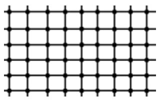
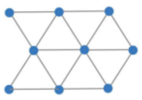
System of spins ½ with isotropic Heisenberg interaction: density matrix parameterization and variational method

Filipp Uskov (Skoltech)

in collaboration with Oleg Lychkovsky and Elena Shpagina

Model





Hamiltonian: $H = J\sum_{<i,j>}(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)$

<i, j> denotes neighboring sites

Scalar and mixed products of Pauli matrices:

$(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j) \equiv \delta^{\alpha\beta}\cdot\sigma_i^\alpha \otimes \sigma_j^\beta$ - rotational and time-inverse symmetric

$(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k) \equiv \varepsilon^{\alpha\beta\gamma}\cdot\sigma_i^\alpha \otimes \sigma_j^\beta \otimes \sigma_k^\gamma$ - rotational symmetric

$\alpha,\beta,\gamma \in \{x,y,z\}$

Squaring parameterization of density matrix [1]

Conditions: $\rho^+ = \rho;\quad \mathrm{Tr}\rho = 1;\quad \rho \geqslant 0\quad;\quad \tau^+ = \tau$

$$\rho \leftarrow \tau:\ \boxed{\rho = \frac{\tau^2}{\mathrm{Tr}\tau^2};\quad a_i = f(b_k) \\ 2^N\rho = a_iA_i;\quad \tau = b_iA_i}$$

Additional symmetry requirement:

$U\tau U^+ = \tau \Rightarrow U\rho U^+ = \rho$

Basis: $\{A_i\} = \{1,\ (\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k),\ (\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)(\boldsymbol{\sigma}_l\boldsymbol{\sigma}_m),\ \ldots\}$

$\{B_j\} = \{(\boldsymbol{\sigma}_p\boldsymbol{\sigma}_r\boldsymbol{\sigma}_s),\ (\boldsymbol{\sigma}_p\boldsymbol{\sigma}_r\boldsymbol{\sigma}_s)(\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k),\ (\boldsymbol{\sigma}_p\boldsymbol{\sigma}_r\boldsymbol{\sigma}_s)(\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)(\boldsymbol{\sigma}_l\boldsymbol{\sigma}_m),\ \ldots\}$

Basis is overcomplete, but we can remove unwanted vectors:

$+(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) - (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_5) - (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) = 0$

- hypothesis, checked only up to 10 spins

Symbolic relations and simplifications

•Algorithm which based on Pauli identity ($\sigma^\alpha\sigma^\beta = \delta^{\alpha\beta} + i\varepsilon^{\alpha\beta\gamma}\sigma^\gamma$) implemented in Wolfram Mathematica

$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)^2 = 3 - 2(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) - i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) = -(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) - 2i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) + 2i(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) = -(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) + 2i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) - 2i(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) - i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) + i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$
$$(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) + i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) - i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)^2 = 6 - 2(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) - 2(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) - 2(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) = -(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) - (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) + 2(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) + i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) + i(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) = +(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_5) - (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) - i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) + i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5)$$

•Scalar product of matrices implemented in Wolfram Mathematica:

$(A,B) \equiv \mathrm{Tr}(A^+B) = \mathrm{Tr}(AB);\qquad A^+ = A$

If sets of spins in A and B differ, then $(A,B) = 0$

$\mathrm{Tr}(\ (\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)\ldots(\boldsymbol{\sigma}_l\boldsymbol{\sigma}_m)(\boldsymbol{\sigma}_m\boldsymbol{\sigma}_i)\ ) = 3\cdot 2^n$ – one cycle

$\mathrm{Tr}(\ (\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_n)\ (\boldsymbol{\sigma}_k\boldsymbol{\sigma}_l)\ldots(\boldsymbol{\sigma}_m\boldsymbol{\sigma}_n)\ ) =$

$= \mathrm{Tr}(\ (\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)\ ) = 6\cdot 2^n$

$(A,B) = 3^C\cdot 2^n$, where C - number of cycles

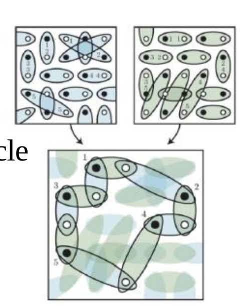


Illustration from [6]

Challenge and main ideas

$$???\leqslant E_{gs} \leqslant \langle\psi|H|\psi\rangle$$

Our challenge — well known variational method

Divide ***full*** lattice to ***cl***usters:

N – number of spins in lattice

M – number of clusters

d - number of bonds per 1 spin

m – number of bonds in cluster

$$M = \frac{Nd}{m}$$

•Anerson bound[3]: $H_{full} = \sum_{i=1}^{M} H_{i\,cl} \;\Rightarrow\; E_{gs\ full} \geqslant \sum_{i=1}^{M} E_{i\ gs\ cl}$

$$\boxed{E_{gs\ full}/N \geqslant \frac{d}{m}E_{gs\ cl}}$$

•Variational method:

$$E_{gs\ full} = \min_\psi\langle\psi|H|\psi\rangle = \min_{\rho_{full}\in S_{full}} \mathrm{Tr}_{\mathrm{full}}H_{full}\rho_{full} = \min_{\rho_{full}\in S^S_{full}} \mathrm{Tr}_{\mathrm{full}}H_{full}\rho_{full} =$$
$$= M\min_{\rho_{full}\in S^S_{full}} \mathrm{Tr}_{\mathrm{full}}H_{cl}\rho_{full} = M\min_{\rho_{full}\in S^S_{full}} \mathrm{Tr}_{\mathrm{cl}}(H_{cl}\mathrm{Tr}_{\mathrm{full}\setminus\mathrm{cl}}\rho_{full}) =$$
$$= M\min_{\rho_{cl}\in S^{trS}_{cl}} \mathrm{Tr}_{\mathrm{cl}}H_{cl}\rho_{cl} \geqslant M\min_{\rho_{cl}\in S^S{}_{cl}} \mathrm{Tr}_{\mathrm{cl}}H_{cl}\rho_{cl}$$

S_{full} - set of density matrices of lattice

$S^S{}_{full}$ - set of density matrices of lattice with the same symmetries as in full hamiltonian

$S^{trS}_{cl} = \{\mathrm{tr}_{\mathrm{full}\setminus\mathrm{cl}}\rho_{full} : \rho_{full}\in S^S_{full}\}$

$S^S{}_{cl}$ - set of density matrices of cluster with the same symmetries as in full hamiltonian

$S^S{}_{cl} \supset S^{trS}_{cl}$

S_{cl} - set of all density matrices of cluster

$$\boxed{E_{gs\ full}/N \geqslant \frac{d}{m}\min_{\rho_{cl}\in S^S{}_{cl}} \mathrm{Tr}_{\mathrm{cl}}H_{cl}\rho_{cl};}$$

•Comparison:

$$E_{gs\ cl} = \min_{\rho_{cl}\in S_{cl}} \mathrm{Tr}_{\mathrm{cl}}H_{cl}\rho_{cl} \leqslant \min_{\rho_{cl}\in S^S{}_{cl}} \mathrm{Tr}_{\mathrm{cl}}H_{cl}\rho_{cl}$$

Variational method in general outperform Anderson bound for the same cluster size

Variational method example

Let consider $H_{cl} = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)$

$\{A_k\} = \{1, (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2), (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3), (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4), (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3), (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4), (\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4),$
$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4), (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4), (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)\}$

$\tau = b_iA_i,\ \ \rho = a_iA_i,\ \ \rho = \tau^2 \ \Rightarrow\ a_k = a_{k,ij}b_ib_j$

Normalization: $a_0 = 1/16$

Lattice symmetries: $a_{(1,2)} = a_{(2,3)} = a_{(3,4)};\ \ a_{(1,3)} = a_{(2,4)}$

Let find: $\min Tr\ H\rho = \min_b \eta_{ij}b_ib_j,$ where $\eta_{ij} = Tr(A_iHA_j)$

with constraints: $\mathrm{a}_{0,ij}b_ib_j - 1/16 = 0$

$c_{k,ij}b_ib_j = 0,\quad k = \{(1,2)(2,3),\ (2,3)(3,4),\ (1,3)(2,4)\},$ where:

$c_{(1,2)(2,3),ij} = a_{(1,2),ij} - a_{(2,3),ij};\ \ \mathrm{c}_{(2,3)(3,4),ij} = a_{(2,3),ij} - a_{(3,4),ij};\ \ \mathrm{c}_{(1,3)(2,4),ij} = a_{(1,3),ij} - a_{(2,4),ij}$

Let use **method of Lagrange multipliers** to find minima with constraints:

$$L(b,c) = \eta_{ij}b_ib_j + \lambda_0(a_{0,ij}b_{bj} - 1/16) + \sum_k \lambda_k c_{k,ij}b_ib_j$$

$$\begin{cases} \frac{1}{2}\frac{\partial L}{\partial b_i} = (\eta_{ij} + \lambda_0 a_{0,ij} + \sum_k \lambda_k c_{k,ij})b_j = 0 \\ \frac{\partial L}{\partial \lambda_0} = a_{0,ij}b_ib_j - 1/16 = 0 \\ \frac{\partial L}{\partial \lambda_k} = c_{k,ij}b_ib_j = 0 \end{cases}$$

Solving this equations in progress…

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