Exact diagonalizations of SU(N) Heisenberg models taking full advantage of SU(N) symmetry

F. Mila
Ecole Polytechnique Fédérale de Lausanne
Switzerland

Collaborators: P. Nataf (Lausanne)
P. Corboz (Amsterdam), A. Läuchli (Innsbruck), K. Penc (Budapest)
M. Lajko (ISSP), M. Troyer (Zürich)
T. Toth and J. Dufour (Lausanne), L. Messio (Paris)
Scope

- Introduction: **SU(N) models** in condensed matter and in ultra-cold atoms
- SU(3) and SU(4) on various 2D lattices
  - color order, VBS, algebraic liquid,…
- SU(N) for N>4
  - how to work in irreps of SU(N)
  - SU(5), SU(8) and SU(10) on square lattice
- Conclusions
Quantum permutations

- Objects with N flavours on a lattice
- Hilbert space = \{ | \sigma_1 \sigma_2 \ldots \sigma_L > \}
  \sigma_i = 1,2, ..., N or \sigma_i = A, B, C, ..., or \( \bullet, \circ, \bigcirc \ldots \)

\[
H = \sum_{\langle i,j \rangle} P_{ij}
\]

\[
P_{ij} | \sigma_1 \ldots \sigma_i \ldots \sigma_j \ldots \sigma_L > = | \sigma_1 \ldots \sigma_j \ldots \sigma_i \ldots \sigma_L >
\]
SU(N) formulation

\[ H = \sum_{\langle i,j \rangle} S^m_n(i) S^n_m(j) \]

\[ S^n_m |\mu\rangle = \delta_{n,\mu} |m\rangle \]

\[ [S^m_n, S^l_k] = \delta_{n,k} S^l_m - \delta_{m,l} S^n_k \]

→ generators of SU(N)

At each site: fundamental N-dimensional representation
Physical realizations I

Magnetic insulators

- N=2 → spin-1/2 Heisenberg
  \[ P_{ij} = 2\vec{S}_i \cdot \vec{S}_j + 1/2 \]

- N=3 → S=1 biquadratic
  \[ P_{ij} = \vec{S}_i \cdot \vec{S}_j + (\vec{S}_i \cdot \vec{S}_j)^2 - 1 \]

- N=4 → symmetric Kugel-Khomskii model
  \[ H = \sum_{ij} J_{ij} \left( 2\vec{s}_i \cdot \vec{s}_j + \frac{1}{2} \right) \left( 2\vec{\tau}_i \cdot \vec{\tau}_j + \frac{1}{2} \right) \]
Mott phases of ultracold atoms

Density profile of $^{133}\text{Cs}$ in an optical lattice with a harmonic trap $\rightarrow$ wedding cake structure

Gemelke et al, Nature 2009
Physical realizations II

N-flavour fermions in optical lattice
\((^{40}\text{K}, \, ^{87}\text{Sr}, \ldots)\)

N-flavour Hubbard model

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\alpha=1}^{N} (c_i^\dagger \sigma_{i,j,\alpha} c_{j,\alpha} + h.c.) + U \sum_{i} \sum_{(\alpha,\beta)} n_{i,\alpha} n_{i,\beta}
\]

\(1/N\) filling \(\downarrow\) 1 fermion per site

\[
\mathcal{H} = \frac{2t^2}{U} \sum_{\langle i,j \rangle} P_{ij}
\]
General properties

- Soluble in 1D with Bethe Ansatz
  → algebraic correlations with periodicity $2\pi /N$
  Sutherland, 1974

- Equivalent of SU(2) dimer singlet: N sites

$$| S > = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \left| \sigma_{P(1)} \sigma_{P(2)} \ldots \sigma_{P(N)} \right>$$

with $\{ \sigma_1 \sigma_2 \ldots \sigma_N \} = \{1, 2 \ldots N\}$

Li, Ma, Shi, Zhang, PRL’98
Mean-field approximation

\[ |\psi\rangle = \prod_i |\varphi_i\rangle \]

\[ \langle \varphi_1 \varphi_2 | P_{12} | \varphi_1 \varphi_2 \rangle = \langle \varphi_1 \varphi_2 | \varphi_2 \varphi_1 \rangle = |\langle \varphi_1 | \varphi_2 \rangle|^2 \]

→ on 2 sites, energy minimal if \( \langle \varphi_1 | \varphi_2 \rangle = 0 \)

→ on a lattice, MF energy certainly minimal if colors on nearest neighbors are different
SU(N) in 2D: methods

- Linear flavor wave theory
  - fluctuations around mean-fied solutions
- Exact diagonalizations
  - exact results on small clusters
- iPEPS (tensor-network algorithm)
  - 2D extension of PEPS formulation of DMRG
- Gutzwiller projected fermionic wfs
  - variational Monte Carlo
SU(N) in 2D: results for N=3 and 4

