uparrow\rangle$

$|i=2\rangle \equiv |\uparrow, \uparrow, \downarrow\rangle$

$|i=3\rangle \equiv |\uparrow, \downarrow, \uparrow\rangle$

$\vdots$

$|i=8\rangle \equiv |\downarrow, \downarrow, \downarrow\rangle$

$\rightarrow$ campo longitudinale:

- $\hat{\sigma}_2^z |i=1\rangle \equiv \hat{\sigma}_2^z |\uparrow,\uparrow,\uparrow\rangle = +|\uparrow,\uparrow,\uparrow\rangle = |i=1\rangle \quad \Rightarrow \langle i=1|\hat{\sigma}_2^z|i=1\rangle = +1$
- $\hat{\sigma}_3^z |i=6\rangle \equiv \hat{\sigma}_3^z |\downarrow,\uparrow,\downarrow\rangle = -|\downarrow,\uparrow,\downarrow\rangle = -|i=6\rangle \quad \Rightarrow \langle i=6|\hat{\sigma}_3^z|i=6\rangle = -1$

$\hat{\sigma}_3^z = \mathbb{1} \otimes \hat{\mathbb{1}} \otimes \hat{\sigma}^z$

elementi diagonali

$\rightarrow$ accoppiamento:

- $\hat{\sigma}_1^z \hat{\sigma}_2^z |i=6\rangle \equiv \hat{\sigma}_1^z \hat{\sigma}_2^z |\downarrow,\uparrow,\downarrow\rangle = -|\downarrow,\uparrow,\downarrow\rangle = -|i=6\rangle \quad \Rightarrow \langle i=6|\downarrow,\uparrow,\downarrow|i=6\rangle = -1$

elemento diagonale

$\rightarrow$ campo trasverso:

- $\hat{\sigma}_1^x |i=1\rangle \equiv \hat{\sigma}_1^x |\uparrow,\uparrow,\uparrow\rangle = |\downarrow,\uparrow,\uparrow\rangle = |i=5\rangle \quad \Rightarrow \langle i=5|\hat{\sigma}_1^x|i=1\rangle = +1$

elemento NON diagonale

27/10/2020

- I fase: Costruzione della matrice corrispondente ad $\hat{H}$ $(2^N \times 2^N)$

- II fase: diagonalizzazione di $\hat{H}$

diag. esatta || diag esatta solamente trovando lo stato fondamentale

"forza bruta"
$\Rightarrow$ trovo tutti autovalori e gli autovettori
$N \sim O(12)$

(eventualmente pochi altri autovalori e autovettori "vicini" a quello fondamentale)
più veloce (meno risorse) ⊛
$N \sim O(24)$

⊛ Lanczos (~1950) ricerca di tipo variazionale del ground state

① • prendiamo uno stato "di partenza" $|\psi_0\rangle$ (es. stato random $|\psi_0\rangle = \sum_n c_n |n\rangle$ dove c_n sono scelti in modo casuale)
$|\psi_0\rangle \in \mathcal{H}$
dove $\mathcal{H} = \mathbb{C}^{2N}$ (N spin)

② • costruisco un secondo stato a partire da $|\psi_0\rangle$
es. $\hat{K}|\psi_0\rangle = |\tilde{\psi}_1\rangle$ $\hat{K}$ è un "generico" operatore

③ • ortonormalizzo $|\tilde{\psi}_1\rangle$ rispetto a $|\psi_0\rangle$

$$|\psi_1\rangle = \frac{\hat{K} - \langle\hat{K}\rangle_0}{\sqrt{\langle K^+ K\rangle_0 - |\langle K\rangle_0|^2}} |\psi_0\rangle$$

$(\langle\hat{A}\rangle_0 = \langle\psi_0|\hat{A}|\psi_0\rangle)$

$\downarrow$
Gram-Schmidt

per costruzione $\langle\psi_1|\psi_0\rangle = 0$
$|\langle\psi_1|\psi_1\rangle|^2 = 1$

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

diagonalizzo l'Hamiltoniana $\hat{H}$ su $\mathcal{H}_1$ e trovo il ground state lì

$$\hat{H}_r = \begin{pmatrix} \langle\psi_0|\hat{H}|\psi_0\rangle & \langle\psi_1|\hat{H}|\psi_0\rangle \\ \langle\psi_0|\hat{H}|\psi_1\rangle & \langle\psi_1|\hat{H}|\psi_1\rangle \end{pmatrix}$$ Matrice 2×2

↳ trovo lo stato fondamentale $|\psi_0^{(1)}\rangle = \alpha|\psi_0\rangle + \beta|\psi_1\rangle$

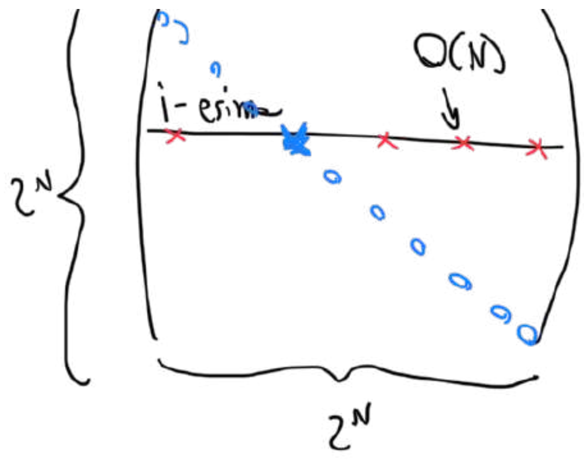
⑤ • itero la procedura da ② sostituendo $|\psi_0\rangle$ con $|\psi_0^{(1)}\rangle$

