An algebraic approach to spin-1/2 systems with isotropic Heisenberg interaction

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MOTIVATION

In many problems involving spin-1/2 systems with isotropic Heisenberg interaction one needs to simplify products of scalar and mixed products of Pauli matrices.

Typical Hamiltonian:

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

where $< i, j >$ denotes neighbouring sites

Typical problems:

- squaring parametrization of density matrices, ρ [1] (see also talk by N. Il'in and poster by E. Spagina)
- variational principle [2]
- Schrodinger equation in the form $H\rho = E\rho$ (see e.g. [3])

Important: account for all (possibly noncommuting) symmetries simultaneously!

STATIONARY SCHRODINGER EQUATION FOR A DENSITY MATRIX

ρ can be used instead of Ψ in a stationary Schrodinger equation (see e.g.[3]):

$$H\rho = E\rho.$$

If the Hamiltonian of N spins 1/2 is invariant w.r.t. rotations (i.e. $SU(2)$) and time reversal one can seek ρ in form

$$\rho = \frac{1}{2^N}\left(1 + a_{i,j}(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j) + b_{i,j,k,l}(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)(\boldsymbol{\sigma}_k\boldsymbol{\sigma}_l) + \ldots\right)$$

Example:

$$H = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)$$

Additional symmetry of the Hamiltonian: $1 \leftrightarrow 3$

$$\rho = \frac{1}{8}\big(1 + a\big((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)\big) + b(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3)\big)$$

$$H\rho = \frac{1}{8}((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3))(1 + a((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)) + b(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3)) =$$
$$= \frac{1}{8}(6a + (1 + b - 2a)(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) + 2a(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3) + (1 + b - 2a)(\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)) =$$
$$= \frac{1}{8}(E + Ea(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) + Ea(\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3) + Eb(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3)) = E\rho$$

System of three quadratic equations: Solution:

$$\begin{cases} 6a - E = 0 \\ 1 - 2a + b - aE = 0 \\ 2a - bE = 0 \end{cases} \qquad \begin{cases} a = -\frac{1}{2} \\ b = \frac{1}{3} \\ E = -4 \end{cases} \quad \begin{cases} a = 0 \\ b = -1 \\ E = 0 \end{cases} \quad \begin{cases} a = \frac{1}{3} \\ b = \frac{1}{3} \\ E = 2 \end{cases}$$

VARIATIONAL PRINCIPLE

A variational principle of [2] allows to bound the ground state energy **from below**. For the Heisenberg model on the square lattice it reads

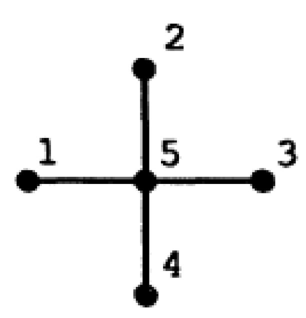
$$E_{gs}/N \geqslant \frac{2}{M} \inf_{\rho_c} \operatorname{tr} H_c \rho_c,$$

where E_{gs}/N is the ground state energy per site, H_c is the Hamiltonian of an arbitrary cluster on the square lattice, M – number of couplings in this cluster, ρ_c – its density matrix respecting all symmetries of the *original model*.

Example: $H_c = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_5)$

To ensure $\rho_c \geq 0$, $\operatorname{tr}\rho_c = 1$, $\rho_c^\dagger = \rho_c$ we use **squaring parametrization** [3]:

$$\rho_c = \frac{\tau^2}{\operatorname{tr}\tau^2}$$



τ accounting for all symmetries:

$$\tau = 1 +$$
$$a_1((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_5) + (\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_5)) +$$
$$a_2((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_4)) +$$
$$a_3((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_1)) +$$
$$b_1((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_4) +$$
$$+ (\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_1) + (\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_1) + (\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) + (\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_2)) +$$
$$b_2((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_1)) +$$
$$b_3(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_4) +$$
$$b_4((\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_3, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_4) + (\boldsymbol{\sigma}_4, \boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3))$$

$$\operatorname{tr} H_c \rho_c = \frac{\begin{array}{c}(24a_1 - 24a_1^2 + 24a_1 a_2 + 48a_1 a_3 + 48a_2 b_1 + 192a_3 b_1 - 192b_1^2 + 192b_1 b_2 + \\ 48b_1 b_3 + 72a_2 b_4 + 48a_3 b_4 - 96b_1 b_4 + 48b_2 b_4 + 72b_3 b_4 - 72b_4^2)\end{array}}{1 + 12a_1^2 + 6a_2^2 + 12a_3^2 + 96b_1^2 + 24b_2^2 + 12b_2 b_3 + 9b_3^2 + 48b_1 b_4 + 36b_4^2}$$

$$NMinimize \to \left\{ -6., \begin{cases} a_1 \to -0.5, & a_2 \to 0.333333, \\ a_3 \to 0.333333, & \\ b_1 \to -0.1, & b_2 \to 0.0666667, \\ b_3 \to 0.0666667, & b_4 \to -0.1 \end{cases} \right\} \quad \Rightarrow \quad E_{gs}/N \geqslant -3$$

