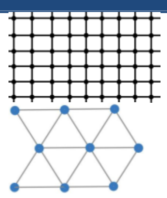
System of spins ½ with isotropic Heisenberg interaction: parameterization density matrix, variational method, exact diagonalization

Skoltech
Skolkovo Institute of Science and Technology

Faculty of Physics of MSU

Filipp Uskov
Skoltech, Moscow State University
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 vectors of Pauli matrices:

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

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

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

Squaring parameterization of density matrix [1]

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

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

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 eject unwanted vectors:
$+(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) - (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_5) - (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) = 0$
- hypotesis, checked only up to 10 spins

Symbolic relations and simplifications

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

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

$(A, B) = 0$ if A and B contain different spins

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

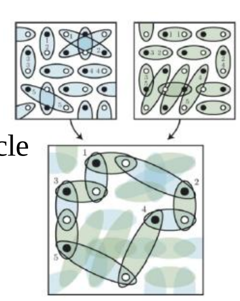
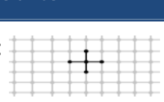


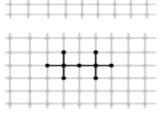
Illustration from [6]

Results

2d:



$E_{gs}/N > 3$



$E_{gs}/N > -2{,}9685$

1d exact theoretical [7]: $E_{gs}/N = 1 - 4\ln 2 = -1.7725$

1d:

cluster	$E_{gs}/N >$
	-2.1547
	-1.92789
	-1.99486
	-1.89083
	-1.92853

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

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

•Schrödinger equation: $H_{full} = \sum_{i=1}^{M} H_{i\,cl} \quad \Rightarrow \quad E_{gs\,full} \geqslant \sum_{i=1}^{M} E_{i\,gs\,cl}$

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

•Variational method:

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

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

S_{full} - set of density matrices of lattice
$S^S{}_{full}$ - set of density matrices of lattice with the same symmetries as in hamiltonian of lattice
$S^{trS}_{cl} = \{\mathrm{tr}_{\mathrm{full}\setminus\mathrm{cl}}\rho_{full} : \rho_{full} \in S^S_{full}\}$
$S'_{cl} \supset S^{trS}_{cl}$

Schrödinger equation

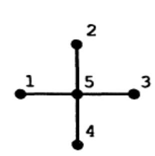
$$H\rho = E\rho \quad \Leftrightarrow \quad H\frac{\tau^2}{\mathrm{Tr}\tau^2} = E\frac{\tau^2}{\mathrm{Tr}\tau^2} \quad \Leftarrow \quad H\tau = E\tau$$

$$HA_j a_j = A_i h_{ij} a_j + B_i d_{ij} a_j = EA_j a_j \quad \Rightarrow \quad \begin{cases} h_{ij}a_j = Ea_i \\ d_{ij}a_j = 0 \end{cases}$$

$$(A_i, A_j) = g_{ij}$$
$$\mathrm{Tr}(A_i H A_j) = \eta_{ij} \qquad h_{ij} = g^{-1}_{ik}\eta_{kj}$$

We take into account the symmetries of commutation of spins in cluster.

Example:



$$A_0 = 1$$
$$A_1 = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_3\boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5)$$
$$A_2 = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_4\boldsymbol{\sigma}_1) + (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4)$$
$$A_3 = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)$$
$$+ (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)$$
$$+ (\boldsymbol{\sigma}_3\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_3\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_3\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4)$$
$$+ (\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$
$$A_4 = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)$$

$$h_{ij} = \begin{pmatrix} 0 & 12 & 0 & 0 & 0 \\ 1 & -2 & 3 & 0 & 0 \\ 0 & 2 & 0 & 10 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 4 & 0 \end{pmatrix}$$

$$d_{ij} = 0$$
$$E_{gs} = -6, -4, 4, 2, 0$$

Variational method

Numeric method: $$\min \mathrm{Tr}H\rho = \min_{\{b_i\}} \frac{b_i b_j}{b_l b_m}\frac{\eta_{ij}}{g_{lm}}$$

Lagrange method:
$$\min \mathrm{Tr}H\rho = \min_{\{b_i\}} b_i b_j \eta_{ij}$$
with condition $b_l b_m g_{lm} = 1$

$$L(\{b_k\}, \lambda) = b_i b_j(\eta_{ij} - \lambda g_{ij}) + \lambda$$
$$\Rightarrow b_i(\eta_{ik} - \lambda g_{ik}) = 0$$
$$\Leftrightarrow \ b_i(g^{-1}_{ij}\eta_{jk}) = b_i h_{ik} = \lambda b_k$$
$$\min_{\{b_i\}} b_i b_j \eta_{ij} = \min \lambda$$

1. N. Il'in, E. Shpagina, F. Uskov, O. Lychkovskiy, Squaring parametrization of constrained and unconstrained sets of quantum states. J. Phys. A: Math. Theor. 51, 085301 (2018)
2. R. Tarrah, R. Valenti, Exact lover bounds to the ground state of spin systems: The two-dimensional S = 1/2 antiferromagnetic Heisenberg model Physical review B , (1990)
3. P. W. Anderson, Limits on the Energy of the Antiferromagnetic Ground State, Letters to the editor (1951)
4. Tillmann Baumgratz1 and Martin B Plenio, Lower bounds for ground states of condensed matter systems. New Journal of Physics 14, 023027 (2012)
5. David A. Mazziotti, Variational minimization of atomic and molecular ground-state energies via the two-particle reduced density matrix, Phys.Rev.A, 65, 062511 (2002)
6. K.S.D. Beach, A.W. Sandvik Some formal results for the valence bond basis Nuclear Physics B 750 [FS] 142–178 (2006)
7. Daniel C. Mattis, C. Y. Pan, Ground-State Energy of Heisenberg antiferromagnet for Spins s=1/2 and s=1 in d=1 and 2 Dimensions. Phys.Rev.Lett., 61, (1988)
8. Маттис. Теория магнетизма. Москва, Мир, 1967