$\langle\psi_0|\hat{H}|\psi_0\rangle \simeq E_0$
$\langle\psi_0^{(1)}|\hat{H}|\psi_0^{(1)}\rangle \leq E_0$

a me non serve costruire tutta $\hat{H}$ $(2^N \times 2^N)$

ma mi basta saper fare $\hat{H}|\psi\rangle = |\phi\rangle$

se $\hat{H}$ è sparsa (piena di zeri)
$\Rightarrow$ è molto più rapido di immagazzinare tutta la matrice H $(2^N \times 2^N)$



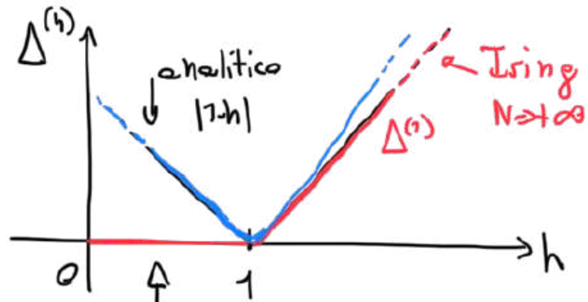
$\rightarrow |0100011101\rangle \Rightarrow |\uparrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\downarrow\rangle$

$\sigma_1^x |\uparrow\downarrow\uparrow\uparrow\uparrow\ldots\rangle = |\downarrow\downarrow\uparrow\uparrow\uparrow\ldots\rangle$ elemento fuori diagonale (uno per ogni spin)

III fase: misure di osservabili / quantità fisicamente interessanti

- energie – primi livelli energetici

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



$\Delta^{(1)} \equiv E_1 - E_0$
gap tra energia del ground state (E_0) e 1° stato eccitato (E_1)

$\Delta^{(2)} \equiv E_2 - E_0$

$h<1 \Rightarrow \Delta^{(1)} \xrightarrow{N\to\infty} 0$

degenerazione dello stato fondamentale per $|h|<1$

NON si vede analiticamente

se fisso le condizioni al contorno per i fermioni

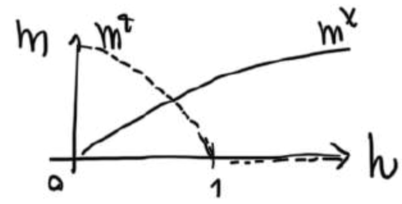
- $m^z = \langle\psi_0|\hat{\sigma}_1^z|\psi_0\rangle$ e $m^x = \langle\psi_0|\hat{\sigma}_1^x|\psi_0\rangle$

"va bene"

$\underline{\underline{m^z = 0}}$
numericamente

è dovuto alla simmetria della "fase ferromagnetica"

va rotta!



$$\hat{H} = -\sum_j \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z - h\sum_j \hat{\sigma}_j^x \left[\underbrace{-\lambda\sum_i \hat{\sigma}_i^z}_{\text{non commuta con } \hat{Z}}\right] \qquad \hat{Z} = \prod_{j=1}^{N} \hat{\sigma}_j^x \quad (\text{simmetria } \mathbb{Z}_2)$$

$\underline{[\hat{H}, \hat{Z}] = 0}$

autovalori $\underline{+1}$ o $\underline{-1}$

$|\psi_1\rangle$ e $|\psi_2\rangle$ sono autostati di $\hat{H}$ che generano il sottospazio del ground state (degenerazione 2, nel limite termodinamico $N\to+\infty$)

$|\psi_1\rangle = \sum_n c_n |n\rangle$

$|\psi_2\rangle = \sum_n c_n |\bar{n}\rangle$

dove $|\bar{n}\rangle$ si ottiene da $|n\rangle$ invertendo tutti gli spin

$|n\rangle = |\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\rangle \Rightarrow |\bar{n}\rangle = |\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\rangle$

$\langle\psi_1|\hat{H}|\psi_1\rangle \approx \langle\psi_2|\hat{H}|\psi_2\rangle$

(= vale se $h=0$, oppure nel limite $N \to +\infty$)

- immaginiamo di calcolare $\langle\psi|\hat{M}^z|\psi\rangle$ dove $\hat{M}^z = \sum_{j=1}^{N}\hat{\sigma}_j^z$

