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

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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 = $\{|\sigma_1\ \sigma_2 \ldots\ \sigma_L\rangle\}$

  $\sigma_i = 1,2, \ldots,N$ or σ_i = A, B, C,… or 

$$\mathcal{H} = \sum_{\langle i,j \rangle} P_{ij}$$

$P_{ij}|\sigma_1 \ldots \sigma_i \ldots \sigma_j \ldots \sigma_L\rangle = |\sigma_1 \ldots \sigma_j \ldots \sigma_i \ldots \sigma_L\rangle$

SU(N) formulation

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

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

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

S^n_m → generators of SU(N)

At each site: fundamental N-dimensional representation

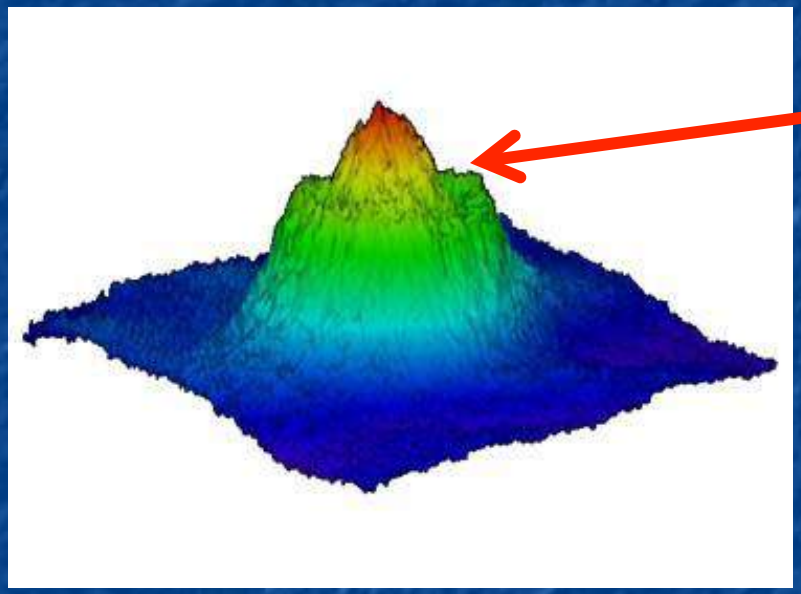
Physical realizations I

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



Mott insulating phase

Density profile of ^{133}Cs in an optical lattice with a harmonic trap → wedding cake structure

Gemelke et al, Nature 2009

Physical realizations II

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

N-flavour Hubbard model

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

1/N filling ↓ 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

$$|S\rangle = (1/\sqrt{N!}) \Sigma_P (-1)^P |\, \sigma_{P(1)}\, \sigma_{P(2)} \ldots \sigma_{P(N)} \rangle$$

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

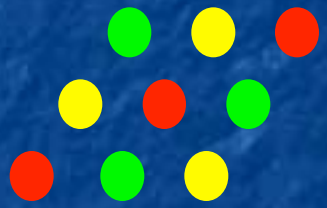
- Linear flavor wave theory
  → fluctuations around mean-fied solutions
- Exact diagonalizations
  → exact results on small clusters
- iPEPS (tensor-network algorithm)
  → 2D extension of PEPS formulation of DMRG
- Gutzwiller projected fermionic wfs
  → variational Monte Carlo

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

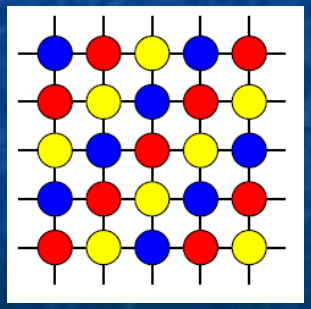
Tsunetsugu, Arikawa, JPSJ 2006
A. Läuchli, FM, K. Penc, PRL 2006

