# Certifying Ground-State Properties of Quantum Many-Body Systems

王杰

中国科学院数学与系统科学研究院

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# Outline

1. The ground state problem
2. Noncommutative polynomial optimization
3. Numerical results

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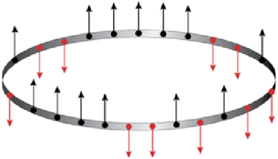
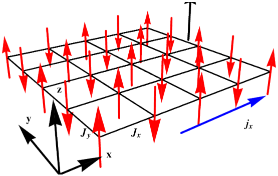
# Quantum many-body systems






- ☞ Ising model
- ☞ Heisenberg model
- ☞ Compute ground state energy: QMA-hard

# Pauli matrices

- Spin-$\frac{1}{2}$ particles
- Pauli matrices:

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^y = \begin{bmatrix} 0 & -\mathbf{i} \\ \mathbf{i} & 0 \end{bmatrix}, \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- For $a \in \{x, y, z\}$ and $i, N \in \mathbb{N}$, let

$$\sigma_i^a = \underbrace{I_2 \otimes \cdots \otimes I_2}_{i-1} \otimes \sigma^a \otimes \underbrace{I_2 \otimes \cdots \otimes I_2}_{N-i} \in M_2(\mathbb{C})^{\otimes N} = M_{2^N}(\mathbb{C})$$

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# Ground state energy of quantum many-body systems

- Ising model: $H_N = -\sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - \sum_{i=1}^{N} \sigma_i^x$
- Heisenberg model: $H_N = \frac{1}{4} \sum_{i=1}^{N} \sum_{a \in \{x,y,z\}} \sigma_i^a \sigma_{i+1}^a$
- $J_1$-$J_2$ Heisenberg model: $H_N = \frac{1}{4} \sum_{i=1}^{N} \sum_{a \in \{x,y,z\}} [\sigma_i^a \sigma_{i+1}^a + J_2 \sigma_i^a \sigma_{i+2}^a]$
- The ground state energy:

$$E_{GS} = \lambda_{\min}(H_N) = \min_{|\psi\rangle \in \mathbb{C}^{2^N}} \langle \psi | H_N | \psi \rangle$$

# Upper bound approaches

☞ Many variational methods produce upper bounds

- The DMRG (density-matrix renormalization group) approach
- Tensor networks
- Neural networks
- Quantum Monte Carlo

☞ No theoretical guarantee

# Noncommutative polynomial optimization reformulation

Consider the Heisenberg chain:

$$
\begin{cases}
\min\limits_{\{|\psi\rangle,\sigma_i^a\}} & \frac{1}{4}\sum_{i=1}^N \sum_{a\in\{x,y,z\}} \langle\psi|\sigma_i^a\sigma_{i+1}^a|\psi\rangle \\
\text{s.t.} & (\sigma_i^a)^2 = 1, \quad i=1,\ldots,N, a\in\{x,y,z\}, \\
 & \sigma_i^x\sigma_i^y = \mathbf{i}\sigma_i^z, \sigma_i^y\sigma_i^z = \mathbf{i}\sigma_i^x, \sigma_i^z\sigma_i^x = \mathbf{i}\sigma_i^y, \quad i=1,\ldots,N, \\
 & \sigma_i^y\sigma_i^x = -\mathbf{i}\sigma_i^z, \sigma_i^z\sigma_i^y = -\mathbf{i}\sigma_i^x, \sigma_i^x\sigma_i^z = -\mathbf{i}\sigma_i^y, \quad i=1,\ldots,N, \\
 & \sigma_i^a\sigma_j^b = \sigma_j^b\sigma_i^a, \quad 1\le i\ne j\le N, a,b\in\{x,y,z\}.
\end{cases}
$$

# Noncommutative polynomial optimization

- Eigenvalue optimization problem:

$$\lambda_{\min}(f, S(\mathbf{g}, \mathbf{h})) = \begin{cases} \inf\limits_{\mathbf{x}\in\cup_{k\geq 1}(\mathbb{S}_k)^n} & \text{eig } f(\mathbf{x}) = f(x_1, \ldots, x_n) \\ \text{s.t.} & g_i(\mathbf{x}) \geq 0, \quad i = 1, \ldots, m, \\ & h_j(\mathbf{x}) = 0, \quad j = 1, \ldots, l. \end{cases}$$

