Spin liquid phases in the SU(4) and SU(3) Heisenberg model on the honeycomb lattice

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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.

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\mathcal{P}_{ij}|\beta_i\alpha_j\rangle = |\alpha_i\beta_j\rangle
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simplest example: SU(2) S=1/2 (fundamental representation) [but not the S=1 !]

Why do we care about SU(N) Heisenberg models?

- (i) Spin models
- (ii) Spin-orbital models
- (iii) f-electron systems
- (iv) Cold alkaline-earth atoms in optical lattices

SU(4) highest symmetry of spin-orbital model (e.g. LiNiO₂ and NaNiO₂)



Spin-orbital models : Microscopic theory



+ the standard perturbation theory to get the effective Hamiltonian.

Spin-orbital models: Kugel-Khomskii Hamiltonian

$$\mathcal{H}_{ij} = -\frac{2}{\tilde{U}+2J_p} \left[2tt'\mathbf{T}_i\mathbf{T}_j - 4tt'T_i^yT_j^y + (t-t')^2(\mathbf{n}_{ij}^z\mathbf{T}_i)(\mathbf{n}_{ij}^z\mathbf{T}_j) + \frac{1}{2}(t^2 - t'^2)\left(\mathbf{n}_{ij}^z\mathbf{T}_i + \mathbf{n}_{ij}^z\mathbf{T}_j\right) + \frac{1}{4}(t^2 + t'^2) \right] \mathcal{P}_{ij}^{S=0} \\ -\frac{2}{\tilde{U}} \left[4tt'T_i^yT_j^y + \frac{1}{2}(t^2 + t'^2) + \frac{1}{2}(t^2 - t'^2)\left(\mathbf{n}_{ij}^z\mathbf{T}_i + \mathbf{n}_{ij}^z\mathbf{T}_j\right) \right] \mathcal{P}_{ij}^{S=0} \\ -\frac{2}{\tilde{U}-J_H} \left[-2tt'\mathbf{T}_i\mathbf{T}_j - (t-t')^2(\mathbf{n}_{ij}^z\mathbf{T}_i)(\mathbf{n}_{ij}^z\mathbf{T}_j) + \frac{1}{4}(t^2 + t'^2) \right] \mathcal{P}_{ij}^{S=1}$$

$$\mathcal{P}_{ij}^{S=0} = \frac{1}{4} - \mathbf{S}_i \mathbf{S}_j \qquad \qquad \mathcal{P}_{ij}^{S=1} = \mathbf{S}_i \mathbf{S}_j + \frac{3}{4}$$

For t=t' and $J_p=0$ $\mathcal{H}_{ij}=\frac{4t^2}{\tilde{U}}\left(\mathbf{T}_i\mathbf{T}_j+\frac{3}{4}\right)\left(\mathbf{S}_i\mathbf{S}_j-\frac{1}{4}\right)+\frac{4t^2}{\tilde{U}-J_H}\left(\mathbf{T}_i\mathbf{T}_j-\frac{1}{4}\right)\left(\mathbf{S}_i\mathbf{S}_j+\frac{3}{4}\right)$ SU(2)×SU(2) symmetric

t=t' and
$$J_p = J_H = 0$$

 $\mathcal{H}_{ij} = \frac{8t^2}{\tilde{U}} \Big(\mathbf{T}_i \mathbf{T}_j + \frac{1}{4} \Big) \Big(\mathbf{s}_i \mathbf{s}_j + \frac{1}{4} \Big) \sim \mathcal{P}_{ij}$ permutation
 $\mathcal{SU}(4)$ symmetric operator

SU(4) on honeycomb lattice

Motivation: Spin-Orbital Short-Range Order on a Honeycomb-Based Lattice

S. Nakatsuji^{1,*}, K. Kuga¹, K. Kimura¹, R. Satake², N. Katayama², E. Nishibori², H. Sawa², R. Ishii³, M. Hagiwara³, F. Bridges⁴, T. U. Ito⁵, W. Higemoto⁵, Y. Karaki⁶, M. Halim⁷, A. A. Nugroho⁷, J. A. Rodriguez-Rivera^{8,9}, M. A. Green^{8,9}, C. Broholm^{8,10}



Ba₃CuSb₂O₉

We consider the Kugel-Khomskii model for the S=1/2 and two Cu orbitals at the symmetric SU(4) point.