SU(3) Square lattice

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

Infinite degeneracy
A, B → C

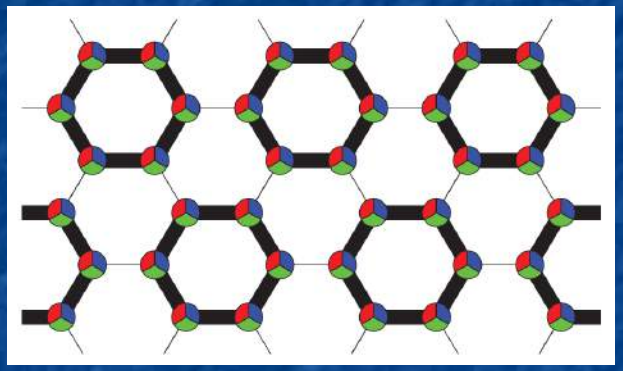
Selection by zero-point fluctuations



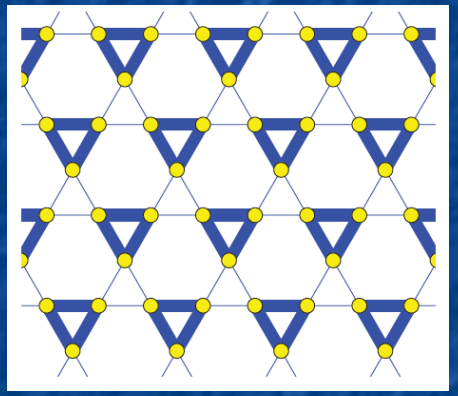
T. Toth, A. Läuchli, FM, K. Penc, PRL 2010

Plaquette order

SU(3)



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

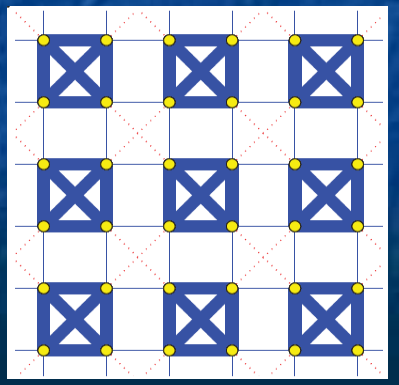


D.Arovas, PRB 2008; P. Corboz, K. Penc, FM, A. Läuchli, PRB 2012

SU(4)



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

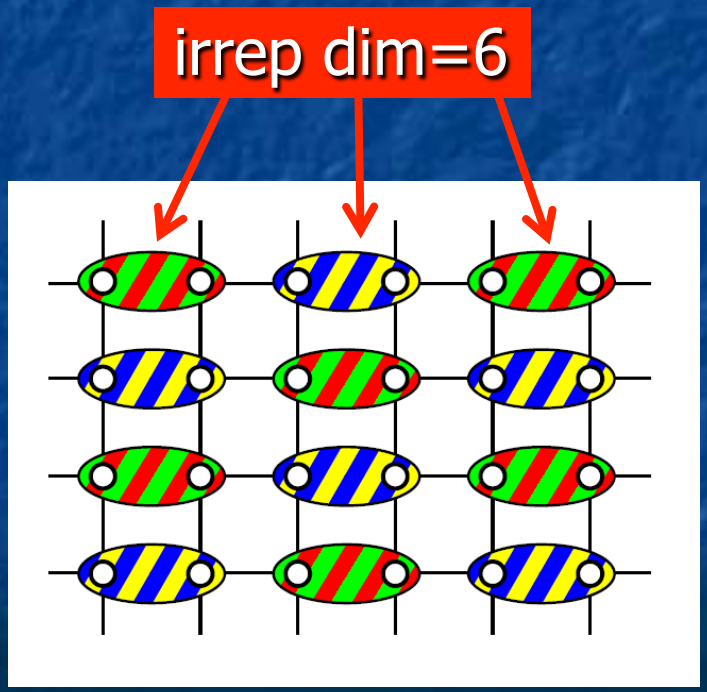


SU(4) on square lattice

iPEPS → Spontaneous dimerization



P. Corboz



Dimerized ground state

+ Néel order

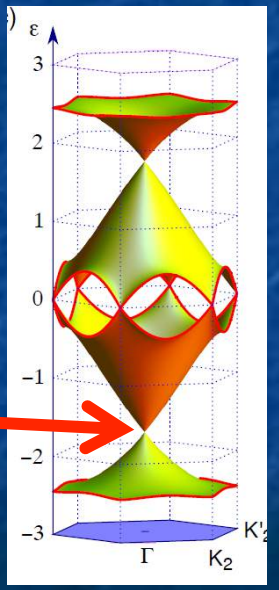
P. Corboz, A.Läuchli, K. Penc,
M. Troyer, FM, PRL 2011

SU(4) on honeycomb lattice

- No color order, no bond-energy order
- Good variational wave function with π-flux per plaquette

  → algebraic quantum liquid

Dirac point at quarter filling



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 AABBCC… + lattice symmetries

  → 2.1×10^{14}

  Singlet sector: 16'796 states only!
- Try to work directly in irreps of SU(N)

Logical way to proceed

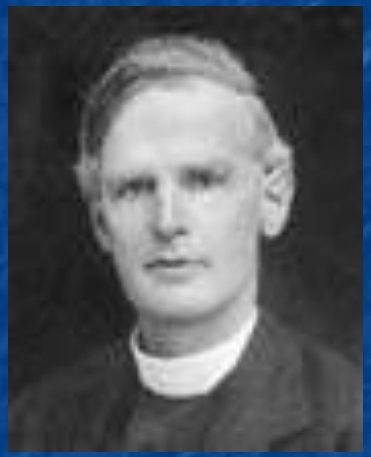
- Use Clebsch-Gordan coefficients to build a basis of a given irrep
- Determine the Hamiltonian in this basis

  → very cumbersome

  → not attempted so far for ED

  → not necessary!