☞ Multiplication noncommutes: $x_i x_j \neq x_j x_i$

☞ Quotient ring ($l > 0$): $\mathbb{C}\langle\mathbf{x}\rangle/(h_1, \ldots, h_l)$

☞ Mathematical foundation: $C^*$-algebra

# Moment matrix and localizing matrix

- Monomial basis: $[\mathbf{x}]_r := [1, x_1, \ldots, x_n, x_1^2, x_1x_2, x_2x_1, x_2^2, \ldots, x_n^r]$
- $\mathbf{y} = (y_w)$: a sequence in $\mathbb{C}$ indexed by monomials
- $r$-th order moment matrix $\mathbf{M}_r(\mathbf{y})$:

$$[\mathbf{M}_r(\mathbf{y})]_{uv} := y_{u^\star v}, \quad \forall u, v \in [\mathbf{x}]_r$$

- Given $g = \sum_w g_w w$, $r$-th order localizing matrix $\mathbf{M}_r(g\mathbf{y})$:

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# The hierarchy of moment relaxations

- The hierarchy of moment relaxations indexed by relaxation order $r$:

$$\theta_r := \begin{cases} \inf_{\mathbf{y}} & L_{\mathbf{y}}(f) := \sum_w f_w y_w \\ \text{s.t.} & \mathbf{M}_r(\mathbf{y}) \succeq 0, \\ & \mathbf{M}_{r-d_i}(g_i\mathbf{y}) \succeq 0, \quad i = 1, \ldots, m, \\ & y_1 = 1. \end{cases}$$

☞ Semidefinite programming (SDP)

# Sum of Hermitian squares and quadratic module

- Sums of Hermitian squares (SOHS): $f = g_1^\star g_1 + g_2^\star g_2 + \cdots + g_t^\star g_t$
- Quadratic module:

$$\mathcal{Q}(\mathbf{g}) := \left\{ \sum_g \tau_g^\star g \tau_g \,\middle|\, \tau_g \in \mathbb{C}\langle \mathbf{x} \rangle, g \in \{1\} \cup \mathbf{g} \right\}$$

- Truncated quadratic module:

$$\mathcal{Q}(\mathbf{g})_{2r} := \left\{ \sum_g \tau_g^\star g \tau_g \,\middle|\, \tau_g \in \mathbb{C}\langle \mathbf{x} \rangle, \deg(\tau_g^\star g \tau_g) \le 2r, g \in \{1\} \cup \mathbf{g} \right\}$$

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# The hierarchy of dual SOHS relaxations

- $f \in \mathcal{Q}(\mathbf{g}) \Rightarrow f \geq 0$ on $S(\mathbf{g})$
- The hierarchy of dual SOHS relaxations:

$$\theta_r^* := \begin{cases} \sup\limits_{\lambda} & \lambda \\ \text{s.t.} & f - \lambda \in \mathcal{Q}(\mathbf{g})_{2r}. \end{cases}$$

☞ SDP

# The NPA hierarchy (2008)

$$
\begin{array}{ccccc}
 & & \lambda_{\min}(f, S(\mathbf{g})) & & \\
 & \rotatebox{-45}{$\geq$} & & \rotatebox{45}{$\leq$} & \\
 & \vdots & & \vdots & \\
 & \geq & & \geq & \\
\textcolor{red}{\text{(Moment relaxation)}} & \theta_r & \text{``}=\text{''} & \theta_r^* & \textcolor{red}{\text{(dual SOHS relaxation)}} \\
 & \geq & & \geq & \\
 & \vdots & & \vdots & \\
 & \geq & & \geq & \\
 & \theta_{r_{\min}} & \text{``}=\text{''} & \theta_{r_{\min}}^* &
\end{array}
$$

# Asymptotical convergence

- Archimedean's condition: there exists $p > 0$ s.t. $p - \sum_{i=1}^{n} x_i^2 \in \mathcal{Q}(\mathbf{g})$

☞ Under Archimedean's condition: $\theta_r, \theta_r^* \nearrow \lambda_{\min}(f, S(\mathbf{g}))$ as $r \to \infty$

(**Helton & McCullough, 2004**)

