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


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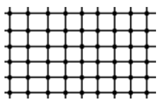
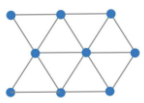
## Model





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

where <i, j> denotes neighboring sites

Scalar and mixed products of vectors of Pauli matrices:

$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) \;\;= \delta^{\alpha\beta}\cdot\sigma_1^\alpha \otimes 1_2 \otimes \sigma_3^\beta \otimes 1_4 \otimes 1_5$$

$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) = \varepsilon^{\alpha\beta\gamma}\cdot\sigma_1^\alpha \otimes 1_2 \otimes \sigma_3^\beta \otimes \sigma_4^\gamma \otimes 1_5$$

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

## Squaring parameterization of density matrix [1]

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

From $\rho$ to $\tau$: $\rho = \dfrac{\tau^2}{\mathrm{Tr}\tau^2}$; for $\tau$ only one condition: $\tau^+ = \tau$

$$\rho = \frac{1}{2^n} a_i A_i; \qquad \tau = b_i A_i$$

Basis:

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

Basis overflow:

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

## 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 $B$ contains different spins

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

$$\mathrm{Tr}(\,(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_n)\,(\boldsymbol{\sigma}_k\boldsymbol{\sigma}_l)\ldots(\boldsymbol{\sigma}_m\boldsymbol{\sigma}_n)\,) =$$
$$= \mathrm{Tr}(\,(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k)\,) = 6\cdot 2^n$$

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

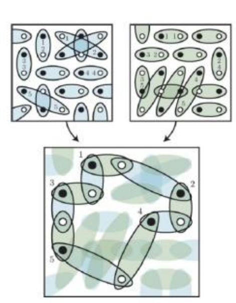
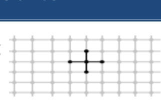


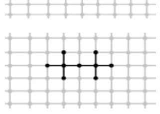
Illustration from [6]

## 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*** crystal to ***cl***usters:

N – number of spins in crystal

M – number of clusters

d - number of bonds by 1 spin

m – number of bonds in cluster

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

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

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

- Variational method:

$$E_{gs\,full} = \min_\psi \langle\psi\,|\,H\,|\,\psi\rangle = \min_{\rho_{full}\in M_{full}} \mathrm{Tr}_{\mathrm{full}} H_{full}\rho_{full} = \min_{\rho_{full}\in M_{full}^S} \mathrm{Tr}_{\mathrm{full}} H_{full}\rho_{full} =$$

$$= M \min_{\rho_{full}\in M_{full}^S} \mathrm{Tr}_{\mathrm{full}} H_{cl}\rho_{full} = M \min_{\rho_{full}\in M_{full}^S} \mathrm{Tr}_{\mathrm{cl}}(H_{cl}\mathrm{Tr}_{\text{full-cl}}\rho_{full}) =$$

$$= M \min_{\rho_{cl}\in M_{cl}^{trS}} \mathrm{Tr}_{\mathrm{cl}} H_{cl}\rho_{cl} \geqslant M \min_{\rho_{cl}\in M'_{cl}} \mathrm{Tr}_{\mathrm{cl}} H_{cl}\rho_{cl}$$

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

## Schrödinger equation

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

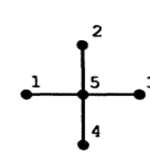
$$HA_j a_j = A_i h_{ij} a_j + B_i d_{ij} a_j = EA_j a_j \;\Rightarrow\; \begin{cases} h_{ij}a_j = Ea_i \\ d_{ij}a_j = 0 \end{cases}$$

$$(A_i, A_j) = g_{ij}$$

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

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

Lagrange method:

$\min \mathrm{Tr}H\rho = \min_{\{b_i\}} b_i b_j \eta_{ij}$

with condition $b_l b_m g_{lm} = 1$

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

If we don't take into account the symmetries of commutation of spins Variational method is identical to Schrodinger equation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