# SU(N) symmetry broken states with long range order in 2D

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## What are the SU(N) symmetric Heisenberg models that we are interested in?





N species on each site that are treated equally.

 $\mathcal{P}_{ij}|\beta_i\alpha_j\rangle = |\alpha_i\beta_j\rangle$ 

simplest example: SU(2) S=1/2 (fundamental representation) [but not the S=1 !]

## What are the SU(N) symmetric Heisenberg models that we are interested in?

$$\mathcal{P}_{i,j} | \begin{array}{c} & \longrightarrow \\ \mathbf{j} & \mathbf{j} \\ \mathbf{S}_1 \cdot \mathbf{S}_2 = S_1^z S_2^z + \frac{1}{2} \left( S_1^+ S_2^- + S_1^- S_2^+ \right) \right)$$

$$\mathbf{S}_{1} \cdot \mathbf{S}_{2} |\uparrow\uparrow\rangle = \frac{1}{4} |\uparrow\uparrow\rangle \qquad \rightarrow \qquad \left(2\mathbf{S}_{1} \cdot \mathbf{S}_{2} + \frac{1}{2}\right) |\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle$$
$$\mathbf{S}_{1} \cdot \mathbf{S}_{2} |\uparrow\downarrow\rangle = -\frac{1}{4} |\uparrow\downarrow\rangle + \frac{1}{2} |\downarrow\uparrow\rangle \qquad \rightarrow \qquad \left(2\mathbf{S}_{1} \cdot \mathbf{S}_{2} + \frac{1}{2}\right) |\uparrow\downarrow\rangle = |\downarrow\uparrow\rangle$$

For the S = 1/2 fundamental representation of the SU(2):

$$\left(2\mathbf{S}_1\cdot\mathbf{S}_2+\frac{1}{2}\right)=\mathcal{P}_{1,2}$$

#### Single-atom-resolved fluorescence imaging of an atomic Mott insulator

Jacob F. Sherson et al., Nature 467, 68 (2010)



#### also

Probing the Superfluid–to–Mott Insulator Transition at the Single-Atom Level W. S. Bakr *et al.*, Science **329**, 547 (2010)

SU(3): Competing spin and quadrupolar ordering in spin models (NiGa<sub>2</sub>S<sub>4</sub>?)

$$\begin{aligned} & \langle \mathbf{x} \rangle &= \frac{i}{\sqrt{2}} \left( |1\rangle - |\overline{1}\rangle \right) \\ & \langle \mathbf{y} \rangle &= \frac{1}{\sqrt{2}} \left( |1\rangle + |\overline{1}\rangle \right) \\ & \langle \mathbf{z} \rangle &= -i|0\rangle \end{aligned}$$
 
$$\hat{\mathbf{Q}}_i \hat{\mathbf{Q}}_j = 2 \left( \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j \right)^2 + \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j - 8/3$$

bilinear-biquadratic Heisenberg model for S=1 spins:

$$\mathcal{H} = J \sum_{i,j} \left[ \cos \vartheta \mathbf{S}_i \mathbf{S}_j + \sin \vartheta \left( \mathbf{S}_i \mathbf{S}_j \right)^2 \right] - h \sum_i S_i^z$$

Increased SU(3) symmetry at  $\vartheta = \pi/4$ :

$$\hat{\mathbf{Q}}_i \hat{\mathbf{Q}}_j + \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j = -2\mathcal{P}_{i,j} - \frac{2}{3}$$

all the 3 states of the S=1 spin become identical

## What methods do we use?

(i) Variational – site factorized wave function
(ii) Flavor wave calculations
(iii) Exact diagonalization of small clusters
(iv) iPEPS: infinite project entangled pair states(variational approach based on tensor ansatz)
(v) Variational – Gutzwiller projected fermionic wave functions

# Triangular lattice, S=1 and SU(3)



. .

even (symmetrical)

even (symmetrical)

## SU(3) irreps on 3 sites

Addition of three SU(3) spins (27 states):

$$3 \times 3 \times 3 = 1 + 2 \times 8 + 10$$
$$\square \otimes \square \otimes \square = \square \oplus 2 \times \square \oplus \square$$

SU(3) singlet

$$= |ABC\rangle + |CAB\rangle + |BCA\rangle - |BAC\rangle - |ACB\rangle - |BCA\rangle$$
  
spins fully antisymmetrized



in the SU(3) singlet the spins are fully entangled: we cannot write it in a product form