$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle$

$$\langle\psi|\hat{M}^z|\psi\rangle = \left(\langle\psi_1|\alpha^* + \langle\psi_2|\beta^*\right)\left(\sum_j \hat{\sigma}_j^z\right)\left(\alpha|\psi_1\rangle + \beta|\psi_2\rangle\right)$$

$$= \sum_n |\alpha|^2|c_n|^2\langle n|\sum_j\hat{\sigma}_j^z|n\rangle + |\beta|^2|c_n|^2\langle\bar{n}|\sum_j\hat{\sigma}_j^z|\bar{n}\rangle +$$

$$+ \cancel{\sum_n \alpha^*\beta|c_n|^2\langle n|\sum\hat{\sigma}_j^z|\bar{n}\rangle + h.c.}$$

perché $\langle n|\bar{n}\rangle = 0$ e $\hat{\sigma}_j^z$ è diagonale

$$\langle n|\sum_j\hat{\sigma}_j^z|n\rangle = -\langle\bar{n}|\sum_j\hat{\sigma}_j^z|\bar{n}\rangle$$

i due valori di aspettazione sono opposti

$$\Rightarrow \langle\psi|\hat{M}^z|\psi\rangle = \sum_n |c_n|^2\langle n|\sum_j\hat{\sigma}_j^z|n\rangle\left(|\alpha|^2 - |\beta|^2\right)$$

se $\alpha = \pm\beta \Rightarrow \langle\psi|\hat{M}^z|\psi\rangle = 0$

$\underline{\alpha=\beta} \Rightarrow |\psi_S\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_2\rangle\right) = \frac{1}{\sqrt{2}}\sum_n |c_n|^2\left(|n\rangle + |\bar{n}\rangle\right)$

$$\underline{\hat{Z}|\psi_S\rangle} = \frac{1}{\sqrt{2}}\sum_n |c_n|^2\left(|\bar{n}\rangle + |n\rangle\right) = \underline{|\psi_S\rangle}$$

simmetrico

$\hat{Z}|n\rangle = |\bar{n}\rangle$

$\hat{Z}|\bar{n}\rangle = |n\rangle$

$\underline{\alpha = -\beta} \Rightarrow |\tilde{\psi}_A\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle - |\psi_2\rangle\right)$ $\qquad \underline{\hat{Z}|\tilde{\psi}_A\rangle = -|\tilde{\psi}_A\rangle}$

antisimmetrico

- numericamente $\langle\psi|\hat{M}^z|\psi\rangle = 0$ dove $|\psi\rangle$ è lo stato fondamentale

$|\psi\rangle = \sum_n d_n|n\rangle$

↳ si può fare: $\tilde{M}_z = \sum_n |d_n|^2 \cdot \left|\langle n|\sum_j\hat{\sigma}_j^z|n\rangle\right|$

prendere il modulo!

$$\langle\psi_S|\tilde{M}^z|\psi_S\rangle = \sum_n |c_n|^2|\alpha|^2\left|\langle n|\sum_j\hat{\sigma}_j^z|n\rangle\right| + |c_n|^2|\beta|^2\left|\langle\bar{n}|\sum_j\hat{\sigma}_j^z|\bar{n}\rangle\right| =$$

se prendo i moduli, sono uguali

$$= \sum_n |c_n|^2\left|\langle n|\sum_j\hat{\sigma}_j^z|n\rangle\right|\underbrace{\left(|\alpha|^2+|\beta|^2\right)}_{1} = \sum_n |c_n|^2\cdot\left|\langle n|\sum_j\hat{\sigma}_j^z|n\rangle\right|$$

caso facile: $\underline{h=0} \Rightarrow \hat{H} = \sum_j \hat{\sigma}_j^z\hat{\sigma}_{j+1}^z$ $\qquad |\psi_1\rangle = |\uparrow\uparrow\ldots\uparrow\rangle$ $\qquad \hat{Z} = \prod_{j=1}^{N}\hat{\sigma}_j^x$

$|\psi_2\rangle = |\downarrow\downarrow\ldots\downarrow\rangle$

$$|\psi_A\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\ldots\uparrow\rangle - |\downarrow\ldots\downarrow\rangle\right) \qquad |\psi_S\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\ldots\uparrow\rangle + |\downarrow\ldots\downarrow\rangle\right)$$

simultaneamente autostati di $\hat{H}$ e $\hat{\mathcal{Z}}$

sono i due stati in competizione, per la fisica a basse energie

$$\langle\psi_A|\hat{M}^z|\psi_A\rangle = \langle\psi_S|\hat{M}^z|\psi_S\rangle = 0 \qquad \text{ma} \quad \langle\psi_+|\hat{M}^z|\psi_+\rangle = 1\,;\ \langle\psi_-|\hat{M}^z|\psi_-\rangle = -1$$

$$\rightarrow \quad \tilde{M}^z = \sum_n |c_n| \cdot \left|\langle n|\sum_j \hat{\sigma}_j^z|n\rangle\right| = \pm 1$$

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- numericamente (2):
  invece di calcolare $M^z = \langle\psi|\sum_j \hat{\sigma}_j^z|\psi\rangle$ (=0 per ragioni di simmetria)

$C^{zz}(r) = \langle\psi|\hat{\sigma}_j^z\hat{\sigma}_{j+r}^z|\psi\rangle$ funzione di correlazione della magnetizzazione longitudinale

$$\langle\psi|\hat{\sigma}_j^z\hat{\sigma}_{j+r}^z|\psi\rangle \xrightarrow{r\to+\infty} \langle\psi|\hat{\sigma}_j^z|\psi\rangle\langle\psi|\hat{\sigma}_{j+r}^z|\psi\rangle \sim (M^z)^2$$

$$\frac{1}{N}M^z \sim \left[\lim_{r\to+\infty} C^{zz}(r)\right]^{1/2}$$

Poco utile se N simulabile è piccolo (con diag. esatta non va bene...)

