QMC simulations on novel quantum magnetism of SU(2N) Hubbard models with large-spin fermions

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1. D. Wang, Y. Li, Z. Cai, Z. Zhou, Y. Wang, C. Wu, Phys. Rev. Lett. 112, 156403 (2014).
2. Z. Cai, H. Hung, L. Wang, D. Zheng, C. Wu, Phys. Rev. Lett. 110, 220401 (2013) .
3. Z. Cai, H. Hung, L. Wang, C. Wu, Phys. Rev. B 88, 125108 (2013).
4. C. Wu, Nature Physics 8, 784 (2012) (News and Views).

Related past works:

5. C. Wu, J. P. Hu, and S. C. Zhang, Phys. Rev. Lett. 91, 186402(2003).
6. C. Wu, Phys. Rev. Lett. 95, 266404 (2005),

BU Conference, May, 2014

Collaborators

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- **Introduction: a novel system for quantum magnetism.**

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

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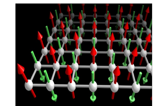
Fermionic Hubbard model:

$$H=-t\sum_{\langle ij\rangle}\sum_{\sigma=\uparrow,\downarrow}(c^\dagger_{i,\sigma}c_{j,\sigma}+h.c)-\mu\sum_i n_i+U\sum_i n_{i\uparrow}n_{i\downarrow}$$

A simplest model describing interacting particles in a lattice with only minimum ingredients.

At half-filling: Free from "sign-problem" in DQMC
Antiferromagnetic long-range ordering in 2D
(D. J. Scalapino et al, 1981, J. E. Hirsch 1983)

Away from half-filling: ?
High-Tc superconductor. MI Mott transition……



SU(2N) generalization of Hubbard model:a mathematic convenience of large N

$$H=-t\sum_{\langle ij\rangle}\sum_{\alpha=1}^{2N}(c^\dagger_{i,\alpha}c_{j,\alpha}+h.c)+\frac{U}{2}\sum_i(n_i-\tilde\mu)^2$$

I. Affeck and J. B. Marston, 1988

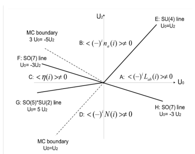
- **Use large spin alkali and alkaline earth to realize symmetries SU(N) and Sp(N) (N=4). (SO(5) ~ Sp(4)). Sp(4) symmetry is generic for spin-3/2 Hubbard model, and SU(4) is a special case of in the Sp(4) phase space.**

VOLUME 91, NUMBER 18 PHYSICAL REVIEW LETTERS week ending 31 OCTOBER 2003

Exact SO(5) Symmetry in the Spin-3/2 Fermionic System

Congjun Wu, Jiang-ping Hu, and Shou-cheng Zhang

Besides the alkali atoms, the trapping and cooling of the alkaline-earth atoms are also exciting recently [25,26]. Among these two families, ^{132}Cs, ^{9}Be, ^{135}Ba, and ^{137}Ba are spin-3/2 atoms. The last two Ba atoms are stable and the resonances of $6s^2\to 6s^16p^1$ are at 553.7 nm [27], thus making them possible candidates. Their scattering lengths are not available now, but that of ^{138}Ba (spin 0) was estimated as $-41a_B$ [25]. Because the 6s shell of Ba is full-filled, both the a_0, a_2 of ^{135}Ba and ^{137}Ba should have similar value. Considering the rapid development in this field, we expect more and more spin-3/2 systems will be realized experimentally.



What is new? Large spin alkaline-earth and alkali atoms

- High symmetries (e.g. Sp(2N)/SU(2N)) difficult to access in solid state systems, which are usually met in high energy physics.

- Theoretical investigations.

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

Azaria, Lecheminant (2006 ---);

V. Gurarie, M. Hermele, A. Rey, J. Ye, P. Zoller, E. Demer, M. Lukin et al. (2010---).

- Strong quantum fluctuations!

