Formalizm Matrix-Product States dla kwantowego modelu Isinga

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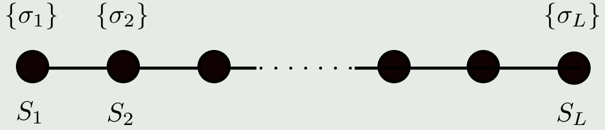
Zdefiniowanie problemu

Układ fizyczny

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{(\sigma_1\ldots\sigma_L)} |\sigma_1 \ldots \sigma_L\rangle$$



Hamiltonian układu

$$\hat{H} = -\sum_{n=1}^{L-1} \hat{S}_n^x \hat{S}_{n+1}^x - \gamma \sum_{n=1}^{L} \hat{S}_n^z$$

gdzie:
$\hat{S}_n^x$,$\hat{S}_n^z$ - operatory spinowe
$\gamma = \frac{h}{J}$

Formalizm Matrix-Product States(MPS)

MPS dla otwartych warunków brzegowych(OBC)

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L}^{d_1,\ldots,d_L} \sum_{a_1,\ldots,a_{L-1}}^{D_1,\ldots,D_{L-1}} M^{\sigma_1}_{1,a_1} M^{\sigma_2}_{a_1,a_2} \ldots M^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} M^{\sigma_L}_{a_{L-1},1} |\sigma_1 \ldots \sigma_L\rangle$$

MPS dla periodycznych warunków brzegowych(PBC)

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L}^{d_1,\ldots,d_L} \sum_{a_1,\ldots,a_L}^{D_1,\ldots,D_L} M^{\sigma_1}_{a_1,a_2} M^{\sigma_2}_{a_2,a_3} \ldots M^{\sigma_{L-1}}_{a_{L-1},a_L} M^{\sigma_L}_{a_L,a_1} |\sigma_1 \ldots \sigma_L\rangle$$

Zapis dowolnego stanu w postaci MPS

Wejście

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{(\sigma_1\ldots\sigma_L)} |\sigma_1 \ldots \sigma_L\rangle$$

Krok 1

$$c_{(\sigma_1\ldots\sigma_L)} = \Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} = \sum_{a_1}^{D_1} U_{\sigma_1,a_1} S_{a_1,a_1} {V^\dagger}_{a_1,(\sigma_2\ldots\sigma_L)}$$

$U_{\sigma_1,a_1} = A^{\sigma_1}_{1,a_1}$
$c_{a_1,(\sigma_2\ldots\sigma_L)} = S_{a_1,a_1} {V^\dagger}_{a_1,(\sigma_2\ldots\sigma_L)}$

Zapis dowolnego stanu w postaci MPS

Krok 2

$$c_{a_1,(\sigma_2\ldots\sigma_L)} = \Psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)} = \sum_{a_2}^{D_2} U_{(a_1\sigma_2),a_2} S_{a_2,a_2} {V^\dagger}_{a_2,(\sigma_3\ldots\sigma_L)}$$

$U_{(a_1\sigma_2),a_2} = A^{\sigma_2}_{a_1,a_2}$
$c_{a_2,(\sigma_3\ldots\sigma_L)} = S_{a_2,a_2} {V^\dagger}_{a_2,(\sigma_3\ldots\sigma_L)}$

Wyjście

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L}^{d_1,\ldots,d_L} \sum_{a_1,\ldots,a_{L-1}}^{D_1,\ldots,D_{L-1}} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1,a_2} \ldots A^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1},1} |\sigma_1 \ldots \sigma_L\rangle$$

Specjalna postać MPS

Lewostronnie unormowany MPS

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L}^{d_1,\ldots,d_L} \sum_{a_1,\ldots,a_{L-1}}^{D_1,\ldots,D_{L-1}} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1,a_2} \ldots A^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1},1} |\sigma_1 \ldots \sigma_L\rangle$$

$$\begin{aligned} \sum_{\sigma_n} \left(A^{\sigma_n \dagger} A^{\sigma_n} \right)_{a_n,a'_n} &= \sum_{a_{n-1},\sigma_n} A^{\sigma_n \dagger}_{a_n,a_{n-1}} A^{\sigma_n}_{a_{n-1},a'_n} \\ &= \sum_{a_{n-1}\sigma_n} U^{\dagger}_{a_n,(a_{n-1}\sigma_n)} U_{(a_{n-1}\sigma_n),a'_n} = \delta_{a_n,a'_n} \end{aligned}$$