The same result was obtained by another method in [4].
We expect that our method outperforms the method of ref. [4] for larger clusters.
Work is underway.

ALGORITHM FOR SIMPLIFICATION OF PRODUCTS OF σ-MATRICES

The algorithm is used, in particular, for simplifying $H\rho$.

$\rightarrow$ Input and output form: $(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j) = d(i,j)$ and $(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k) = t(i,j,k)$.

Algorithm:

1. • $d(i,j) \to \sigma(i,\alpha)\sigma(j,\alpha)$
   • $t(i,j,k) \to \varepsilon(\alpha,\beta,\gamma)\sigma(i,\alpha)\sigma(j,\beta)\sigma(k,\gamma)$

   (we assume that different site indices are different: $i \neq j \neq k \neq i$ etc)
2. σ-matrices with different site indices are commuting, so we can stable(!) sort it:
   (a) first σ in multiplication $\to \tilde{\sigma}$
   (b) while found $\tilde{\sigma}\sigma$
      i. $\tilde{\sigma}\sigma \to \tilde{\sigma}\boxed{\sigma}$
      ii. while found $\tilde{\sigma}\boxed{\sigma}$
         A. if(site indices of $\tilde{\sigma}$ and $\boxed{\sigma}$ are equal) push spin index of $\boxed{\sigma}$ to the back of $\tilde{\sigma}$ (for example $\tilde{\sigma}(i,\alpha,\beta)\boxed{\sigma}(i,\gamma) \to \tilde{\sigma}(i,\alpha,\beta,\gamma)$)
         B. else swap $\tilde{\sigma}$ and $\boxed{\sigma}$: $\tilde{\sigma}\boxed{\sigma} \to \boxed{\sigma}\tilde{\sigma}$
      iii. if $\boxed{\sigma}$ is in first position, $\boxed{\sigma} \to \tilde{\sigma}$
3. $\tilde{\sigma}(i,\alpha,\beta,\gamma) = \sigma_i^\alpha\sigma_i^\beta\sigma_i^\gamma$

   apply Pauli formula while $\tilde{\sigma}$ has more than one spin index

   $$\sigma(i,\alpha,\beta,\gamma,\ldots) \to \delta(\alpha,\beta)\sigma(i,\gamma,\ldots) + i\varepsilon(\alpha,\beta,\mu)\sigma(i,\mu,\gamma,\ldots)$$
4. in each term σ-matrices commute
   • simplify δ and ε symbols
   • isolate scalar and mixed products $d(i,j)$ and $t(i,j,k)$

This algorithm was implemented in Wolfram Mathematica and Nikhef Form.

ALTERNATIVE BASIC ALGEBRAIC RELATIONS

We can use this formulas recursively to simplify products of scalar and mixed products of σ-matrices.

$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)^2 = 3 - 2(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) \tag{1}$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) = -i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) + (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) \tag{2}$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) = -(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) - 2i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) + 2i(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) \tag{3}$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) = -(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) + 2i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) - 2i(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) \tag{4}$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) - i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) + i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) \tag{5}$$
$$(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) = (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) + i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) - i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) \tag{6}$$
$$(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)^2 = 6 - 2(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) - 2(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3) - 2(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) \tag{7}$$
$$\begin{aligned}(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) = &+ i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) + i(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4) \\ &- (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4) - (\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3) + 2(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)\end{aligned} \tag{8}$$
$$\begin{aligned}(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) = &- i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) + i(\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3)(\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4\boldsymbol{\sigma}_5) \\ &+ (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_4)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_5) - (\boldsymbol{\sigma}_2\boldsymbol{\sigma}_5)(\boldsymbol{\sigma}_3\boldsymbol{\sigma}_4)\end{aligned} \tag{9}$$

ALGORITHM FOR GENERATION OF SYMMETRIC ρ

Accounts for symmetries w.r.t. to permutations etc.

