Power-law correlated 2D SU(6) quantum paramagnets

Congjun Wu

Department of Physics, University of California, San Diego

Ref: Z. Cai, H. H. Hung, L. Wang, Yi Li, and C. Wu, arxiv:1207.6843.

Z. Cai, H. H. Hung, L. Wang, D. Zheng, and C. Wu, arxiv1202.6323.

C. Wu, Physics 3, 92 (2010).

Related past works:

C. Wu, J. P. Hu, and S. C. Zhang, Phys. Rev. Lett. 91, 186402 (2003).
C. Wu, Mod. Phys. Lett. B 20, 1707 (2006) (brief review).
H. H. Hung, Y. P. Wang, C. Wu, Phys. Rev. B 84, 054406 (2011).

KITP, Sept 18, Frustrated magnet workshop ¹

C	Collaborators
Zi Cai	(UCSD→Ludwig-
	Maximilians Univ.)
Hsiang-hsuan Hung	$(UCSD \rightarrow UIUC \rightarrow UT Austin)$
Yi Li	(UCSD)
Dong Zheng	(Tsinghua/UCSD \rightarrow industry
Lei Wang	(ETH, Zurich)
Collaborators on past related	d works: S. C. Zhang (Stanford), 🦂



Acknowledgments: J. Hirsch (UCSD), Y. Takahashi (Kyoto Univ.), Kivelson(Stanford), F. Zhou (UBC), T. L. Ho (OSU). Supported by AFOSR, NSF.

J. P. Hu (Purdue), S. Chen and Y. P. Wang (IOP, CAS).



<u>Outline</u>

• Introduction: a novel system for quantum magnetism.

Large hyperfine-spin ultra-cold alklai and alklaine-earth fermions in optical lattices.

Why they are interesting?

Large spin enhances rather than suppresses quantum spin fluctuations due to large symmetries of SU(2N), Sp(2N).

• Brief-review the generic Sp(4) symmetric in spin-3/2 systems – unification of AFM, SC and CDW.

http://online.kitp.ucsb.edu/online/coldatoms07/wu2/

• Evidence of power-law correlated spin-correlations of SU(6) Hubbard model at half-filling – a Quantum Monte-Carlo study.

• Thermodynamic properties of SU(6) Hubbard model: enhancement of Pomeranchuk cooling - QMC

Analytic and numeric efforts for spin-liquids

• Bosonic large N – Neel, dimer ordering.

Arovas, Auerbach PRB1988, Sachdev and Read, Nucl. Phy. B 1989.

• Fermionic large N -- spinon Fermi surface, Dirac point, etc.

Affleck and Maston PRB1988, Hermele et al PRB2004, Lee, Nagaosa, Wen, RMP2006

• RVB, quantum dimer model, etc.

Anderson 1973; Rokhsar, Kivelson PRL1988; Fradkin, Kivelson Mod. Phys. Lett 1990; Moessner and Sondhi PRL 2001.

• Frustration -- ring exchange, J1-J2 square lattice, Kagome, etc.

Jiang, Fisher, Sheng, Motrunich et al 2008-2012; Jiang, Yao, Balents PRB 2012; Yan, Huse, White Science 2011.

• Weak Mott-insulators – QMC: honeycomb lattice, square lattice with π -flux.

Meng et al, Nature 2010, Sorella et al arxiv2012, Chang and Scalettar PRL 2012.

Large spin fermions with alkaline-earth and alkali atoms

• High symmetries (e.g. Sp(2N)/SU(2N)) difficult to access in solid state systems.

Theoretical investigations.

Wu, Hu, Zhang, Chen, Wang (2003 ---);

Azaria, Lecheminant (2006 ---);

V. Gurarie, M. Hermele, A. Rey, P. Zoller, et al. (2010 ---).

• Why are they related to this workshop?

Strong quantum spin fluctuations!

Another system for quantum disordered Mott-insulating states besides solid state systems.

Experiment progress of multi-component fermions







Current experiment progress on alkaline-earth atoms

- ¹³²Yb (F=5/2) and ⁸⁷Sr (F=9/2) \rightarrow quantum degeneracy in optical traps.
- ¹³²Yb fermions \rightarrow 3D cubic optical lattices \rightarrow Mott-insulating states.
- Temperatures can reach the order of t, but are still higher than the AF exchange energy scale J.
- An interesting T scale difficult to reach in solids S. Kivelson.
 - S. Taie et al, arXiv:1208.4883.



Observation of Mott gap

- The Mott-state of one fermion per site.
- Create charge excitations (doublons) from periodically modulating lattice potentials.
- The charge gap measured from resonance spectra.



