Variational Ansätze for frustrated quantum magnetism: reconstructing correlations, entanglement and the sign structure

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Find the ground state of frustrated quantum magnetism systems

Wave function :

$$|\psi\rangle = \sum_{\vec{\sigma}} W_{\vec{\sigma}} \, |\vec{\sigma}\rangle$$

where $\vec{\sigma} = (\sigma_1, \cdots, \sigma_N)$, $|\sigma_i\rangle$ is the eigenvector of S_i^z

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Without frustration : $W_{\vec{\sigma}} \geqslant 0$ (up to a canonical transformation in H)

(*Feynman no-node theorem* [Feynman, Statistical Physics])

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$\Rightarrow$ Quantum Monte Carlo

scalable unbiaised numerical method

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$\Rightarrow$ **Sign problem** with Quantum Monte Carlo

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$\Rightarrow$ **biaised** Quantum Monte Carlo

Generally : No theoretical insight of the sign structure

Variational methods scalable but biaised

Wave function :

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* The least possible : $poly(N)$.

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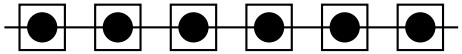
How to choose the variables $\{C_\alpha\}$?

* The least possible : *poly*(N).
* Enough to reproduce the quantum correlations.
* $W_\sigma(\{C_\alpha\})$ efficiently computable (time $\propto$ *poly*(N)).
* Freedom in the sign structure.

Variational Ansatz

N : System size $\quad d$: dimension of the local Hilbert space



Mean Field Ansatz

$$W_\sigma(a_{\sigma_i}) = a_{\sigma_1} a_{\sigma_2} \dots a_{\sigma_N}$$

$N \times d$ variables

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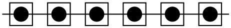

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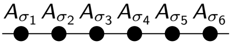

Tensor network states

$$W_\sigma(A_{\sigma_i}) = \mathrm{Tr}(A_{\sigma_1} A_{\sigma_2} \ldots A_{\sigma_N})$$

$N \times d \times D^z$ variables

$$A_i : \text{Tensor of size } \overbrace{D \times \cdots \times D}^{z\,:\,\text{coordination number}}$$

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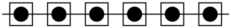

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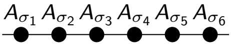

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1D : Density matrix renormalisation group/Matrix product states

Variational Ansatz

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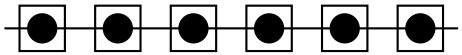

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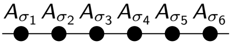

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1D : Density matrix renormalisation group/Matrix product states

Higher dimension : Tensor network states

Tensor network contraction $\rightarrow$ grows exponentially

Variational Ansatz

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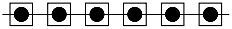

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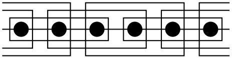

EPS Ansatz short range plaquettes of size N_p

$$W_\sigma(C_{P,\vec{\sigma_p}}) = \prod_P C_{P,\vec{\sigma_p}}$$

$N \times d^{N_P}$ variables

Entangled-plaquette states (EPS) [F.Mezzacapo et al NJP 2009]

Correlator product states [H.J.Changlani et al PRB 2009, S.Al-Assam et al PRB 2011]

Generalization of Spin-jastrow states [T.Pang PRB 1990]

Variational Ansatz

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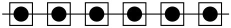

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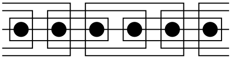
$N \times d$ variables



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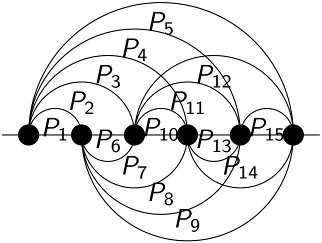
Studying 2D frustrated systems