$\rightarrow$ We get input data as generators of permutation group which rest Hamiltonian.

1. generate all elements of this group
2. for each number pairs

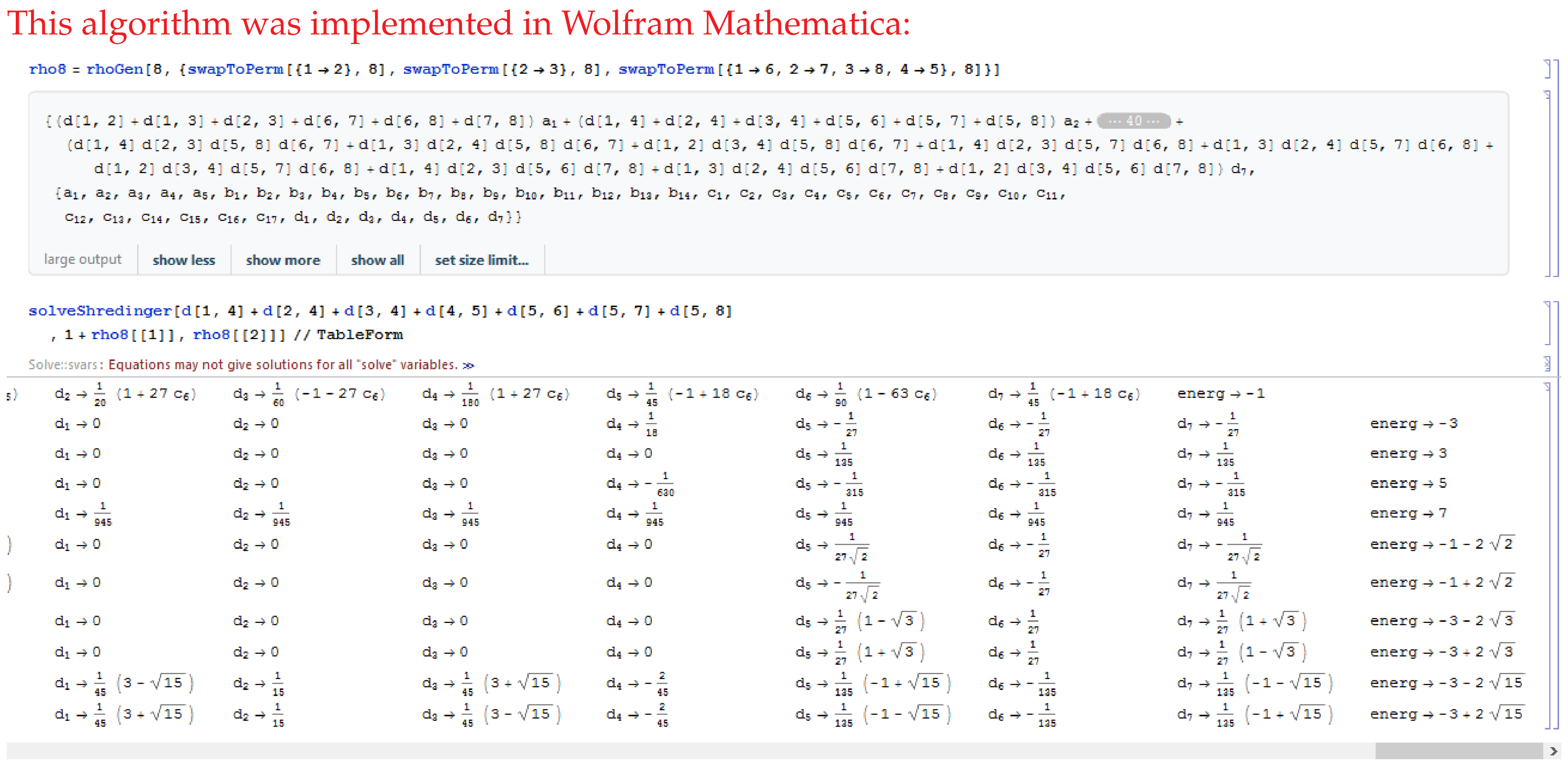
   For each Construction of Pairs (CP) we can get next CP.

   We need split all CPs to "groups" of CPs which map into themselves by any permutation of Hamiltonian's group.

   We do this by brute force.
3. We parameterize each "group" of CPs by new parameter

   and convert each CP to expression and sum them

This algorithm was implemented in Wolfram Mathematica:



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