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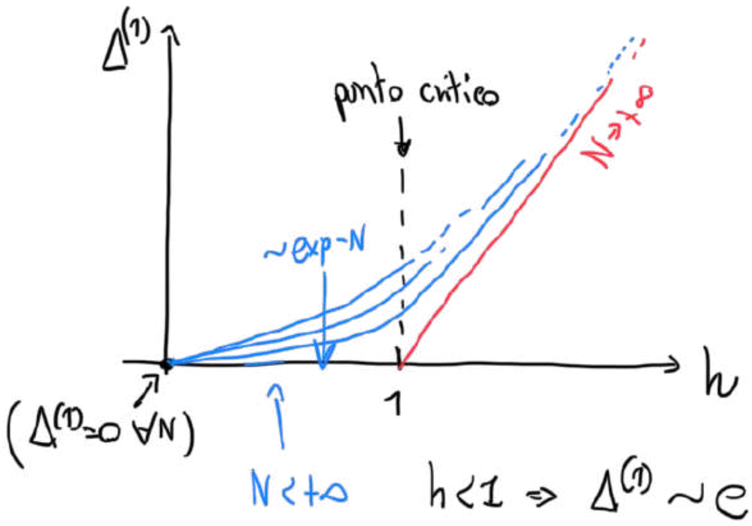
gap $\Delta^{(1)} = E_1 - E_0$



$h<1 \Rightarrow \Delta^{(1)} \sim e^{-N/\alpha(h)}$

$\alpha(h)$: $\alpha(0)=0$

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

- a Temperatura $T=0$
  (stato fondamentale)

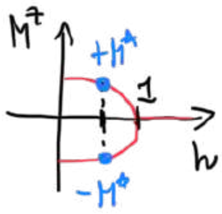
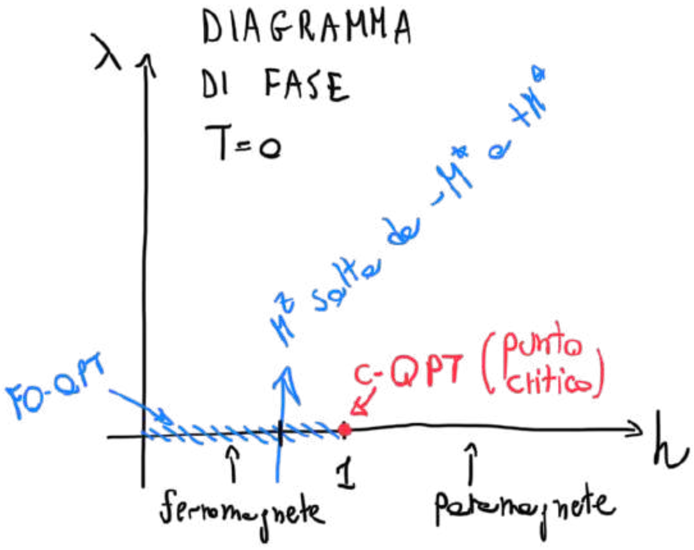


DIAGRAMMA DI FASE $T=0$



il punto critico ($h=1, \lambda=0$) è associato a esponenti critici UGUALI al modello

$$\lim_{h\to 0}\lim_{N\to+\infty}\langle\psi|\hat{\sigma}_j^z|\psi\rangle = M^z$$

c-QPT: quantum phase

corrispondente classico
in dimensione $1+1=2$

quantum phase transition (continuous)

FO-QPT: quantum phase transition (1^{o} order)

(quantistici (d)-dimensionali
$\Updownarrow$
classici $(d+1)$-dimensionali)

- finite-size scaling (come classico $T \to h$)

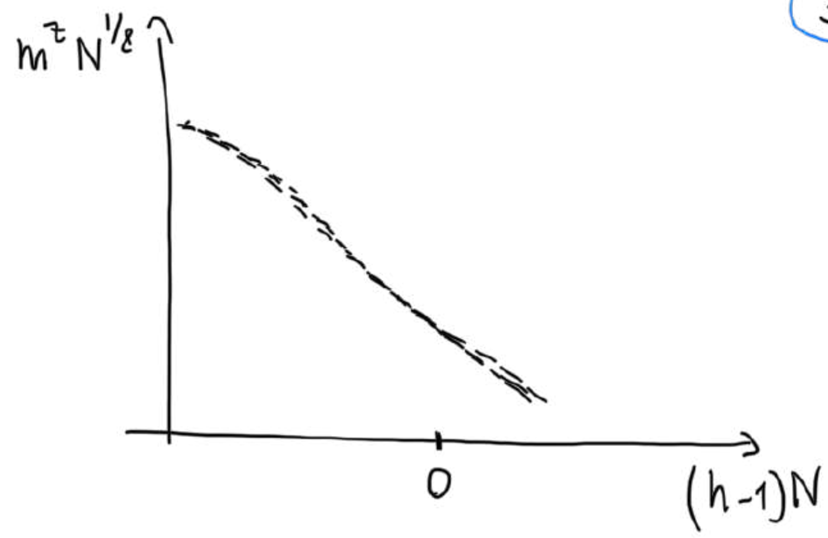
$$m^z(h,N) = N^{-\beta/\nu} \cdot \mathcal{M}\left[(h-1)N^{1/\nu}\right] \qquad (\lambda=0)$$

