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

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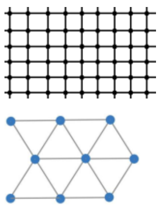
Model



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

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

$$\rho = \frac{1}{2^n}a_iA_i;\qquad \tau = b_iA_i$$

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

See illustrations in poster by Elena Shpagina

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

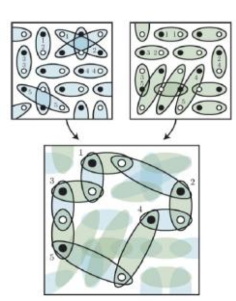
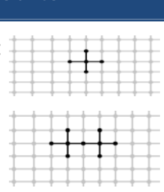


Illustration from [6]

Results

2d:

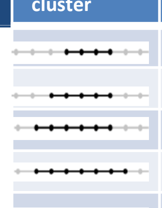


$E_{gs}/N > 3$

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

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:

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

Schrödinger equation

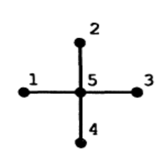
$$H\rho = E\rho \;\Leftrightarrow\; H\frac{\tau^2}{\mathrm{Tr}\tau^2} = E\frac{\tau^2}{\mathrm{Tr}\tau^2} \;\Leftarrow\; H\tau = E\tau$$

$$HA_ja_j = A_ih_{ij}a_j + B_id_{ij}a_j = EA_ja_j \;\Rightarrow\; \begin{cases} h_{ij}a_j = Ea_i \\ d_{ij}a_j = 0 \end{cases}$$

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

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

Example:



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

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

$$d_{ij} = 0$$

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

Variational method

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

Lagrange method:

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

with condition $b_lb_mg_{lm} = 1$

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

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

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