Complexify the coefficients

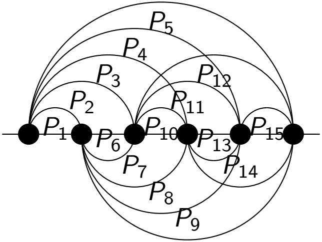
$$C_{P,\sigma_P} = V_{P,\sigma_P} e^{i\theta_{P,\sigma_P}}$$

F. Mezzacapo, JI Cirac NJP 2010
F. Mezzacapo, M. Boninsegni PRB 2012
F. Mezzacapo PRB 2012

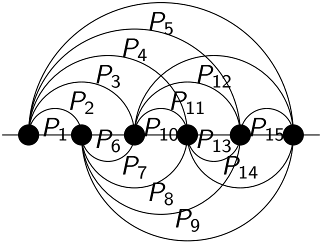
Long Range EPS of size 2



Long Range EPS of size 2



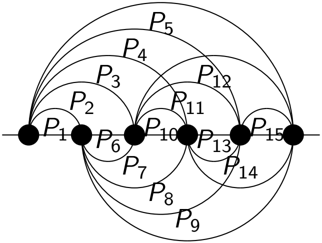
$\propto N^2$ variables



$\propto N$ variables (translation invariance)

Long Range EPS of size 2

$$H = -J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$$



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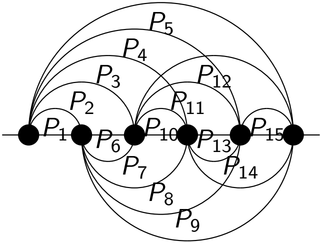

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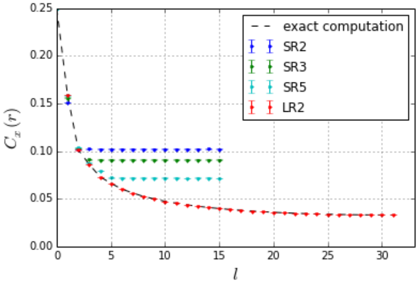
Correlations along x

$$C_x(r) = \langle S_i^x S_{i+r}^x \rangle - \langle S_i^x \rangle^2$$



$N = 62$

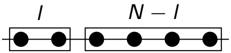
Entanglement Entropy

Reduced density matrix

$$\rho_l = \mathrm{Tr}_{N-l}\ \rho$$

Renyi entanglement entropy

$$S = -\log(\mathrm{Tr}_l\ \rho_l^2)$$



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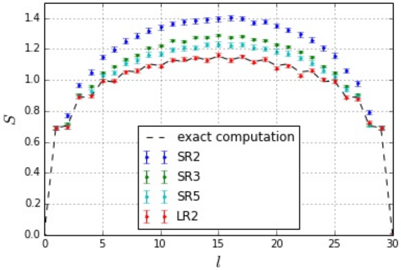
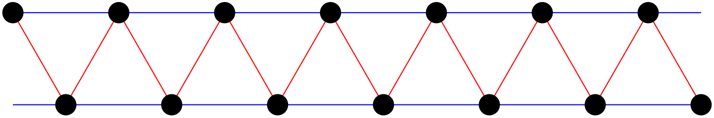


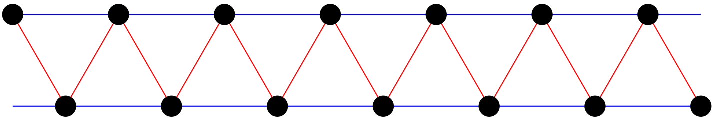
XX-chain $N = 30$

$J_1 J_2$-chain [White, Affleck PRB 1996]



$$H = J_1 (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z) + J_2 (S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + S_i^z S_{i+2}^z)$$

$J_1 J_2$-chain [White, Affleck PRB 1996]



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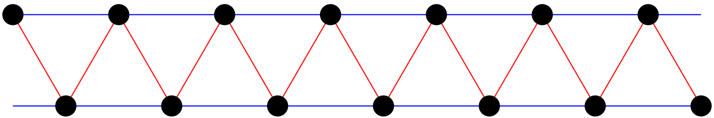