$$\beta = 1/8 \; ; \; \nu = 1 \quad \Rightarrow \quad m^z(h,N) = N^{-1/8}\mathcal{M}\left[(h-1)N\right]$$

$$\chi^z(h,N) = \frac{\partial m}{\partial h} \qquad \chi^z(h,N) = N^{\gamma/\nu}\,\tilde{\chi}\left[(h-1)N^{1/\nu}\right]$$

$$\gamma = 7/4$$

3/11/2020

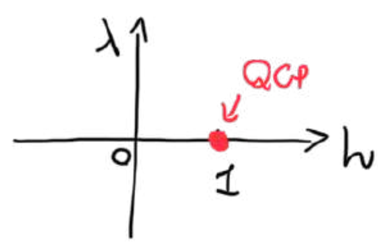


$$\hat{H} = -\sum_j \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z \underbrace{-h\sum_j \hat{\sigma}_j^x}_{\text{"temperature classica"}} -\lambda \sum_j \hat{\sigma}_j^z$$

$$\chi^z = \left.\frac{\partial m^z}{\partial \lambda}\right|_{\lambda=0} \qquad \chi^z \cdot N^{\gamma/\nu} = \tilde{\chi}\left(\lambda N^{y_\lambda}\right) \qquad y_\lambda = 15/8$$

$$\begin{cases} \tilde{h} = (h-h_c)N^{y_h} & \text{con } y_h = 1 \\ \tilde{\lambda} = (\lambda-\lambda_c)N^{y_\lambda} & \text{con } y_\lambda = \frac{15}{8} \end{cases}$$

$(h_c = 1)$ e $(\lambda_c = 0)$



$$\chi^z \sim N^{-\gamma/\nu}\,\tilde{\chi}(\tilde{h})$$
$$\chi^z \sim N^{-\gamma/\nu}\,\tilde{\chi}(\tilde{\lambda})$$

$$\chi^z = \left.\frac{\partial m^z}{\partial \lambda}\right|_{\lambda\to 0} = \frac{m^z(\lambda_2) - m^z(\lambda_1)}{\lambda_2 - \lambda_1} \qquad \lambda_1, \lambda_2 \sim O(10^{-2}/10^{-3})$$

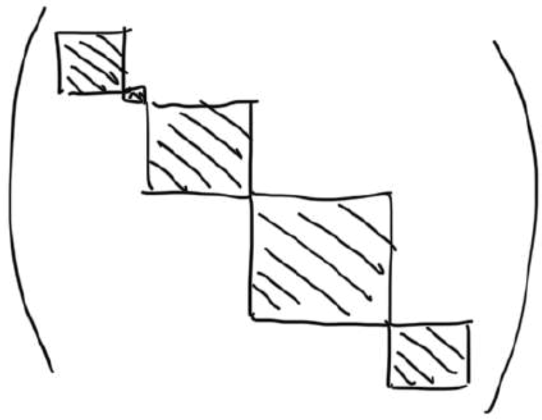
SIMMETRIE:

$$\hat H = -\sum_j \Big(\overbrace{\hat\sigma^x_j \hat\sigma^x_{j+1} + \hat\sigma^y_j \hat\sigma^y_{j+1}}^{(\hat\sigma^+_j \hat\sigma^-_{j+1} + \hat\sigma^-_j \hat\sigma^+_{j+1})} + \Delta \hat\sigma^z_j \hat\sigma^z_{j+1}\Big) + h\sum_j \hat\sigma^z_j$$

XXZ - in campo magnetico

$$\hat M^z = \sum_j \hat\sigma^z_j \Rightarrow [\hat M^z, \hat H] = 0$$

se $[\hat H, \hat M^z] = 0 \Rightarrow \hat H$ è diagonale a blocchi sulla base computazionale



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

$\dim(\text{blocco più grande}) = \binom{N}{N/2} \Leftrightarrow \left(\frac{N}{2} \text{ spin} \uparrow\right)$ e $\left(\frac{N}{2} \text{ spin} \downarrow\right)$

es. $N = 10 \Rightarrow 2^{10} = 1024$; $\binom{10}{5} = 252$

$N = 16 \Rightarrow 2^{16} = 65536$; $\binom{16}{8} = 12870$

Implementazione della DINAMICA dopo un quench

$$|\psi(t)\rangle = e^{-i\hat H t} |\psi(0)\rangle$$ dove $|\psi(0)\rangle$ NON è autostato di $\hat H$

eq. di Schrödinger è lineare

① decomposizione di Suzuki-Trotter

$\hat U = e^{-i\hat H t}$ operatore di evoluzione temporale

(metodo zero è calcolare esplicitamente $\hat U$, diagonalizzando $\hat H$)

