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

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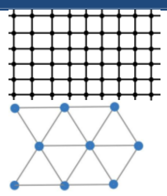
Model



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

$$\rho\ \leftarrow\ \tau:\boxed{\begin{array}{ll}\rho=\dfrac{\tau^2}{\mathrm{Tr}\tau^2}; & a_i=f(b_k)\\ 2^N\rho=a_iA_i; & \tau=b_iA_i\end{array}}$$

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

$$\begin{aligned}
&(\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)
\end{aligned}$$

•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

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

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

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

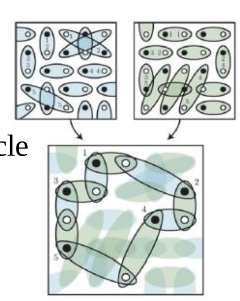
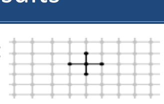


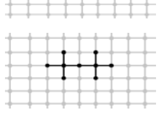
Illustration from [6]

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

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

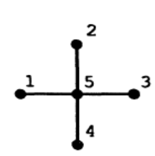
$$HA_ja_j=A_ih_{ij}a_j+B_id_{ij}a_j=EA_ja_j\quad\Rightarrow\quad\begin{cases}h_{ij}a_j=Ea_i\\ d_{ij}a_j=0\end{cases}$$

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

$$\mathrm{Tr}(A_iHA_j)=\eta_{ij}\qquad h_{ij}=g^{-1}_{ik}\eta_{kj}$$

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

Example:



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

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

$d_{ij}=0$

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

Variational method

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

Lagrange method:

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

with condition $b_lb_mg_{lm}=1$

$$L(\{b_k\},\lambda)=b_ib_j(\eta_{ij}-\lambda g_{ij})+\lambda$$

$$\Rightarrow b_i(\eta_{ik}-\lambda g_{ik})=0$$

$$\Leftrightarrow\ b_i(g^{-1}_{ij}\eta_{jk})=b_ih_{ik}=\lambda b_k$$

$$\min_{\{b_i\}}b_ib_j\eta_{ij}=\min\lambda$$

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