## Variational (classical) approach

a site-product wave function for e.g. SU(3):

$$\begin{split} |\Psi\rangle &= \prod_{i} |\psi_{i}\rangle \\ |\psi_{i}\rangle &= d_{A,i} |A\rangle_{i} + d_{B,i} |B\rangle_{i} + d_{C,i} |C\rangle_{i} \end{split}$$

$$E_{\text{var}} = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = J \sum_{\langle i, j \rangle} \left| \mathbf{d}_i \cdot \bar{\mathbf{d}}_j \right|^2$$

minimal, when the  $\boldsymbol{d}_i$  and  $\boldsymbol{d}_j$  on the bond are orthogonal different colors on a bond



## The fate of SU(3) on triangular lattice SU(2) frustrated!



crystal of singlets?



### "classical" solution?

SU(3) classical state is perfectly happy on the triangular lattice - the 3 mutually perpendicular **d**'s form a 3 sublattice structure.

H. Tsunetsugu and M. Arikawa, J. Phys. Soc. Jpn. **75**, 083701 (2006) [NiGa2S4, Nakatsuji]

A. M. Läuchli, F. Mila, and K. Penc, Phys. Rev. Lett. 97, 087205 (2006)

### Phase diagram

### mean field

 $\langle \hat{\mathbf{Q}}_i \cdot \hat{\mathbf{Q}}_j \rangle = 2(\mathbf{d}_i \cdot \mathbf{d}_j)^2 - \frac{2}{3} \quad \begin{array}{l} \text{max., if } \mathbf{d}_i \ \text{II} \ \mathbf{d}_j \\ \text{min., if } \mathbf{d}_i \perp \mathbf{d}_j \end{array}$ 

### exact diagonalization



PRL 97, 087205 (2006)

### SU(3) on triangular lattice - exact diagonalization



Signature of SU(3) breaking in the excitation spectrum: Anderson tower compatible with 3 sublattice order

C2 - Casimir operator, analog of the total spin S^2

K. Penc, A. M. Läuchli, in <u>Introduction to Frustrated</u> <u>Magnetism', p. 331-362</u>, Springer Series in Solid-State Sciences, Vol. **164**, eds. C. Lacroix, F. Mila, and P. Mendels (Springer, 2011)

## SU(3) flavour-wave theory

N. Papanicolaou, Nucl. Phys. B **305**, 367 (1988) A. Joshi *et al.* PRB **60**, 6584 (1999)



We enlarge the fundamental to the fully symmetric representation of M boxes.

States in the fully symmetric multiplet can be represented by 3 Schwinger bosons  $a_A, a_B$  and  $a_C$ 

$$a_{A,i}^{\dagger}a_{A,i} + a_{B,i}^{\dagger}a_{B,i} + a_{C,i}^{\dagger}a_{C,i} = M$$

$$\mathcal{P}_{ij} = \sum_{\mu,\nu\in\{A,B,C\}} a^{\dagger}_{\mu,i} a^{\dagger}_{\nu,j} a_{\nu,i} a_{\mu,j}$$

The site product wave function is the "classical"

solution (no quantum entanglement between sites)

 $|\Psi
angle = \prod_i |\psi_i
angle$ 

$$\psi_i \rangle = d_{A,i} |A\rangle_i + d_{B,i} |B\rangle_i + d_{C,i} |C\rangle_i$$

cf. SU(2) spin coherent state for SU(2)  $|\vartheta,\varphi\rangle = \cos\frac{\vartheta}{2}|\uparrow\rangle + \sin\frac{\vartheta}{2}e^{i\varphi}|\downarrow\rangle$ 

### SU(3) flavour-wave theory

$$\mathcal{P}_{ij} = \sum_{\mu,\nu \in \{A,B,C\}} a^{\dagger}_{\mu,i} a^{\dagger}_{\nu,j} a_{\nu,i} a_{\mu,j}$$