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

Experiment breaking through of large-spin fermions

PHYSICAL REVIEW LETTERS — PRL 105, 190401 (2010)

Realization of a SU(2) × SU(6) System of Fermions in a Cold Atomic Gas

Shintaro Taie, Yosuke Takasu, Seiji Sugawa, Rekishu Yamazaki, Takuya Tsujimoto, Ryo Murakami, and Yoshiro Takahashi

PHYSICAL REVIEW LETTERS — PRL 105, 030402 (2010)

Degenerate Fermi Gas of ^{87}Sr

B. J. DeSalvo, M. Yan, P. G. Mickelson, Y. N. Martinez de Escobar, and T. C. Killian

Viewpoint — Physics 3, 92 (2010)

Exotic many-body physics with large-spin Fermi gases

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Published November 1, 2010

The experimental realization of quantum degenerate cold Fermi gases with large hyperfine spins opens up a new opportunity for exotic many-body physics.

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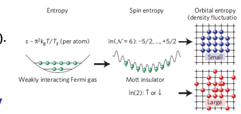
nature physics — ARTICLES — PUBLISHED ONLINE: 23 SEPTEMBER 2012 | DOI: 10.1038/NPHYS2430

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

Shintaro Taie*, Rekishu Yamazaki, Seiji Sugawa and Yoshiro Takahashi

S. Taie,et.al, Nature phys. 8, 825(2012).



QUANTUM GASES

Mott made easy

The realization of a Mott insulating state in a system of ultracold fermions comprising far more internal components than the electron, provides an avenue for probing many-body physics that is difficult to access in solids.

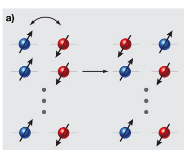
C. Wu, Nature phys. 8, 784 (2012).

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

- Hund's rule coupled electrons 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

$$\frac{t^2}{U}\vec S_i\cdot\vec S_j+\frac{t^4}{U^3}(\vec S_i\cdot\vec S_j)^2+\ldots$$



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

Large-spin cold atoms: **Not classical but quantum!**

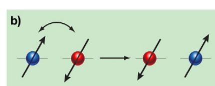
- Large-spin cold fermion moves as a whole object. The exchange of a pair of fermions can completely flip spin-configurations.

$$\Delta S_z=\pm1,\pm2,\ldots\pm S$$

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

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

$$S_i\cdot S_j,(S_i\cdot S_j)^2,(S_i\cdot S_j)^3$$



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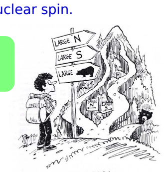
C. Wu, Mod. Phys. Lett. (2006); Physics 3, 92 (2010).

Large N NOT large S! SU(2N), Sp(2N) (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 2N components are equivalent.

- SU(2N) symmetry is not generic for spin-dependent interactions, say, alkali fermions with unpaired electrons.
- SU(2N) 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. Wu Physics 3, 92 (2010).

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The simplest case spin-3/2: **Hidden symmetry**!

- Spin 3/2 atoms: 132Cs, 9Be, 135Ba, 137Ba, 201Hg. C. Wu et al. Phys. Rev. Lett. 91, 186402 (2003).

- **Sp(4) (SO(5))** symmetry without fine tuning regardless of dimensionality, particle density, and lattice geometry!

Sp(4) in spin 3/2 systems SU(2) in spin ½ systems

- SU(4) symmetry is realized iff the interaction is spin-independent.

- Importance of high symmetries: unification of competing orders, description of strong spin fluctuations, etc.