CeB_6 : almost SU(4) on cubic lattice





Anisotropic SU(4) spin wave treatment sufficient. (R. Shiina et al, J. Phys. Soc. Jpn. **66**, 1741 (1997)

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

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



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

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

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also

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

SU(6) Mott physics in cold atoms

An SU(6) Mott insulator of an atomic **Fermi** gas realized by large-spin Pomeranchuk cooling

Shintaro Taie, Rekishu Yamazaki, Seiji Sugawa & Yoshiro Takahashi

Nature Physics 8, 825-830 (2012) doi:10.1038/nphys2430





SU(2) vs. SU(3) – two sites $\mathcal{P}_{12}(|\alpha\beta\rangle - |\beta\alpha\rangle) = -(|\alpha\beta\rangle - |\beta\alpha\rangle) \quad \text{E}=-1$, odd wave function $\mathcal{H} = \mathcal{P}_{12} \quad \mathcal{P}_{12}(|\alpha\beta\rangle + |\beta\alpha\rangle) = +(|\alpha\beta\rangle + |\beta\alpha\rangle) \quad \text{E}=+1$, even wave function







 $|ac\rangle + |ca\rangle$, and $|bc\rangle + |cb\rangle$.

even (symmetrical)

 $\square |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle \text{ triplet}$ even (symmetrical)

SU(3) irreps on 3 sites

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

$$3 \times 3 \times 3 = 1 + 2 \times 8 + 10$$
$$\Box \otimes \Box \otimes \Box = = 2 \times 10 \oplus 2 \times 100 \oplus 100$$

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

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

Variational (classical) approach

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

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

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

minimal, when the \mathbf{d}_i and \mathbf{d}_j on the bond are orthogonal



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:

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

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

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

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, 087205/1-4 (2006)

SU(3) on triangular lattice - exact diagonalization



Signature of SU(3) breaking in the excitation spectrum: Anderson towers 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) square lattice, classical solutions: macroscopically degenerate

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









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



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

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

structure of the flavor wave Hamiltonian



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

each term separately $E_{ZP} = 0$

the 3-site term gives $E_{ZP} > 0$

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



SU(4) irreps on 4 sites

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



SU(4) irreps on 4 sites

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



SU(4) on 2D-square lattice



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



D = 12 and a unit cell 4×2

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) honeycomb: Lifting of the degeneracy in flavor wave theory

Basic building blocks: nearest (mean field) and next nearest (fluctuations) neighbor colors different.



Order by disorder does not work!



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Order by disorder does not work!





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



Summary of iPEPS results [SU(4) honeycomb]

- dimerization vanishes

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



spin-orbital liquid

How to characterize it?

fermionic representation:

 $\mathcal{P}_{ij} = \sum f_{\alpha,i}^{\dagger} f_{\beta,i} f_{\beta,i}^{\dagger} f_{\alpha,i}$ $\mu,\nu\in$ colors

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

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

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

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



two-fold degenerate bands

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

$$\langle S_{\bullet}S_{\delta}\rangle\propto \langle P_{\bullet,\delta}
angle-rac{1}{4}$$



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

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

$$\langle S_{\bullet}S_{\delta}\rangle\propto \langle P_{\bullet,\delta}
angle-rac{1}{4}$$



marked differences in 3rd neighbor correlations

Majoranna fermions for 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



comparison to 1D chains



comparison to 1D chains



Y. Yamashita, N. Shibata, K. Ueda Phys. Rev. B **58**, 9114-9118 (1998) Beat Frischmuth, Frederic Mila, Matthias Troyer Phys. Rev. Lett. **82**, 000835 (1999)



SU(4) honeycomb: Tetramerization



J_1-J_2 SU(4) honeycomb: Tetramerization



SU(3) honeycomb lattice: flavor wave

Lee and Yang,

Phys. Rev. B 85, 100402 (2012)



SU(3) honeycomb lattice: tensor network

S=1 bilinear-biquadratic model

H.H.Zhao,C.Xu,Q.N.Chen,Z.C.Wei, M.P.Qin,G.M. Zhang, and T. Xiang, Phys. Rev. B **85**, 134416 (2012).







SU(3) honeycomb lattice: projected fermions











Friday, June 14, 2013

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SU(3) honeycomb lattice: cartoon picture

Resonance of SU(3) singlets





SU(N) on honeycomb

SU(2) is a Néel state



SU(3) is a plaquette state

[Y.-W. Lee and M.-F. Yang, Phys. Rev. B **85**, 100402 (2012). H.H.Zhao,C.Xu,Q.N.Chen,Z.C.Wei,M.P.Qin,G.M. Zhang, and T. Xiang, Phys. Rev. B **85**, 134416 (2012).]

SU(4) is most probably an algebraic flavor liquid [P. Corboz, M. Lajkó, A. M. Läuchli, K. Penc, F. Mila, <u>arXiv:1207.6029</u>]



SU(6) is possibly a chiral flavor liquid [G. Szirmai E. Szirmai, A. Zamora, and M. Lewenstein, Phys. Rev. A **84**, 011611 (2011)], similarly, SU(N) is also a chiral liquid [extending the results of M. Hermele, V. Gurarie, & A. M. Rey, Phys. Rev. Lett. **103**, 135301 (2009)]

honeycomb optical lattices can be realized



the end thank you for your attention