Działania na MPSach

Iloczyn wewnętrzny

$$\langle\phi|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} \tilde{M}^{\sigma_L\dagger} \ldots \tilde{M}^{\sigma_1\dagger} M^{\sigma_1} \ldots M^{\sigma_L}$$

Wartość oczekiwana

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{\substack{\sigma_1,\ldots,\sigma_L \\ \sigma_i'}} \tilde{M}^{\sigma_L\dagger} \ldots \tilde{M}^{\sigma_i\dagger} \ldots \tilde{M}^{\sigma_1\dagger} O^{\sigma_i,\sigma_i'} M^{\sigma_1} \ldots M^{\sigma_i'} \ldots M^{\sigma_L}$$

gdzie:

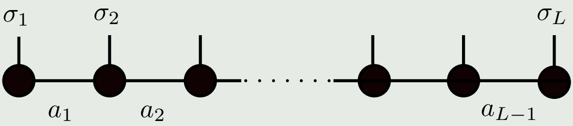
$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} M^{\sigma_1} \ldots M^{\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle$

$|\phi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} \tilde{M}^{\sigma_1} \ldots \tilde{M}^{\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle$

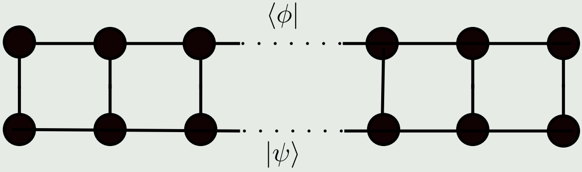
$\hat{O} = \sum_{\sigma_i,\sigma_i'} O^{\sigma_i,\sigma_i'} |\sigma_i\rangle\langle\sigma_i'|$

Graficzna reprezentacja

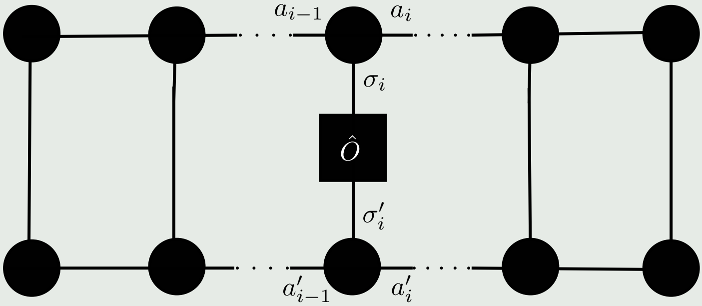
MPS



Iloczyn wewnętrzny



Wartość oczekiwana



Metoda wariacyjna w dziedzinie MPS (VMPS)

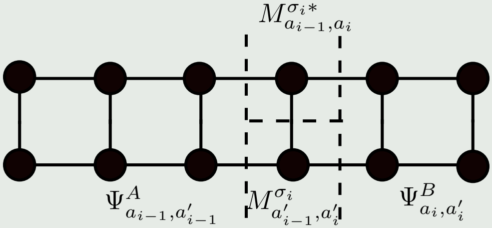
Podstawa metody

$$\langle\psi|\hat{H}|\psi\rangle = \sum_n \sum_m c_m^* c_n E_n \langle\psi_m|\psi_n\rangle = \sum_n E_n |c_n|^2 \geqslant E_0$$

Metoda mnożników Lagrange'a

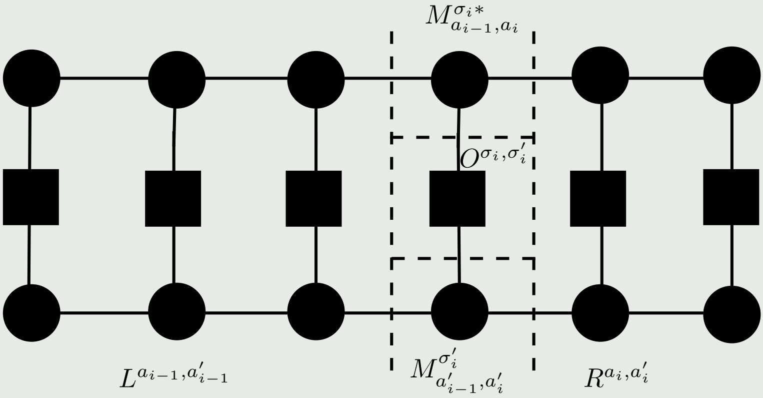
$$L = \langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle$$