ED in the irreps of SU(N)



Alfred Young



Pierre Nataf

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

Alfred Young's papers on S_n

1) On quantitative substitutional analysis

Proc. London Math. Soc. 1900

2) On quantitative substitutional analysis (second paper)

Proc. London Math. Soc. 1902

Alfred Young's papers on S_n

1) On quantitative substitutional analysis

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).

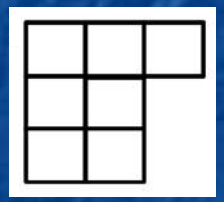
By ALFRED YOUNG.

[Received and read 18 June, 1931.]

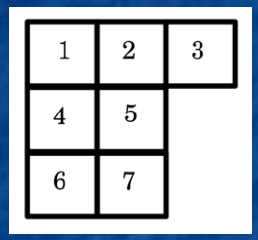
This paper is a continuation of the fourth paper in the series*. In the first paragraph a second proof of Theorem II in that paper is given. Section 2 gives a proof of Frobenius' generating function for the characters of the symmetric group by the methods of this analysis—a proof which I believe throws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

Standard tableaux I

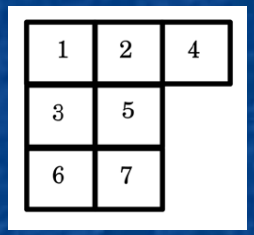
- irrep of SU(N): Young tableau



- Multiplicity of an irrep
  = number of
  standard tableaux



,



...

- Permutation between consecutive integers
  → same line: only diagonal, +1
  → 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

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

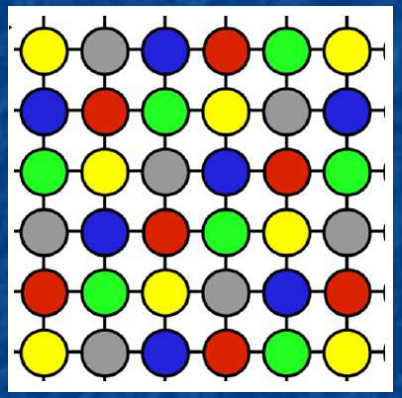
ρ=1/axial distance

- Non-consecutive integers

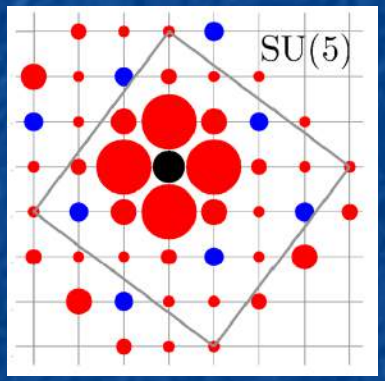
$$\tau_{i,j} = \tau_{i,i+1}\tau_{i+1,i+2}\cdots\tau_{j-1,j}\tau_{j-2,j-1}\cdots\tau_{i+1,i+2}\tau_{i,i+1}$$