Classical (large S): large-spin solid state systems

- Hund's rule coupled electrons \rightarrow large onsite spin.
- Inter-site coupling is dominated by exchanging a single pair of electrons.
- ΔS_z only +1 or -1. Quantum spin-fluctuations are suppressed by 1/S.
- In solid state systems, the larger the spin is, the more classical the physics is.
- Bilinear exchange dominates

$$\frac{t^{2}}{U}\vec{S}_{i}\cdot\vec{S}_{j}+\frac{t^{4}}{U^{3}}(\vec{S}_{i}\cdot\vec{S}_{j})^{2}+...$$



C. Wu, Mod. Phys. Lett. (2006); Physics 3, 92 (2010).

Large-spin cold atoms: Not classical but quantum!

• Large-spin cold fermion moves as a whole object. The exchange of a pair of fermions can completely flip spin-configuration.

$$\Delta S_{z} = \pm 1, \pm 2, \dots \pm S$$

• Quantum fluctuations are enhanced by the large number of spin components.

• Bilinear, bi-qudratic, bi-cubic terms, etc., are all at equal importance.

$$\vec{S}_i \cdot \vec{S}_j, (\vec{S}_i \cdot \vec{S}_j)^2, (\vec{S}_i \cdot \vec{S}_j)^3$$



10

C. Wu, Mod. Phys. Lett. (2006); Physics 3, 92 (2010).

Large N NOT large S! SU(2N), Sp(2N=2S+1)

• Alkaline-earth atoms have fully-filled electron-shells, thus their hyperfine spin is just nuclear spin.

• Interactions are insensitive to nuclear spin components \rightarrow an obvious SU(2N) symmetry.

• SU(2N) symmetry is not generic for spin-dependent interactions, say, alkali fermions.

• $SU(2N) \rightarrow Sp(2N)$: SU(2N) generators which are **odd** under time-reversal transformation span the Sp(2N) algebra.



From Auerbach's book.

C. Wu et al, PRL 2003, C. Wu and S. C. Zhang PRB 2005; C. Wu, Mod. Phys. Lett. (2006); C. Wu₁₁ Physics 3, 92 (2010).

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Spin-3/2 atoms are special with hidden Sp(4) symmetry!

- Spin 3/2 atoms: ¹³²Cs, ⁹Be, ¹³⁵Ba, ¹³⁷Ba, ²⁰¹Hg.
- Extend Hubbard model to spin-3/2 fermions. Only two independent interaction parameters U₀ and U₂.

$$H = \sum_{\langle ij \rangle, \alpha} -t \{ c_{i,\alpha}^{+} c_{j,\alpha}^{-} + h. c. \} - \mu \sum_{i} c_{i,\alpha}^{+} c_{i,\alpha}^{-} \qquad \eta^{+}(i) = \sum_{\alpha\beta} \langle 00 \mid \frac{3}{2} \frac{3}{2}; \alpha\beta \rangle c_{\alpha}^{+}(i) c_{\beta}^{+}(i)$$
$$+ U_{0} \sum_{i} \eta^{+}(i) \eta(i) + U_{2} \sum_{m=\pm 2, \pm 1, 0} \chi_{m}^{+}(i) \chi_{m}(i) \qquad \chi_{m}^{+}(i) = \sum_{\alpha\beta} \langle 2m \mid \frac{3}{2} \frac{3}{2}; \alpha\beta \rangle c_{\alpha}^{+}(i) c_{\beta}^{+}(i)$$

• Exact **Sp(4)** symmetry regardless of dimensionality, external potential, and lattice geometry!

Sp(4) in spin 3/2 systems $\leftrightarrow \rightarrow$ SU(2) in spin $\frac{1}{2}$ systems

C. Wu et al, PRL 2003, C. Wu, Mod. Phys. Lett. (2006); Physics 3, 92 (2010).

$U(4) \rightarrow Sp(4)$ algebra

- Total degrees of freedom: $\psi_{\alpha}^{+}M_{\alpha\beta}\psi_{\beta}$ 4²=16=1+3+5+7.
- 1 density operator and 3 spin operators are far from complete.

rank: 0 1,
1
$$S_x, S_y, S_z$$

 $M_{\alpha\beta}$ 2 $\xi_{ij}^a S_i S_j (a = 1 \sim 5)$: $\{S_x^2 - S_y^2, S_z^2 - \frac{5}{4}, \{S_x, S_y\}, \{S_y, S_z\}, \{S_z, S_x\}\}$
3 $\xi_{ijk}^a S_i S_j S_k (a = 1 \sim 7)$

• Spin-quadrupole matrices: the same Γ -matrices in Dirac equation.

$$\Gamma^{a} = \xi^{a}_{ij} F_{i} F_{j}, \quad \{\Gamma^{a}, \Gamma^{b}\} = 2\delta_{ab}, \quad (1 \le a, b \le 5)$$

Hidden conserved quantities: spin-octupoles

• Both $S_{x,y,z}$ and $\xi_{ijk}^{a} S_{j} S_{k}$ are conserved, which span the Sp(4) algebra. Spin-3/2 Hubbard model is Sp(4) invariant!!