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Spin-3/2 Hubbard model in optical lattices

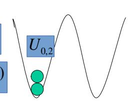
$$H=\sum_{\langle ij\rangle,\alpha}-t\{c^+_{i,\alpha}c_{j,\alpha}+h.c.\}-\sum_i c^+_{i,\alpha}c_{i,\alpha}+U_0\sum_i\eta^+(i)\eta(i)+U_2\sum_{i}\sum_{a=1\sim5}\chi^+_a(i)\chi_a(i)$$

$$\uparrow\left|\tfrac{3}{2}\right\rangle\ \uparrow\left|\tfrac{1}{2}\right\rangle\quad \downarrow\left|-\tfrac{1}{2}\right\rangle\ \downarrow\left|-\tfrac{3}{2}\right\rangle$$

- Fermi statistics: only Ftot=0, 2 are allowed; Ftot=1, 3 are forbidden.

singlet: $\eta^+(i)=\sum_{\alpha\beta}\langle 00|\tfrac32\tfrac32;\alpha\beta\rangle c^+_\alpha(i)c^+_\beta(i)$

quintet: $\chi^+_a(i)=\sum_{\alpha\beta}\langle 2a|\tfrac32\tfrac32;\alpha\beta\rangle c^+_\alpha(i)c^+_\beta(i)$



- For arbitrary values of t, , U₀, U₂ and lattice geometry, there is an **exact** Sp(4), or SO(5) symmetry.

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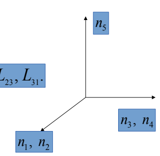
What is Sp(4)(SO(5)) group?

- SU(2) (SO(3)) group.

3-vector: x, y, z; 3-generators: L_{12},L_{23},L_{31}.

2-spinor: $|\uparrow\rangle$, $|\downarrow\rangle$



- Sp(4)(SO(5)) group.

5-vector: n_1,n_2,n_3,n_4,n_5

10-generators: $L_{ab}\ (1\le a<b\le5)$

4-spinor: $\uparrow\left|\tfrac32\right\rangle\ \uparrow\left|\tfrac12\right\rangle\ \downarrow\left|-\tfrac12\right\rangle\ \downarrow\left|-\tfrac32\right\rangle$

- We will see what quantities correspond to these 5-vector and 10-generator.

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spin-3/2 algebra $\psi^+_\alpha M_{\alpha\beta}\psi_\beta$

- Total degrees of freedom: 42=16=1+3+5+7.

1 density operator and 3 spin operators are far from complete.

rank:	$M_{\alpha\beta}$
0	I,
1	F_x,F_y,F_z
2	$\xi^a_{ij}F_iF_j\ (a=1\sim5)$:
3	$\xi^a_{ijk}F_iF_jF_k\ (a=1\sim7)$

→ $F_x^2-F_y^2,\ F_z^2-\frac54$, $\{F_x,F_y\},\{F_y,F_z\},\{F_z,F_x\}$

- **Spin-quadrupole matrices** (rank-2 tensors) form five-Γ matrices (SO(5) vector) --- the same Γ-matrices in Dirac equation.

$$\Gamma^a=\xi^a_{ij}F_iF_j,\quad \{\Gamma^a,\Gamma^b\}=2\delta_{ab},\quad (1\le a,b\le5)$$

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Hidden conserved quantities: spin-octupoles

- Both $F_{x,y,z}$ and $\xi^a_{ijk}F_iF_jF_k$ commute with Hamiltonian. 10 SO(5) generators: 10=3+7.
- **7 spin-octupole operators** are the hidden conserved quantities.

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

- **SO(5): 1 scalar + 5 vectors + 10 generators = 16**

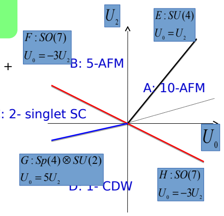
		Time Reversal
1 density:	$n=\psi^+\psi;$	even
5 spin-quadrupole:	$n_a=\frac{1}{2}\psi^+\Gamma^a\psi;$	even
3 spins + 7	$L_{ab}=\frac{1}{2}\psi^+\Gamma^{ab}\psi;$	odd

Unify AF, SC, CDW with **exact** symmetries extended from Sp(4) in bipartite lattice at half-filling

- AF (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 C. N. Yang's eta-pairing.
- AFM(10-spin+spin octupole) +SC (10-quintet)+ CDW by the adjoint rep. of SO(7).