1/M expansion:

$$\begin{split} \tilde{a}_{A}^{\dagger}, \tilde{a}_{A} &\to \sqrt{M - \tilde{a}_{B}^{\dagger} \tilde{a}_{B} - \tilde{a}_{C}^{\dagger} \tilde{a}_{C}} \\ &\to \sqrt{M} - \frac{1}{2\sqrt{M}} \begin{pmatrix} \tilde{a}_{B}^{\dagger} \tilde{a}_{B} + \tilde{a}_{C}^{\dagger} \tilde{a}_{C} \end{pmatrix} + \dots \\ & \bullet & \bullet \\ & \bullet & \bullet \\ \end{split}$$
Holstein-Primakoff  $\mathcal{H} = (a^{\dagger} + b)(a + b^{\dagger})$ 

quadratic in operators: we know how to diagonalize it (spin wave)

$$\mathcal{H} = -MJL + M\sum_{\nu}\sum_{\mathbf{k}}\omega_{\nu}(\mathbf{k})\left(\alpha_{\nu}^{\dagger}(\mathbf{k})\alpha_{\nu}(\mathbf{k}) + \frac{1}{2}\right)$$



Structure factors in S=1 bilinear-biquadratic Heisenberg model QMC (A. Völl and S. Wessel) Phys. Rev. B **91**, 165128 (2015)



FIG. 5. (Color online) Dynamical spin and quadrupolar structure factors  $S_S(\omega, q)$  and  $S_Q(\omega, q)$  for different values of  $\theta$  along the path  $\Gamma \to K \to M \to \Gamma$  through the Brillouin zone  $[\Gamma = (0,0)^{\mathsf{T}}, K = (4\pi/3,0)^{\mathsf{T}}, M = (2\pi/3,\pi/\sqrt{3})^{\mathsf{T}}]$ . The dashed lines indicate the quadrupolar wave dispersion relations obtained within flavor-wave  $10^{-\text{theory.}}$ 

# Triangular lattice, SU(4)

### SU(4) on triangular lattice - exact diagonalization





Signature of SU(4) breaking in the excitation spectrum: Anderson tower compatible with 4 sublattice order for large enough second neighbor J'

C2 - Casimir operator, analog of the total spin S^2



K. Penc, M. Mambrini, P. Fazekas, F. Mila, Phys. Rev. B **68**, 012408 (2003)

# Square lattice, SU(3)

## SU(3) square lattice, classical solutions: macroscopically degenerate





All bonds happy at the mean field level, frustration due to abundance of choices

Order by disorder: the zero point energy of the quantum fluctuations over a mean field solution selects the ground state

$$E_{ZP} = \frac{M}{2} \sum_{\nu} \sum_{\mathbf{k}} \omega_{\nu}(\mathbf{k})$$

### SU(3) flavour-wave: helical states



 $q=\pi$  2-sublattice  $q=2\pi/3$  3-sublattice

### SU(3) flavour-wave theory: 1/M expansion

quadratic in operators  $\rightarrow$  we know how to diagonalize it (spin wave)

$$\mathcal{H} = -MJL + M\sum_{\nu}\sum_{\mathbf{k}}\omega_{\nu}(\mathbf{k})\left(\alpha_{\nu}^{\dagger}(\mathbf{k})\alpha_{\nu}(\mathbf{k}) + \frac{1}{2}\right)$$

Order by disorder: if classically degenerate, quantum fluctuations decide the winner

$$E_{ZP} = \frac{M}{2} \sum_{\nu} \sum_{\mathbf{k}} \omega_{\nu}(\mathbf{k})$$

### SU(3) flavour-wave: helical dispersion, zero-point energy



### structure of the flavor wave Hamiltonian



$$\begin{aligned} \mathcal{H} &= & \qquad \mathbf{a} \\ &+ (a^{\dagger} + b)(b^{\dagger} + a) \\ &+ (b^{\dagger} + c)(c^{\dagger} + b) \end{aligned} \qquad \begin{array}{c} \mathbf{b} \\ \mathbf{c} \end{aligned}$$

disconnected (commuting) terms, each of them gives  $E_{ZP} = 0$ 

the connected term gives  $E_{ZP} > 0$ 

fluctuation energy minimal if next nearest neighbor spins are also of different color





### SU(2) coupled chains



decoupled SU(2) spin chain: Luttinger liquid with a spinon continuum



coupled SU(2) spin chain: antiferromagnetic LRO, with magnons as bound states developing from the lower edge of the continuum

KCuF3







ladder in field

## SU(3) coupled chains







decoupled SU(3) spin chain: Luttinger liquid, excitations form a continuum

softening at 2Pi/3 leads to 3 sublattice LRO for the coupled SU(3) chains?