3+7=10
$$\Gamma^{ab} = \frac{i}{2} [\Gamma^{a}, \Gamma^{b}] \ (1 \le a < b \le 5)$$

• The time-reversal odd kernel of U(4) is Sp(4).

1 scalar + 5 vectors + 10 generators = 16

		lime Reversal
1 density:	$n=\psi^{+}\psi$;	even
5 spin-quadrupole:	$n_{a} = \frac{1}{2} \psi^{+} \Gamma^{a} \psi;$	even
3 spins + 7 spin- octupole:	$L_{_{ab}} = rac{1}{2} \psi^{+} \Gamma^{ab} \psi;$	odd

<u>Unify AFM, SC, CDW with **exact** symmetries extended</u> <u>from Sp(4) in bipartite lattice at half-filling</u>

• AFM (5-spin quadrupole) + SC (singlet) by SO(7) symmetry.

c.f. SO(5) theory of high Tc: 3-AF + 2 SC=5.

- CDW + SC (singlet) by pseudo-spin SU(2) symmetry. Generalization of eta-pairing.
- AFM(10-spin+spin octupole) +SC (10-quintet)+ CDW by the adjoint rep. of SO(7).



More technical details

Brief Review

Modern Physics Letters B, Vol. 20, No. 27 (2006) 1707–1738 © World Scientific Publishing Company



HIDDEN SYMMETRY AND QUANTUM PHASES IN SPIN-3/2 COLD ATOMIC SYSTEMS

CONGJUN WU

Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA wucj@kitp.ucsb.edu

Received 31 August 2006

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SU(2N) Hubbard model at half-filling

$$H = -t \sum_{\langle ij \rangle, \sigma=1}^{2N} \{c_{i,\sigma}^{+} c_{j,\sigma}^{-} + h. c.\} + \frac{U}{2} \sum_{i} (n_{i} - N)^{2} \qquad n_{i}^{-} = \sum_{\sigma=1}^{2N} n_{i,\sigma}^{-}$$

In the atomic
$$\Delta E = U$$

Imit, t=0.

• Turning on t, number of super-exchange processes scales as N^2 .



Enhancement of quantum spin fluctuations

• As increasing 2N, the Neel states become unfavorable.

Λ

$$\Delta E = -2N \frac{t^2}{U}$$

$$E = -2N(N+1) \frac{t^2}{U}$$

- Bond dimer state consists of $\binom{2N}{N}$ resonating Neel configurations.
- As N goes infinity, bond dimer ordering is realized (Sachdev + Read).

SU(2N) generators and Casimir

• The SU(2N) generators on each site *i*.

$$J_{\alpha\beta}(i) = c_{\alpha}^{+}(i)c_{\beta}(i) - \frac{\delta_{\alpha\beta}}{2N}\sum_{\sigma=1}^{2N}c_{\sigma}^{+}(i)c_{\sigma}(i) \qquad \sum_{\alpha}J_{\alpha\alpha}(i) = 0$$

• If a site is half-filled (N-fermions per site). Its degeneracy is $\binom{2N}{N}$ and the Casimir is

$$C_{2}(2N,N) = \frac{1}{2} \sum_{\alpha\beta} J_{\alpha\beta}(i) J_{\beta\alpha}(i) = \frac{N(2N+1)}{4}$$

• SU(2N) Heisenberg model with self-conjugate Rep.

$$H_{_{Heisenberg}} = \frac{2t^2}{U} \sum_{\alpha\beta} \{J_{\alpha\beta}(i)J_{\beta\alpha}(j) - \frac{1}{2}n(i)n(j)\} + \text{bi} - \text{quadratic} \text{ terms}$$

Sign-problem free QMC at half-filling

• Hubbard-Stratonovich transformation in the density-channel involving imaginary numbers.