Graficzna reprezentacja $\langle\psi|\psi\rangle$



VMPS

Graficzna reprezentacja $\langle\psi|\hat{H}|\psi\rangle$



Minimalizacja na *i*-tym węźle

$$
\begin{aligned}
0 &= \sum_{\sigma_i'} \sum_{a_{i-1}', a_i'} L^{a_{i-1}, a_{i-1}'} O^{\sigma_i, \sigma_i'} R^{a_i, a_i'} M^{\sigma_i'}_{a_{i-1}', a_i'} \\
&- \lambda \sum_{a_{i-1}', a_i'} \Psi^A_{a_{i-1}, a_{i-1}'} M^{\sigma_i}_{a_{i-1}', a_i'} \Psi^B_{a_i, a_i'}
\end{aligned}
$$

VMPS

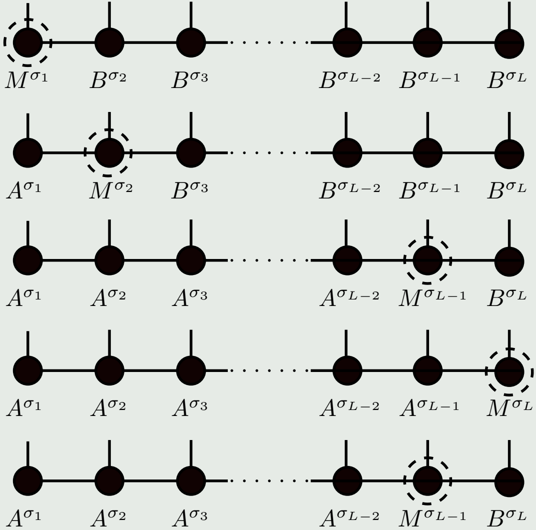
Minimalizacja na *i*-tym węźle

$$H^{ef}_{(\sigma_i a_{i-1} a_i)(\sigma'_i a'_{i-1} a'_i)} = \sum_{b_{i-1},b_i} L^{a_{i-1},a'_{i-1}} O^{\sigma_i,\sigma'_i}_{b_{i-1},b_i} R^{a_i,a'_i}$$
$$N_{(\sigma_i a_{i-1} a_i)(\sigma'_i a'_{i-1} a'_i)} = \Psi^A_{a_{i-1},a'_{i-1}} \Psi^B_{a_i,a'_i} \delta_{\sigma_i,\sigma'_i}$$
$$\nu_{(\sigma'_i a'_{i-1} a'_i)} = M^{\sigma'_i}_{a'_{i-1},a'_i}$$