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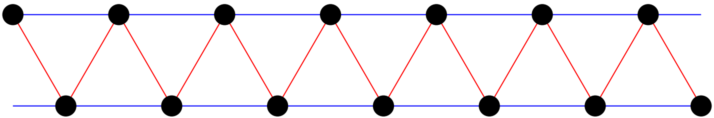
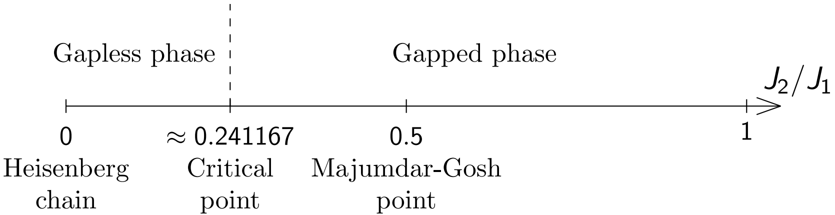
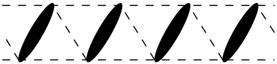
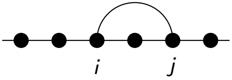






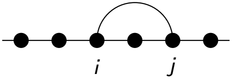
Long range EPS



LR2

$C_{ij}(\sigma_i, \sigma_j)$ spin-spin correlations

Long range EPS



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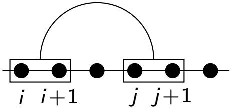

LR4

$C_{i,j}(\sigma_i, \sigma_{i+1}, \sigma_j, \sigma_{j+1})$ spin-spin correlations / dimer-dimer correlations

Case $J_2 = 0$: Heisenberg chain

Known sign structure : Marshall sign rule

$$\mathrm{sgn}(W_\sigma) = (-1)^{N_{\uparrow A}}$$

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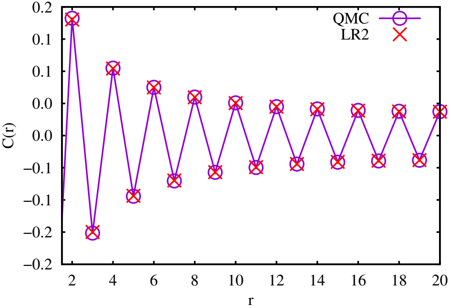
$$\mathrm{sgn}(W_\sigma) = (-1)^{N_{\uparrow A}}$$

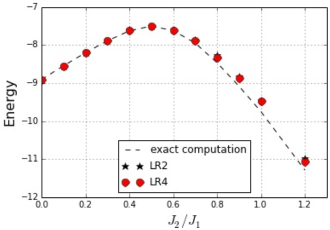
Correlations

$$C(r) = \langle S_i S_{i+r} \rangle - \langle S_i \rangle^2$$

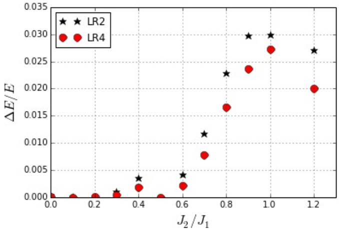


$N = 40$

Case $J_2 \neq 0$



$N = 20$



$N = 20$

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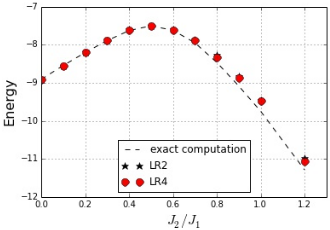
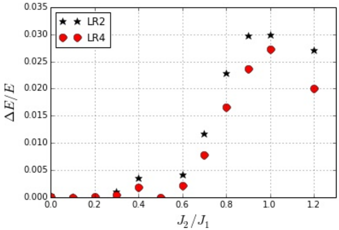