☞ Detect global optimality: flatness condition

☞ Extract a solution: Gelfand-Naimark-Segal construction

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# Choose a smaller monomial basis

- Length of $[\mathbf{x}]_r$: $\frac{n^{r+1}-1}{n-1}$
- When the polynomials are sparse, possibly use a smaller monomial basis

☞ Choose $\mathcal{B}_r \subsetneq [\mathbf{x}]_r$ such that

$$\left(\operatorname{supp}(f) \cup \bigcup_{i=1}^{m} \operatorname{supp}(g_i)\right) \subseteq \mathcal{B}_r^{\star} \cdot \mathcal{B}_r$$

# Exploit symmetries

1. Determine the symmetry group of the system
2. Compute irreducible representations of the symmetry group
3. Compute a basis for each isotypic component
4. Construct block diagonal SDP relaxations

# Structures of the Heisenberg model

1. Quotient ring
2. Sparsity
3. Sign symmetry of the model
4. Sign symmetry of the Hamiltonian
5. Translation symmetry
6. Permutation symmetry of the Hamiltonian
7. Mirror symmetry of the 2D Heisenberg model

# Quotient ring

- Normal form: $\mathrm{NF}(u) := c\sigma_{i_1}^{a_1}\sigma_{i_2}^{a_2}\cdots\sigma_{i_r}^{a_r}$ with $c \in \{1, -1, \mathbf{i}, -\mathbf{i}\}$ and

$1 \leq i_1 < i_2 < \cdots < i_r \leq N$

- Quotient ring: $\mathbb{C}\langle\mathbf{x}\rangle/I$, where $I$ is the ideal generated by all constraints

$$\begin{cases} \min\limits_{\mathbf{y}} & \frac{1}{4}\sum_{i=1}^{N}\sum_{a\in\{x,y,z\}} y_{\sigma_i^a\sigma_{i+1}^a} \\ \text{s.t.} & \widetilde{\mathbf{M}}_r \succeq 0 \end{cases}$$

# Sparse monomial basis

Let

$$\mathcal{P}_d := \left\{\sigma_i^{a_1}\sigma_{i+1}^{a_2}\cdots\sigma_{i+d-1}^{a_d} \mid i = 1, \ldots, N, a_j \in \{x, y, z\}, j = 1, \ldots, d\right\}$$

Use the sparse monomial basis:

$$\mathcal{B}_r := \bigcup_{d=0}^{r} \mathcal{P}_d$$

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# Sign symmetry of the model

The Heisenberg model is invariant under

$$(\sigma_i^x, \sigma_i^y, \sigma_i^z)_{i=1}^N \longrightarrow (-\sigma_i^x, -\sigma_i^y, \sigma_i^z)_{i=1}^N$$

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☞ Yield a block diagonal structure of 4 blocks in the moment matrix $\mathbf{M}_r$

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# Sign symmetry of the Hamiltonian

The Hamiltonian of the Heisenberg model is invariant under

$$(\sigma_i^x, \sigma_i^y, \sigma_i^z)_{i=1}^N \longrightarrow (-\sigma_i^x, \sigma_i^y, \sigma_i^z)_{i=1}^N$$

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☞ Yield $y_u = 0$ if $\mathrm{NF}(u)$ is variant under the above transformations

# Translation symmetry

- Periodic boundary condition: $x_{i+N} = x_i$
- Translation symmetry: $(x_1, \ldots, x_N) \to (x_{1+k}, \ldots, x_{N+k})$

☞ Yield a block structure on the moment matrix $\widetilde{\mathrm{M}}_r$ where each block is an Hermitian circulant matrix ($\mathcal{B}_r$ appropriately sorted)

☞ Every Hermitian circulant matrix can be diagonalised by a discrete Fourier transform:

$$P_{i,j} = \frac{1}{\sqrt{N}} e^{-2\pi \mathbf{i}(i-1)(j-1)/N}, \quad i, j = 1, \ldots, N$$

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# Permutation symmetry

• Permutation symmetry: The Hamiltonian $H_N$ is invariant under any permutation of $\{x, y, z\}$