More technical details

Brief Review

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

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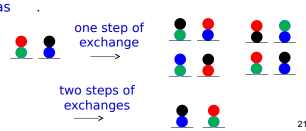
SU(2N) Hubbard model at half-filling

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

- In the atomic limit, t=0. SU(4) $\Delta E=U$
- Turning on t, number of super-exchange processes scales as N^2.

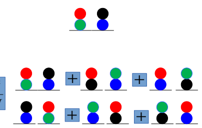


Enhancement of quantum spin fluctuations

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

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

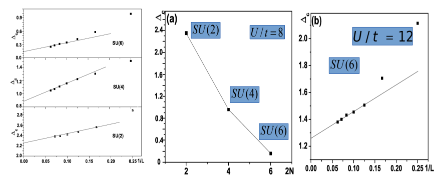
$\Delta E=-2N(N+1)\frac{t^2}{U}$ bond SU(2N) singlet



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

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

$$G(i,i,\tau)=\langle G\,|\,c^+_\alpha(i,\tau)c_\alpha(i,0)\,|\,G\rangle\to e^{-\Delta_{sp}\tau}$$

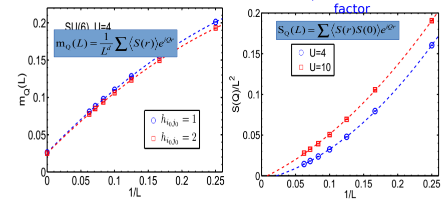


- Single-particle gap is weakened by increasing 2N.

QMC with pinning field: sensitive to weak Neel ordering

- Local pinning field $H_{pin,n}=2Nh_{j_0}\{m_{j_0}-m_{j_0}\}$
- Long range order parameter $m_Q=\lim_{L\to\infty}m_Q(L)$

Comparison: structure factor

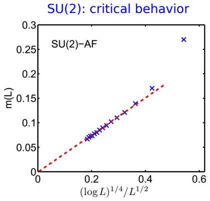


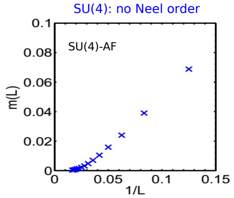
Pinning field method: NOT oversensitive to weak ordering

- 1D Hubbard model:

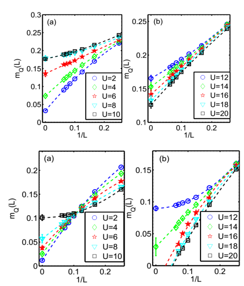
SU(2): critical behavior

SU(4): no Neel order

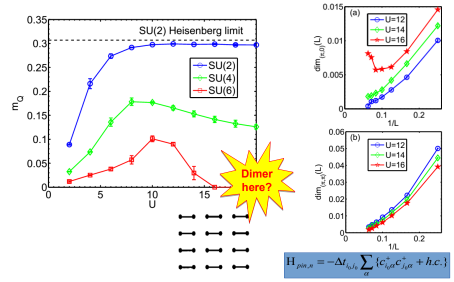




Non-monotonic behavior of Neel ordering v.s. U

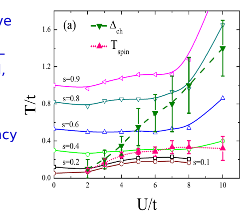


QMC with pinning field: AF dome in phase diagram



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).

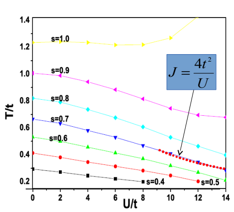
Pomeranchuk cooling for SU(6) fermions at half-filling

- Iso-entropy curve at half-filling (three-particle per site).

$S_{su(2N)}=S/(NL^2)$

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

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



Sample size 10×10

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

Conclusion

- **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).
- Novel magnetic behavior as increasing U in the SU(2N) Hubbard model.
- Pomeranchuk cooling of the SU(6) Hubbard model.