SU(5) on square lattice

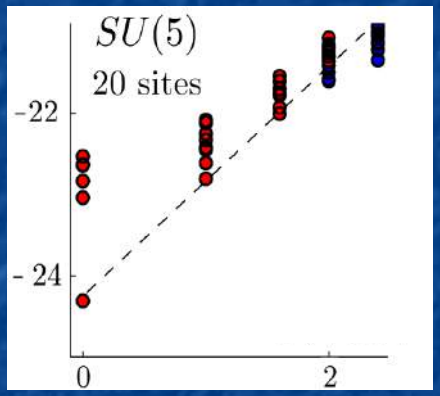
LFWT



ED



ED

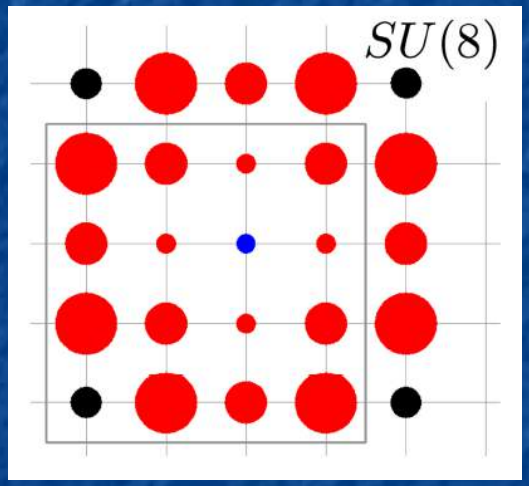


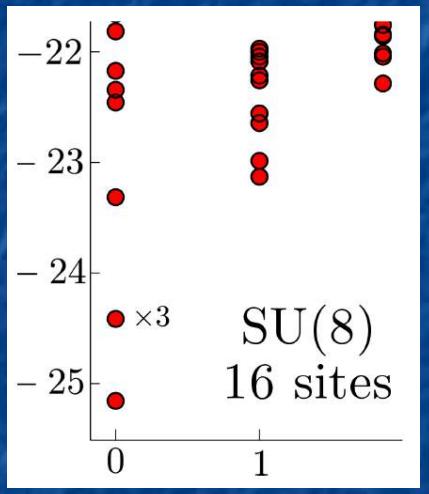
Tower of states

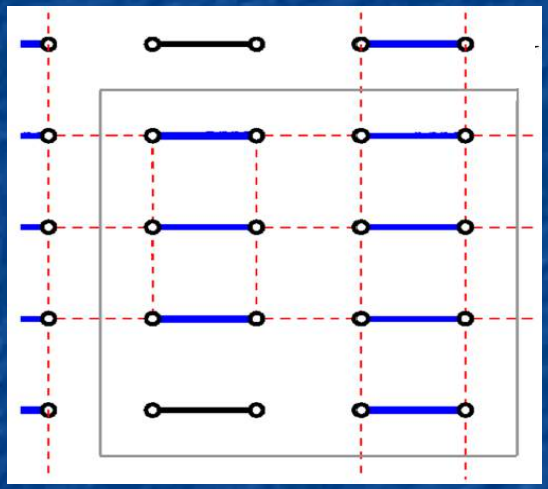
5-sublattice color order

P. Nataf, FM, PRL 2014

SU(8) on square lattice



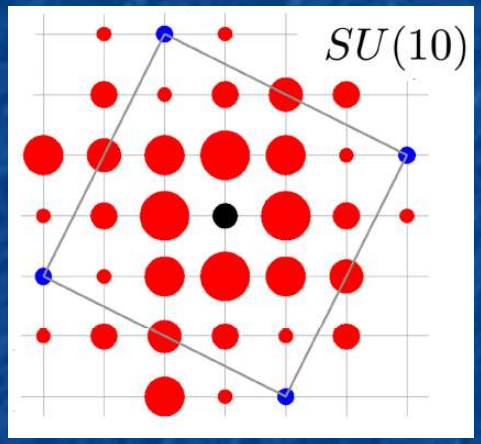


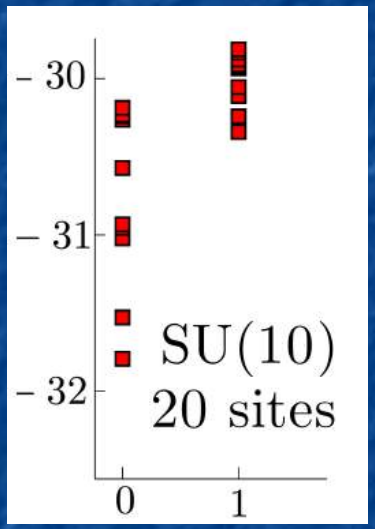


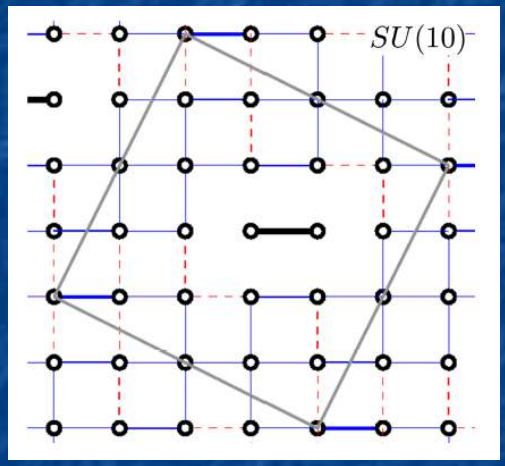
Spontaneous dimerization

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?