↳ oppure: $\hat U = \sum_{n=0}^{+\infty} \frac{(-i\hat H t)^n}{n!}$

↳ $\hat H = \hat H_a + \hat H_b$ dove $[\hat H_a, \hat H_b] \neq 0$

(BCH)

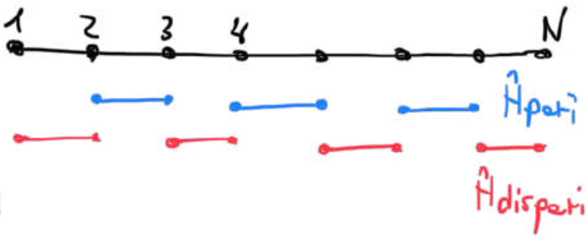
$\Rightarrow$ posso utilizzare lo sviluppo di Baker-Campbell-Hausdorff

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{Z}} \quad \text{con} \quad \hat{Z} = \hat{A} + \hat{B} + \frac{1}{2}[\hat{A},\hat{B}] + \frac{1}{12}\left\{[\hat{A},[\hat{A},\hat{B}]] + [\hat{B},[\hat{B},\hat{A}]]\right\} + \dots$$

se $[\hat{A},\hat{B}] = 0 \Rightarrow e^{\hat{A}} e^{\hat{B}} = e^{\hat{A}+\hat{B}}$

nel nostro caso abbiamo: $\hat{H} = \sum_{i=1}^{N} \hat{h}_{i,i+1}$

$\hat{H} = \hat{H}_p + \hat{H}_d$



$\hat{H}_p = \sum_{i \in pari} \hat{h}_{i,i+1}$; $\hat{H}_d = \sum_{i \in dispari} \hat{h}_{i,i+1}$

$[\hat{H}_p, \hat{H}_d] \neq 0$ però tutti i "pezzi" in $\hat{H}_p$ (o in $\hat{H}_d$) commutano tra loro !

$\Downarrow$

$$e^{-i\hat{H}_p t} = \prod_{i \in pari} e^{-i\hat{h}_{i,i+1} t}$$

agisce solo su 2 siti $\Rightarrow$ facile da implementare numericamente

(e analogo per $\hat{H}_d$)

$$\hat{U}(t) = e^{-i\hat{H}t} = \left(e^{-i\hat{H}\,dt}\right)^{t/dt} \quad \text{con } dt \ll 1 \quad (\text{piccolo})$$

$e^{-i\hat{H}\,dt}$ si può trattare con la formula BCH

BCH: $$e^{\tau(\hat{A}+\hat{B})} = \prod_{i=1}^{k} e^{c_i \tau \hat{A}} e^{d_i \tau \hat{B}} + \mathcal{O}(\tau^n)$$

$k = k(n)$ con n: ordine dello sviluppo ; $\{c_i\}, \{d_i\} \in \mathbb{R}$

$(n=1)$ $k=1$; $c_1 = d_1 = 1$ $\rightarrow e^{\tau(\hat{A}+\hat{B})} = e^{\tau\hat{A}} e^{\tau\hat{B}} + \mathcal{O}(\tau)$

$(n=2)$ $k=2$; $c_1 = c_2 = 1/2$; $d_1 = 1$, $d_2 = 0$

$\rightarrow e^{\tau(\hat{A}+\hat{B})} = e^{\frac{1}{2}\tau\hat{A}} e^{\tau\hat{B}} e^{\frac{1}{2}\tau\hat{A}} + \mathcal{O}(\tau^2)$

$(n=4)$ $k=4$; $c_1 = c_4 = \left(2(2-2^{1/3})\right)^{-1}$; $c_2 = c_3 = (1-2^{1/3})c_1$

$d_1 = d_3 = 2c_1$; $d_2 = -2^{4/3} c_1$; $d_4 = 0$

• es. $(n=2)$ $$\hat{U} = e^{-i\hat{H}t} = \left(e^{-i\hat{H}\,dt}\right)^{t/dt} \simeq \left[e^{-\frac{1}{2} i\,dt\,\hat{H}_p} e^{-i\,dt\,\hat{H}_d} e^{-\frac{1}{2} i\,dt\,\hat{H}_p}\right]^{t/dt}$$

$$\simeq \left[\left(\prod e^{-\frac{1}{2} i\,dt\,\hat{h}_{j,j+1}}\right)\left(\prod e^{-i\,dt\,\hat{h}_{j,j+1}}\right)\left(\prod e^{-\frac{1}{2} i\,dt\,\hat{h}_{j,j+1}}\right)\right]^{t/dt}$$

L'$j \in$ pari $\quad$ ' $j \in$ dispari $\quad$ ' $j \in$ pari $\quad$]

$\rightarrow$ Suzuki-Trotter al II ordine

② metodo di Runge-Kutta (integrazione numerica di equazioni differenziali)

eq. di Schrödinger:

$$i \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle \qquad |\psi(t)\rangle \text{ da } |\psi(0)\rangle$$

$$\begin{cases} f(t, |\psi\rangle) = -i\hat{H}(t)|\psi(t)\rangle \\ y_n = |\psi(t_n)\rangle \end{cases}$$

$$\begin{cases} y'(t) = f(t, y(t)) \\ y(t_0) = y_0 \end{cases} \qquad t \in [t_0, t_f]$$

campionare l'intervallo $t_j = t_0 + jh$ $\quad (h = (t_f - t_0)/n)$

Runge-Kutta IV ordine:

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$t_{n+1} = t_n + h$$

e

$$\begin{cases} k_1 = f(t_n, y_n) \\ k_2 = f(t_n + h/2, y_n + k_1 h/2) \\ k_3 = f(t_n + h/2, y_n + k_2 h/2) \\ k_4 = f(t_n + h, y_n + k_3 h) \end{cases}$$

per implementare RK mi serve saper fare $|\phi\rangle \rightarrow \hat{H}|\phi\rangle$ (stesso passo richiesto da Lanczos)

STATI TERMICI

5/11/2020

Evoluzione temporale in tempo immaginario (medie termiche)

ρ matrice densità

$$\begin{cases} \rho = \frac{1}{Z} e^{-\beta\hat{H}} \\ A = Tr[\hat{A}\rho] \end{cases}$$

"Purificazione"

allargare lo spazio di Hilbert $\mathcal{H}$ del sistema S introducendo uno spazio ausiliario (ancillare) A

($\dim A = \dim S$)

$$\rho_\beta = \frac{1}{Z} e^{-\beta\hat{H}} \qquad Z = Tr[e^{-\beta\hat{H}}]$$

$$= \frac{1}{Z} e^{-\frac{\beta}{2}\hat{H}} \mathbb{1} e^{-\frac{\beta}{2}\hat{H}} \qquad (\mathbb{1} = Z(\beta=0) \cdot \rho_0)$$

temperatura infinita

$$(\rho_0 = Tr_A |\psi_0\rangle\langle\psi_0| \qquad |\psi_0\rangle \in \mathcal{H}_S \otimes \mathcal{H}_A$$

$$\Rightarrow \rho_\beta = \frac{1}{Z(\beta)} e^{-\frac{\beta}{2}\hat{H}} \{Z(\beta=0) \cdot \rho_0\} e^{-\frac{\beta}{2}\hat{H}} = \frac{Z(0)}{Z(\beta)} \left\{ e^{-\frac{\beta}{2}\hat{H}} Tr_A\left[|\psi_0\rangle\langle\psi_0|\right] e^{-\frac{\beta}{2}\hat{H}} \right\}$$

definisco $|\psi(\beta)\rangle = e^{-\beta\hat{H}/2}|\psi_0\rangle$ $\quad$ evoluzione in tempo immaginario $(t \to -i\beta)$

$$\rho_\beta = \frac{Z(0)}{Z(\beta)} \, \mathrm{Tr}_A \left[|\psi(\beta)\rangle\langle\psi(\beta)| \right]$$

$\hat{H}$ sta in $\mathcal{H}_S$ quindi posso portare $e^{-\frac{\beta}{2}\hat{H}}$ dentro $\mathrm{Tr}_A[\dots]$

$$\langle O \rangle_\beta = \mathrm{Tr}_S[\rho_\beta \hat{O}] =$$

$$= \frac{Z(0)}{Z(\beta)} \mathrm{Tr}_S \left[\mathrm{Tr}_A \left[|\psi(\beta)\rangle\langle\psi(\beta)| \right] \hat{O} \right] = \frac{Z(0)}{Z(\beta)} \langle\psi(\beta)| \hat{O}_S \otimes \hat{\mathbb{1}}_A |\psi(\beta)\rangle$$

$$1 = \langle \mathbb{1} \rangle_\beta = \mathrm{Tr}_S[\rho_\beta] = \frac{Z(0)}{Z(\beta)} \mathrm{Tr}_S \left[\mathrm{Tr}_A \left[|\psi(\beta)\rangle\langle\psi(\beta)| \right] \right] = \frac{Z(0)}{Z(\beta)} \langle\psi(\beta)|\psi(\beta)\rangle$$

$$\hookrightarrow \frac{Z(0)}{Z(\beta)} = \frac{1}{\langle\psi(\beta)|\psi(\beta)\rangle}$$

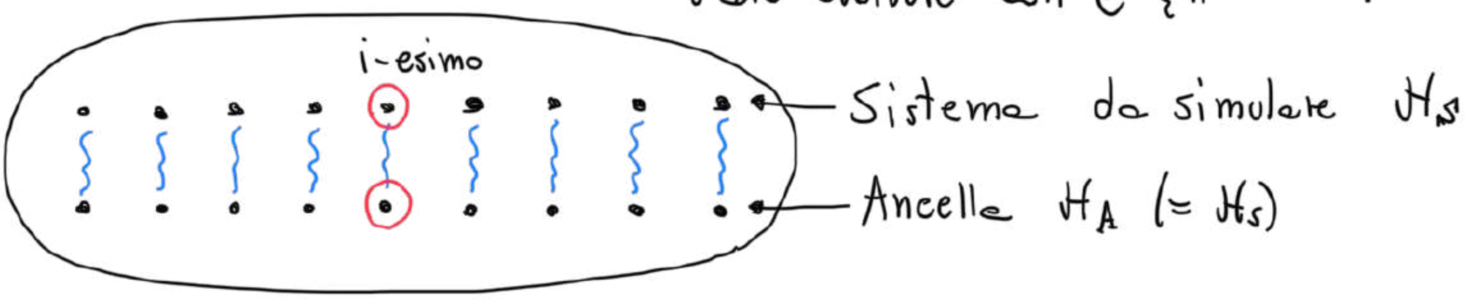
$$\rightarrow \langle O \rangle_\beta = \frac{\langle\psi(\beta)| \hat{O}_S \otimes \hat{\mathbb{1}}_A |\psi(\beta)\rangle}{\langle\psi(\beta)|\psi(\beta)\rangle}$$