$$e^{-U\Delta\tau(n_i-N)^2} = \sum_{l=\pm 1,\pm 2} \gamma_i(l) e^{i\eta_i(l)\sqrt{U\Delta\tau}(n_i-N)} + O(\Delta\tau^4)$$

$$\begin{aligned} \gamma(\pm 1) &= 1 + \frac{\sqrt{6}}{3}, \quad \gamma(\pm 2) = 1 - \frac{\sqrt{6}}{3}, \\ \eta(\pm 1) &= \pm \sqrt{2(3 - \sqrt{6})}, \quad \eta(\pm 2) = \pm \sqrt{2(3 + \sqrt{6})}. \end{aligned}$$

F. F. Assaad, cond-mat/9806307.F. F. Assaad, and M. Imada, J. Phys.Soc. Jpn 65, 189 (1996)

• Particle-hole transformation for •=N+1, ..., 2N.

$$c_{i,\sigma} \rightarrow (-)^{i} c_{i,\sigma}^{+}, \quad c_{i,\sigma}^{+} \rightarrow (-)^{i} c_{i,\sigma}^{-}, \quad n_{i} - N \rightarrow \sum_{\sigma=1}^{N} n_{i,\sigma}^{-} - \sum_{\sigma=N+1}^{2N} n_{i,\sigma}^{-}$$

• The functional determinant after integrating out fermions is a product of complex-conjugate pairs, thus positive-definite.

QMC at half-filling

• Thermodynamic and ground-state properties can be simulated with a high numeric precision.

• Our simulation results:

AFM long-range order for SU(4) --- weaker ordering than SU(2)

Evidence for algebraic spin correlations for SU(6) – gapless quantum paramagnets, or, spin liquid?.

Enhancement of Pomeranchuk cooling at half-filling in the SU(6) case.

Z. Cai, H. H. Hung, L. Wang, Yi Li, and C. Wu, arxiv:1207.6843. Z. Cai, H. H. Hung, L. Wang, C. Wu, arXiv:1202.632.

Confirm Mott gap: extracting single particle gap from Green's function

$$G(i,i,\tau) = \left\langle G \mid c_{\alpha}^{+}(i,\tau)c_{\alpha}(i,0) \mid G \right\rangle \rightarrow e^{-\Delta_{ch}\tau}$$



• Single-particle gap is weakened by increasing 2N.

AFM long-range-ordering of SU(4) Hubbard model

• AF spin structure factor: equal time spin-spin correlation.

 $\frac{1}{I^2} S_{SU(2)}(\vec{Q}) \to 0.125$



SSE on Heisenberg model, Sandvik, PRB, 56, 11678.

Vanishing of spin gap of the SU(4) Hubbard model

• Spin gap scales to zero: measured from non-equal time decay.

$$S_{structure}\left(\vec{Q},\tau\right) = \left\langle G \mid J_{\alpha\beta}\left(\vec{Q},\tau\right) J_{\beta\alpha}\left(-\vec{Q},0\right) \mid G \right\rangle \rightarrow e^{-\Delta_{sp}\tau}$$

- Consistent with the AFM long-range order.
- 6 dimensional
 Goldstone manifold
 U(4)/[U(2)*U(2)].
- Our result is consistent with the variational MC study.

A. Paramekanti and J. B. Marston, J. Phys. Cond. Matt. 19, 125215 (2007).



SU(6) at half-filling: single-particle gap (U/t=12)

- Finite scaling of the charge gap \sim 1.26 \rightarrow Mott insulator
- Green's function: $G(i,i,\tau) = \langle G | c_{\alpha}^{+}(i,\tau) c_{\alpha}(i,0) | G \rangle \rightarrow e^{-\Delta_{ch}\tau}$



SU(6) Hubbard model: vanishing of Neel ordering and spin gap

spin structure factor

spin gap scaling



SU(6) Hubbard mode at U=12: farthest points spin correlation

• Power-law spin correlation. $\eta \approx 1.17$ for U=12.

$$C_{SU(6)}(L/2, L/2) = \frac{1}{C_{2}(6,3)} \sum_{\alpha\beta} \frac{1}{2} \left\langle G \mid J_{\alpha\beta}(0,0) J_{\beta\alpha}(\frac{L}{2}, \frac{L}{2}) \mid G \right\rangle \sim L^{-\eta}$$



SU(6) Hubbard mode U=12: vanishing of dimer ordering

 Structure-factor of bond kinetic energy operators at Q=(□, 0)

$$D_{ij} = \sum_{\alpha} c^{\dagger}_{i,\alpha} c_{j,\alpha} + h.c.$$

• Fitted with $AL^{-2} \rightarrow$ shortrange correlation.