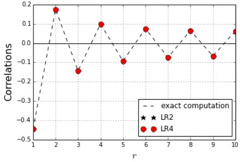
$N = 20$



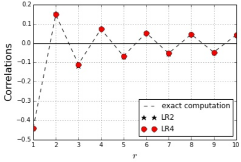
$N = 20$

See also Ferrari et al PRB 2018

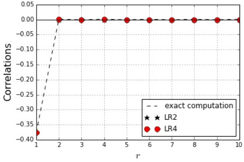
Correlations ($N = 20$)



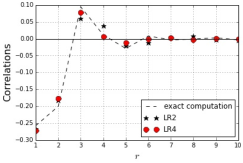
$J_2/J_1 = 0.1$



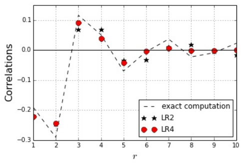
$J_2/J_1 = 0.3$



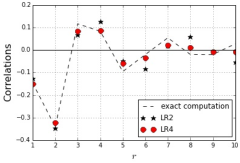
$J_2/J_1 = 0.5$



$J_2/J_1 = 0.7$



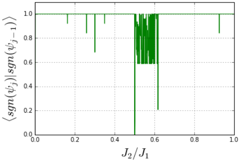
$J_2/J_1 = 0.8$



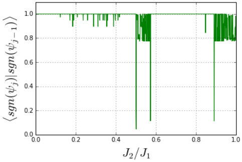
$J_2/J_1 = 1$

Sign structure

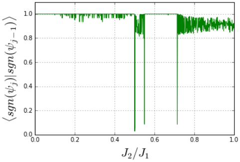
$$|sgn(\psi_j)\rangle = \frac{1}{\sqrt{\mathcal{D}}}\left(\ldots, sign(W_{\vec{\sigma}}^{(j)}), \ldots\right)$$



$N = 10$

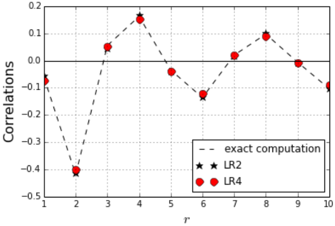


$N = 12$

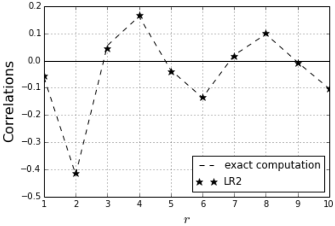


$N = 14$

Case $J_2 > 1$ ($N = 20$)



$J_2/J_1 = 1.2$



$J_2/J_1 = 2$

Conclusion

Aim : Access variationally to systems with non trivial sign structure with a sign-unbiaised method

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Coming soon: systematic comparison of the sign structure of the Ansatz with that of exact diagonalization for $0.5 < J_2/J_1 < 1$

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We can variationally reconstruct non-trivial sign structures (e.g. Marshall sign rule)

Coming soon: systematic comparison of the sign structure of the Ansatz with that of exact diagonalization for $0.5 < J_2/J_1 < 1$

Coming soon(2): enrich the sign structure of LR-EPS states using mixed LR/SR-EPS

$$W_{\vec{\sigma}} = W_{\vec{\sigma}}^{\mathrm{LR-EPS}} \times W_{\vec{\sigma}}^{\mathrm{SR-EPS}}$$

Perspectives

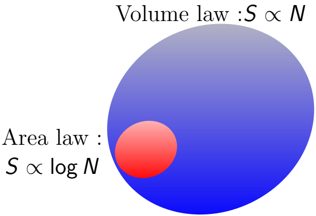
Go to 2D systems : Heisenberg antiferromagnet square and triangular lattice

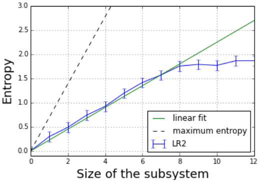
In progress ...

Go to 2D systems : Heisenberg antiferromagnet square and triangular lattice

In progress ...

Study non equilibrium dynamics





Entropy of a random LR2 state for a chain of size 24