- Long-range color order
  → SU(3) on triangular and square lattice

- Plaquette order
  → SU(3) on kagome, honeycomb,…

- Dimerization + long-range order
  → SU(4) on square lattice

- Algebraic order
  → SU(4) on honeycomb
Long-range color order

SU(3) Triangular lattice

3-sublattice order

SU(3) Square lattice

A B A B
B A B A
A B A B

Infinite degeneracy
A, B \rightarrow C

Selection by zero-point fluctuations

Tsunetsugu, Arikawa, JPSJ 2006
A. Läuchli, FM, K. Penc, PRL 2006

T. Toth, A. Läuchli, FM, K. Penc, PRL 2010
Plaquette order

SU(3)

P. Corboz, M. Lajko, K. Penc, FM, A. Läuchli, PRB 2013

SU(4)

M. Van Den Bossche, P. Azaria, P. Lecheminant, FM, PRL 2001

D. Arovas, PRB 2008; P. Corboz, K. Penc, FM, A. Läuchli, PRB 2012
SU(4) on square lattice

iPEPS $\rightarrow$ Spontaneous dimerization

Dimerized ground state $+$ Néel order

SU(4) on honeycomb lattice

- No color order, no bond-energy order
- Good variational wave function with $\pi$-flux per plaquette
  $\rightarrow$ algebraic quantum liquid

P. Corboz, M. Lajko, A. Läuchli, K. Penc, FM, PRX 2012
SU(N) in 2D for larger N

- 2D-DMRG, iPEPS: difficult to converge
- ED: Hilbert space too large
  - SU(10) on 20 sites
    - Hilbert space: \(10^{20}\)
    - Sector AABBC... + lattice symmetries
    - \(\rightarrow 2.1 \times 10^{14}\)
    - Singlet sector: 16'796 states only!
- Try to work directly in irreps of SU(N)
Logical way to proceed

- Use Clebsch-Gordan coefficients to build a basis of a given irrep
- Determine the Hamiltonian in this basis
  - very cumbersome
  - not attempted so far for ED
  - not necessary!
ED in the irreps of SU(N)

Construct the Hamiltonian matrix without explicitly constructing the basis
Alfred Young’s papers on $S_n$

1) On quantitative substitutional analysis
   Proc. London Math. Soc. 1900
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1) On quantitative substitutional analysis
   Proc. London Math. Soc. 1900

2) On quantitative substitutional analysis (second paper)
   Proc. London Math. Soc. 1902
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   Proc. London Math. Soc. 1900

2) On quantitative substitutional analysis (Second Paper)
   Proc. London Math. Soc. 1902

8) On quantitative substitutional analysis (Eighth Paper)
   Proc. London Math. Soc. 1933
ON QUANTITATIVE SUBSTITUTIONAL ANALYSIS

(Sixth Paper).

By Alfred Young.

[Received and read 18 June, 1931.]

This paper is a continuation of the fourth paper in the series*. In the first paragraph a second proof of Theorem II in that paper is given. Section 2 gives a proof of Frobenius’ generating function for the characters of the symmetric group by the methods of this analysis—a proof which I believe throws light on its nature.
Standard tableaux I

- irrep of SU(N): Young tableau
- Multiplicity of an irrep = number of standard tableaux
- Permutation between consecutive integers
  \( \rightarrow \) same line: only diagonal, +1
  \( \rightarrow \) same column: only diagonal, -1
Standard tableaux II

→ Not on the same line or column:
2 x 2 matrix for standard tableaux connected by the permutation

\[
\begin{pmatrix}
-\rho & \sqrt{1 - \rho^2} \\
\sqrt{1 - \rho^2} & \rho
\end{pmatrix}
\]

\(\rho = 1/\text{axial distance}\)

- Non-consecutive integers

\[
\tau_{i,j} = \tau_{i,i+1} \tau_{i+1,i+2} \cdots \tau_{j-1,j} \tau_{j-2,j-1} \cdots \tau_{i+1,i+2} \tau_{i,i+1}
\]
SU(5) on square lattice

LFWT

ED

ED

Tower of states

5-sublattice color order

P. Nataf, FM, PRL 2014
SU(8) on square lattice

Spontaneous dimerization

P. Nataf, FM, PRL 2014
SU(10) on square lattice

Low-lying singlets (as in S=1/2 kagome) → Quantum liquid?

P. Nataf, FM, PRL 2014
Conclusions

- SU(N) on simple 2D lattices
  - color order
  - singlet plaquettes
  - spontaneous dimerization
  - algebraic order
  - ...

Perspectives

- Use the basis of the irreps of SU(N) for other methods: DMRG, iPEPS,…
- Investigate other SU(N) models
  - antisymmetric representation with several fermions per site
- Look for more exotic quantum GS
  - chiral spin liquid?