media termica a temperatura $T = \frac{1}{k_B \beta}$

stato a temperatura infinita $\rho_0 = \frac{1}{d} \hat{\mathbb{1}}$ (d: dimensione di $\mathcal{H}_S$)

$$\rho_0 = \mathrm{Tr}_A |\psi_0\rangle\langle\psi_0|$$

Come faccio a trovare $|\psi_0\rangle$ lo stato di partenza dal quale fare evolvere con $e^{-\frac{\beta}{2}\hat{H}}$?



$|\psi_0\rangle$

•〰• ≡ stato massimamente entangled (coppia di Bell per spin-1/2)

$$|\psi_0\rangle = |\phi_0\rangle_1 \otimes |\phi_0\rangle_2 \otimes \dots \otimes |\phi_0\rangle_N$$

1° sito 2° sito N° sito

$|\phi_0\rangle \equiv$ S•〰•A $\mathrm{Tr}_A |\phi_0\rangle\langle\phi_0| = \mathbb{1}_S$ se S ed A sono massimamente entangled (per definizione)

[es: per spin-1/2 $\quad |\phi_0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_S \otimes |\uparrow\rangle_A + |\downarrow\rangle_S \otimes |\downarrow\rangle_A \right)$

$$\mathrm{Tr}_A[|\phi_0\rangle\langle\phi_0|] = {}_A\langle\uparrow| \{ |\phi_0\rangle\langle\phi_0| \} |\uparrow\rangle_A + {}_A\langle\downarrow| \{ |\phi_0\rangle\langle\phi_0| \} |\downarrow\rangle_A =$$

$$= \frac{1}{2} \{ |\uparrow\rangle_S\langle\uparrow| + |\downarrow\rangle_S\langle\downarrow| \} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$]

Coppie di Bell: (2 spin 1/2)

$$\left.\begin{aligned} |\psi^\pm\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle \pm |\downarrow,\uparrow\rangle\right) \\ |\phi^\pm\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow,\uparrow\rangle \pm |\downarrow,\downarrow\rangle\right) \end{aligned}\right\}$$ stati massimamente entangled

per ogni stato $|\psi^\pm\rangle$ oppure $|\phi^\pm\rangle$ (4 stati)

$$\Rightarrow \quad \mathrm{Tr}_2 |\psi\rangle\langle\psi| = \mathbb{1}_1 \cdot \left(\frac{1}{2}\right)$$

$$|\phi^+\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow,\uparrow\rangle + |\downarrow,\downarrow\rangle\right)$$

$$\downarrow$$

$$\rho = |\phi^+\rangle\langle\phi^+| = \frac{1}{2}\left(|\uparrow,\uparrow\rangle + |\downarrow,\downarrow\rangle\right)\left(\langle\uparrow,\uparrow| + \langle\downarrow,\downarrow|\right)$$

$|\uparrow\rangle \equiv |0\rangle$
$|\downarrow\rangle \equiv |1\rangle$

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

stato di Bell massimamente entangled

è diverso da $\tilde{\rho} = \frac{1}{2}\left(|\uparrow,\uparrow\rangle\langle\uparrow,\uparrow| + |\downarrow,\downarrow\rangle\langle\downarrow,\downarrow|\right)$

$$\tilde{\rho} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

stato non è entangled

- checks numerici:

- Ising 1D in campo trasverso $\quad \hat{H} = -\sum_{j=1}^{N-1} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z - \sum_{j=1}^{N} \hat{\sigma}_j^x \quad (h=1)$

$\rightarrow E_{g.s.}(L, h=1) = 1 - \dfrac{1}{\sin\left(\frac{\pi}{2(2L+1)}\right)}$ $\quad$ condizioni al contorno aperte

$$\rightarrow m^x = \frac{1}{\pi}\int_0^\pi \frac{dq}{w(q,h^{-1})} + \frac{1}{h}\cdot\frac{1}{\pi}\int_0^\pi \frac{\cos q \, dq}{w(q,h^{-1})}$$

limite termodinamico $(L \to +\infty)$

$$w(q,h) = \sqrt{1 + h^2 + 2h\cos q}$$

$\left(\text{se } h=1 \quad m^x = \frac{2}{\pi}\right)$

$\rightarrow \langle \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z \rangle = \dfrac{16}{3\pi^2}$ $\quad$ se $h=1$, $L \to +\infty$