SU(6) Hubbard mode U=12: vanishing of DDW ordering



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Pomeranchuk cooling

• Fermions in Mott-insulating states can hold more entropy than in the Fermi liquid states.

• In Mott-insulators, all the sites contribute to entropy through spin-configurations, while in Fermi liquids, only fermions close to Fermi surfaces contributes.

• Driving a spinful Fermi liquid to Mott-insulating states, or, crystalline solids, leads to cooling --- Pomeranchuk cooling proposed in He-3 system.

• Pomeranchuk cooling is more efficient for large spin systems due to the enhanced entropy capability.

S. Taie, arXiv 1208.4883; K. R. Hazzard, et al PRA 2012, Z. Cai et al, arXiv:1207.6843.

Inefficiency of Pomeranchuk cooling of SU(2) fermions

- The iso-entropy curve for spin-1/2 Hubbard model at half-filling – QMC by T. Paiva et al, PRL 2010.
- The ordering tendency of the SU(2) AFM suppresses the spin entropy.



T. Paiva, et al, PRL 104, 066406 (2010).

Entropy capability per particle for half-filled SU(2N) Hubbard model



• Entropy per particle at $U \rightarrow$ infinity and $N \rightarrow$ infinity.

$$\frac{S_{Su(2N)}}{k_{R}} = \frac{1}{N} \ln \frac{(2N)!}{N!N!} \xrightarrow[N \to \infty]{} \ln 4$$

FIG. 1: Entropy per particle $S_{su(2N)}$ for the SU(2N) Hubbard model at half-filling v.s. 2N in a 10 × 10 square lattice. The temperature is fixed at $T/t = \frac{1}{3}$. The line of $U/t = \infty$ is from the results of Eq. 3.

Pomeranchuk cooling for SU(6) fermions at half-filling

• Iso-entropy curve at halffilling (three-particle per site).

$$\frac{S_{su(2N)}}{k_B} = \frac{S}{(NL^2)}$$
$$\frac{S_{su(2N)}(T)}{k_B} = \ln 4 + \frac{E(T)}{T} - \int_T^\infty dT' \frac{E(T')}{T'^2},$$

• As entropy per particle s<0.7, increasing U can cool the system below the anti-ferro energy scale J.

Z. Cai, H. H. Hung, L. Wang, D. Zheng, and C. Wu, arxiv1202.6323.



Sample size 10×10

Compressibility

• Charge fluctuation energy scale.

$$\kappa_{SU(2N)} = \frac{1}{L^2} \frac{\partial N_f}{\partial \mu} = \frac{1}{TL^2} \left(\left\langle \hat{N}_f^2 \right\rangle - \left\langle \hat{N}_f \right\rangle^2 \right)$$



Sample size 10×10

U / t = 4

Z. Cai, H. H. Hung, L. Wang, D. Zheng, and C. Wu, arxiv1202.6323.

The normalized compressibility $\kappa_{su(2N)}/(2N)$ v.s. T

Magnetic susceptibility v.s. T



FIG. 4: The normalized SU(2N) susceptibilities $\chi_{su(2N)}$ v.s. T with fixed U/t = 4 for 2N = 2, 4, 6

<u>1/4-filling (one particle per site) -- "color magnetism"</u>

C. Wu, Phys. Rev. Lett. 95, 266404 (2005); Hung, Wang, and Wu, PRB 05446, (2011)

- Strong spin fluctuations: N=4.
- When the onsite Neel ordering is suppressed, multi-site correlations develop.
- spin-1/2: 2 sites to form an SU(2) singlet.



• 4 sites to form an SU(4) singlet. Each site belongs to the fundamental Rep.

baryon-like
$$\frac{\varepsilon_{\alpha\beta\gamma\delta}}{4!}\psi_{\alpha}^{+}(1)\psi_{\beta}^{+}(2)\psi_{\gamma}^{+}(3)\psi_{\delta}^{+}(4)|0\rangle$$

Bossche et. al., Eur. Phys. J. B 17, 367 (2000).

• c. f. QCD. At least three quarks form an SU(3) color singlet: baryons; multi-particle color/magnetic correlations.

<u>Conclusion</u>

• Large-spin cold fermions are quantum-like NOT classical!

• Spin-3/2 Hubbard model unifies AFM, SC and CDW phases with exact symmetries extended from Sp(4).

• Power-law spin correlations in the half-filled SU(6) Hubbard model.

• Pomeranchuk cooling of the SU(6) Hubbard model.

• Exotic "color magnetism" exhibits dominant multi-particle correlations.