# Square lattice, SU(4)



 $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$  triplet even (symmetrical) comb.

even (symmetrical).

## SU(4) irreps on 4 sites

Addition of four SU(4) spins (256 states):



## SU(4) ladder

# GS twofold degenerate (translational invariance broken):



gapped excitation spectrum, situation similar to  $J_1-J_2$  SU(2) Heisenberg chain:



M. van den Bossche et al., Phys. Rev. Lett. **86**, 4124 (2001).





Exact diagonalization, 16 sites

M. van den Bossche et al., Eur. Phys. J. B **17**, 367 (2000).

## SU(4) on 2D-square lattice: iPEPS

iPEPS: infinite project entangled pair states



D = 12 and a unit cell  $4 \times 2$ 

dimerization and Neel-like state: both spatial and the SU(4) symmetry is broken



the 6 dimensional irreducible representation is realized on the dimers, can Neel order

### 2-step scenario:

- (i) Dimerization: 6-dimensional irreps are formed
- (ii) the 6-imensional irreps can possibly Néel order

P. Corboz, A. M. Läuchli, K. Penc, M. Troyer, F. Mila, PRL **107**, 215301 (2011).

## SU(4) on square lattice: 2 step scenario

### 2-step scenario:

- (i) Dimerization: **6**dimensional irreps are formed
- (ii) the antipodal pairs in the 6-imensional irreps can possibly Néel order Sublattice  $\Lambda_{\overline{AB}}$





Sublattice  $\Lambda_{\overline{CD}}$ 

P. Corboz, A. M. Läuchli, K. Penc, M. Troyer, F. Mila, PRL 107, 215301 (2011).

## SU(4) 6-dim irrep on square lattice



## SU(4) 6-dim irrep on square lattice



$$R_{\text{Spin}}(L) = 1 - \frac{S_{\text{Spin}}(\mathbf{Q} - (0, 2\pi/L))}{S_{\text{Spin}}(\mathbf{Q})}.$$

changing the anisotropy (decreasing the coupling between the chains), there is a phase transition between the VBS and ordered state deconfined quantum critical point ?



# Honeycomb, SU(4)

### Lifting of the degeneracy in flavor wave theory



### iPEPS - local magnetization vanishes



P. Corboz, M. Lajkó, A. M. Läuchli, K. Penc, F. Mila: Phys. Rev. X **2**, 041013/1-11 (2012).

### iPEPS - dimerization vanishes



P. Corboz, M. Lajkó, A. M. Läuchli, K. Penc, F. Mila: Phys. Rev. X **2**, 041013/1-11 (2012).

## Summary of iPEPS results

- dimerization vanishes (actually no point group symmetry breaking)
- local magnetization vanishes (no SU(4) symmetry breaking)



spin-orbital liquid

How to characterize it?

## Fermionic mean-field

we use the fermionic 
$$\mathcal{P}_{ij} = \sum_{\mu,\nu \in \text{colors}} f^{\dagger}_{\alpha,i} f_{\beta,i} f^{\dagger}_{\beta,j} f_{\alpha,j}$$

$$\mathcal{P}_{ij}^{\mathrm{MF}} = \sum_{\alpha,\beta\in\mathrm{colors}} \langle f_{\beta,i} f_{\beta,j}^{\dagger} \rangle f_{\alpha,i}^{\dagger} f_{\alpha,j}$$
$$= -\sum_{\alpha\in\mathrm{colors}} t_{ij}^{\alpha} f_{\alpha,i}^{\dagger} f_{\alpha,j}$$

Mean-field decoupling of the fermionic Hamiltonian gives a hopping Hamiltonian and a variational wave function

$$|\Psi_{\mathrm{vari}}\rangle = P_{\mathrm{Gutzwiller}}|\Psi_{\mathrm{FS}}\rangle$$

Using different Ansätze for the hoppings, we evaluate the expectation value of the Hamiltonian

$$E_{\rm vari} = \frac{\langle \Psi_{\rm vari} | \mathcal{H} | \Psi_{\rm vari} \rangle}{\langle \Psi_{\rm vari} | \Psi_{\rm vari} \rangle}$$

The fermionic wave function of the pi-flux state



#### The fermionic wave function of the pi-flux state



Brillouin zone

two-fold degenerate bands

# 96-site cluster - real space correlations from Gutzwiller projected wavefunction



square lattice: F. Wang and A. Vishwanath, Phys. Rev. B **80**, 064413 (2009).