☞ This yields

$$y_{\tau(\sigma_{i_1}^{a_1}\sigma_{i_2}^{a_2}\cdots\sigma_{i_r}^{a_r})} = y_{\sigma_{i_1}^{a_1}\sigma_{i_2}^{a_2}\cdots\sigma_{i_r}^{a_r}},$$

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# Mirror symmetry

- Consider 2D Heisenberg model

$$H_N = \frac{1}{4} \sum_{a=x,y,z} \sum_{i=1}^{L} \sum_{j=1}^{L} \sigma^a_{(i,j)} \left( \sigma^a_{(i+1,j)} + \sigma^a_{(i,j+1)} \right)$$

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$$\omega : (i,j) \longrightarrow (j,i)$$

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$$y_{\omega(u)} = y_u$$

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# Ground state energy of the Heisenberg chain

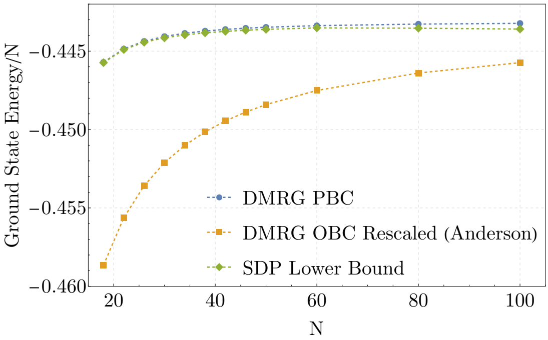


图: Ground state energy of the Heisenberg chain

# Certifying any observable at the ground state

- For any observable $O(\mathbf{x})$ at the ground state:

$$o_{\mathrm{lb}} := \begin{cases} \min\limits_{\{|\psi\rangle,\mathbf{x}\}} & \langle\psi|O(\mathbf{x})|\psi\rangle \\ \text{s.t.} & g_i(\mathbf{x}) \succeq 0, \quad i = 1,\ldots,m \\ & \langle\psi|E_{\mathrm{ub}} - H_N(\mathbf{x})|\psi\rangle \geq 0 \\ & \langle\psi|H_N(\mathbf{x}) - E_{\mathrm{lb}}|\psi\rangle \geq 0 \end{cases}$$

☞ Obtain $o_{\mathrm{GS}} \in [o_{\mathrm{lb}}, o_{\mathrm{ub}}]$

# First-neighbour spin correlations

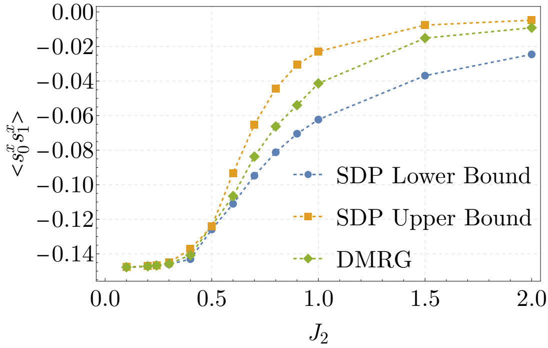


图: First-neighbour spin correlations in the $J_1$-$J_2$ Heisenberg chain for all values of $J_2$ and $N = 40$

# Spin-spin correlation at the ground state

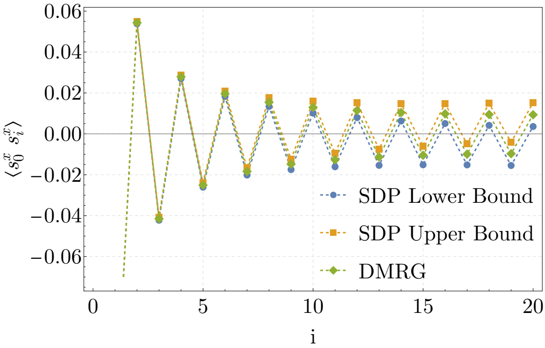


图: Spin-spin correlation in the $J_1$-$J_2$ Heisenberg chain for $J_2 = 0.2$ and $N = 40$

# Our paper

☞ **Jie Wang**, Jacopo Surace, Irénée Frérot, Benoît Legat, Marc-Olivier Renou, Victor Magron, and Antonio Acín, Certifying Ground-State Properties of Many-Body Systems, arXiv:2310.05844, 2023.

# Thank You!

https://wangjie212.github.io/jiewang