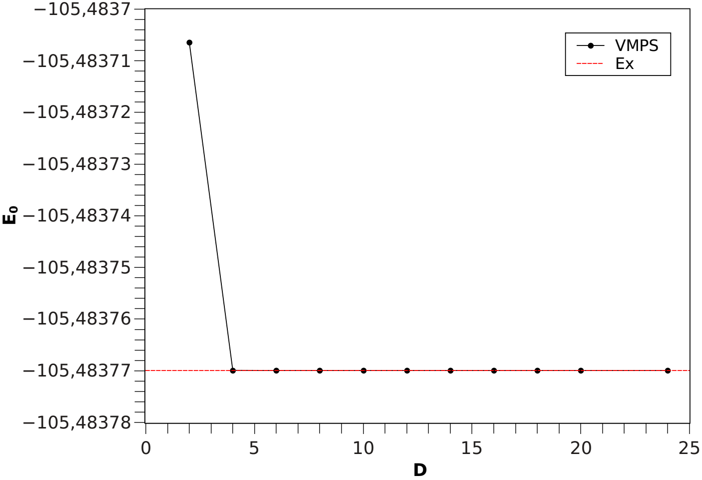
Końcowy wzór

$$H^{ef}\nu = \lambda N \nu$$

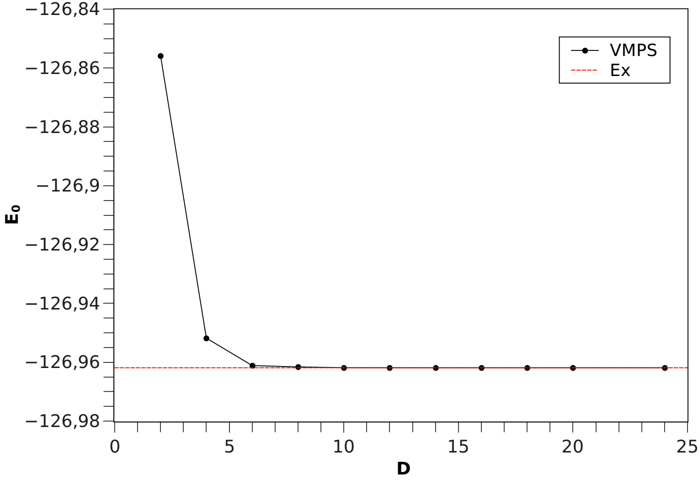
Algorytm VMPS



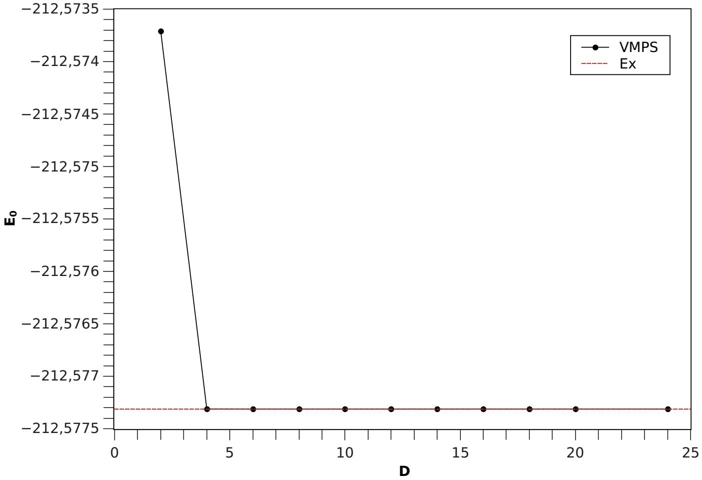
$E_0(D)$, dla $L = 100$, $\gamma = 0.5$



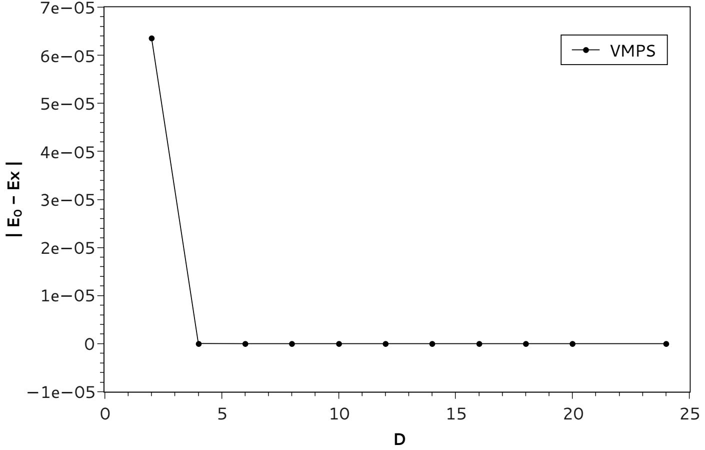
$E_0(D)$, dla $L = 100$, $\gamma = 1$



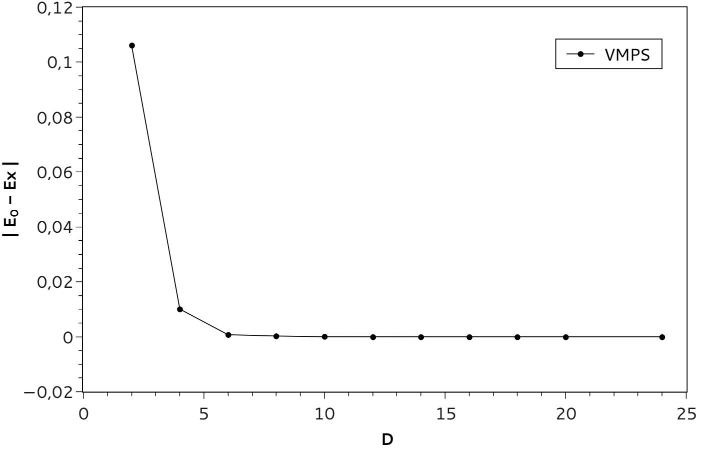
$E_0(D)$, dla $L = 100$, $\gamma = 2$



$|E_0 - Ex|(D)$, dla $L = 100$, $\gamma = 0.5$



$|E_0 - Ex|(D)$, dla $L = 100$, $\gamma = 1$



$|E_0 - Ex|(D)$, dla $L = 100$, $\gamma = 2$