#### Ground state energy from different methods



#### 24-site cluster - real space correlations



Dimension of the Hilbert space is  $24!/(6!)^4 = 2308743493056$ using symmetries makes it tractable



#### Model for the metal-insulator transition in graphene superlattices and beyond

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(Received 27 March 2018; published 3 July 2018)

We propose a two-orbital Hubbard model on an emergent honeycomb lattice to describe the low-energy physics of twisted bilayer graphene. Our model provides a theoretical basis for studying metal-insulator transition, Landau level degeneracy lifting, and unconventional superconductivity that are recently observed.



#### Emergent SU(4) Symmetry in $\alpha$ -ZrCl<sub>3</sub> and Crystalline Spin-Orbital Liquids

Masahiko G. Yamada,<sup>1,\*</sup> Masaki Oshikawa,<sup>1</sup> and George Jackeli<sup>2,3,†</sup>



PHYSICAL REVIEW B 100, 205131 (2019)

#### SU(4) Heisenberg model on the honeycomb lattice with exchange-frustrated perturbations: Implications for twistronics and Mott insulators

W. M. H. Natori,<sup>1,2</sup> R. Nutakki,<sup>3</sup> R. G. Pereira,<sup>4</sup> and E. C. Andrade

# Triangular with ring exchange, SU(N)

### The model

Hubbard model with artificial flux:

$$H = -t \sum_{\langle i,j \rangle} \sum_{\alpha=1}^{N} (e^{\phi_{ij}} c_{i,\alpha}^{\dagger} c_{j,\alpha} + \text{H.c.}) + U \sum_{i,\alpha < \beta} n_{i,\alpha} n_{i_{\beta}}.$$

the effective low energy model includes ring exchange:

$$H = J \sum_{\langle i,j \rangle} P_{ij} + K_3 \sum_{(i,j,k)} (e^{i\Phi} P_{ijk} + \text{H.c.}),$$

$$J = 2t^2 / U_1 \quad K_3 = 6t^3 / U^2$$

The ground state is chiral: a gaped featureless liquid which breaks time reversal invariance

P. Nataf, M. Lajkó, A. Wietek, K. Penc, F. Mila, A. M. Läuchli: *Chiral spin liquids in triangular lattice SU(N) fermionic Mott insulators with artificial gauge fields* Phys. Rev. Lett. **117**, 167202/1-6 (2016)

#### Exact diagonalization vs. variational Monte Carlo





FIG. 3. Summed squared overlaps of the VMC model wave functions with ED eigenstates for N = 3 and  $N_s = 12$ . The blue crosses denote ED eigenstates, while the area of the filled red circles denotes the total squared overlap on those eigenstates. Around  $\theta/\pi \approx 0.25$ , the summed overlaps on the lowest three ED eigenstates (degeneracy 1 + 2) account for over 75% of the total weight, while the ground state alone is at 90%.

P. Nataf, et al., Phys. Rev. Lett. 117, 167202 (2016)

#### N-fold ground state degeneracy



FIG. 2. VMC ground space degeneracy: ordered sequence of eigenvalues of the overlap matrix of Gutzwiller projected wave functions with 30 random values of threaded flux. The overlap matrix has precisely N large eigenvalues for an SU(N) CSL.

P. Nataf, et al., Phys. Rev. Lett. 117, 167202 (2016)

#### spectrum of the edge modes



FIG. 4. Edge states in SU(N) CSLs: the leftmost panel displays the  $N_s = 19$  site triangular cluster with open boundary conditions used. In the various other panels we exhibit the low energy spectrum as a function of the angular momentum around the central site ( $l_0$ denotes the ground state angular momentum). The chiral edge states are clearly visible, with a characteristic SU(N) multiplet structure, which corresponds to a particular sector of a chiral  $SU(N)_1$  Wess-Zumino-Novikov-Witten conformal field theory. The analytical predictions are indicated by the dimensions of the SU(N) multiplets and can be found in Table I of the Supplemental Material [37].

P. Nataf, et al., Phys. Rev. Lett. 117, 167202 (2016)



frustrated

happy

resonating liquid

# Thank you for your attention!