Novel Sp(2N) and SU(2N) quantum magnetism and Mott physics – large spins are different

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Current work:

Earlier work:
2. C. Wu, Phys. Rev. Lett. 95, 266404 (2005),
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Outline

• **Introduction: what is large?**

  Large symmetry (large N) rather than **large spin magnitude** (large S). Quantum spin fluctuations are **enhanced** rather than **suppressed**.

• **Generic Sp(4) symmetry (spin-3/2).**

  Unification of antiferromagnetism, superconductivity, and charge-density-wave.  
  http://online.kitp.ucsb.edu/online/coldatoms07/wu2/

• **Slater v.s. Mott: quantum phase transition at SU(6) -- QMC**

  Interplay between charge and spin degrees of freedom

• **Pomeranchuk effect (thermodynamics) -- QMC.**
The simplest interacting model of lattice fermions

\[ H = - \sum_{{(ij)},\sigma} t \{ c_{{i,\sigma}}^+ c_{{j,\sigma}} + h.c. \} - \mu \sum_{{i,\sigma}} c_{{i,\sigma}}^+ c_{{i,\sigma}} + U \sum_{{i}} n_{{i,\uparrow}} n_{{i,\downarrow}} \]

- Hubbard 1963: itinerant ferromagnetsim (FM), not successful.

- But successful for metal-Mott insulator transitions.

- Can the single band Hubbard describe high T\textsubscript{c} cuprates?

--- Still in debates.
Some rigorous results

• **1D Mott physics:** half-filled (U>0).

  1. Charge gap opens at infinitesimal U (relevance of Umklapp term)
  2. Spin channel remains critical – no symmetry breaking

  C. N. Yang, PRL 19, 1312 (1967); Lieb and F. Y. Wu, PRL 20, 1445, (1968).

  Field theoretical methods, DMRG simulations

• **2D AFM long-range-order:** the square lattice (half-filled).

  Determinant quantum Monte-Carlo (DQMC): Sign-problem free at half filling -- non-perturbative method, asymptotically exact

Hidden symmetry (pseudo-spin)

- Yang and Zhang’s $\eta$-pairing $\rightarrow$ generators of SU(2) in the charge channel.

$$\eta^- = \sum_i (-)^i c_{i\downarrow} c_{i\uparrow}, \quad \eta^+ = \sum_i (-)^i c_{i\uparrow} c_{i\downarrow}, \quad [\eta^-, \eta^+] = 2N$$

- Degeneracy between charge-density-wave (CDW) and superconductivity (SC) at half-filling ($U<0$)

$$0_{cdw} = \sum_i (-)^i n_i, \quad \Delta = \sum_i c_{i\uparrow} c_{i\downarrow}, \quad \Delta^+ = \sum_i c_{i\downarrow} c_{i\uparrow}, \quad [\eta^+, \Delta] = O_{CDW}$$

- Pseudo-Goldstone: $\eta$-mode

$$H(\eta^+ | G_{SC}) = (\mu - \mu_0) (\eta^+ | G_{SC}), \quad (\mu \geq \mu_0)$$
Exotic spin states in the Mott-insulating phase

- **Bosonic large-$N$ -- Neel, dimer ordering.**
  

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

- **RVB, quantum dimer model, etc.**
  

- **Frustration -- ring exchange, $J_1$-$J_2$ square lattice, Kagome, etc.**
  
Theory progress with large-spin fermions

- Novel physics inaccessible in usual solid state systems.

- Early work by Ho and Yip (PRA and PRL 1999).

Richer Fermi liquid properties and Cooper pairing structures than those in spin-1/2 electron systems.

- **A new view point: high symmetries, Sp(2N), SU(2N).**

Sp(4), SO(5), SU(4): (spin $-\frac{3}{2}$) $^{132}\text{Cs}$, $^{9}\text{Be}$, $^{135}\text{Ba}$, $^{137}\text{Ba}$, $^{201}\text{Hg}$


A new strongly correlated system: optical lattices

- Interaction effects tunable by varying laser intensity.

\[ t : \text{inter-site tunneling} \]
\[ U : \text{on-site interaction} \]
Experiment breakthrough of large-spin fermions

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

Shintaro Taie,¹,* Yosuke Takasu,¹ Seiji Sugawa,¹ Rekishu Yamazaki,¹,² Takuya Tsujimoto,¹ Ryo Murakami,¹ and Yoshiro Takahashi¹,²

**Degenerate Fermi Gas of ^{87}\text{Sr}**

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

**Viewpoint**

**Exotic many-body physics with large-spin Fermi gases**

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_The experimental realization of quantum degenerate cold Fermi gases with large hyperfine spins opens up a new opportunity for exotic many-body physics._
An SU(6) Mott insulator of an atomic Fermi gas realized by large-spin Pomeranchuk cooling

Shintaro Taie¹*, Rekishu Yamazaki¹,², Seiji Sugawa¹ and Yoshiro Takahashi¹,²

Many recent progresses: Fallani et al; Jun Ye et al; K. Sengstock et al; Foelling/Bloch et al, .......
What is large?

- High symmetry (large N, SU(2N), Sp(2N)) rather than large spin magnitude (large S).

- High symmetries do not occur frequently in nature, since every new symmetry brings with itself a possibility of new physics, they deserve attention.

  --- comment from D. Controzzi and A. M. Tsvelik, cond-mat/0510505

- Quantum spin fluctuations are enhanced NOT suppressed.

- SU(2N) and Sp(2N) were introduced to condensed matter physics as a formal tool, say, 1/N-expansion.
Transition metal oxides (**large S → classical**)

- **Large spin magnitude** from Hund’s coupling.

- **Inter-site coupling**: exchange a **single pair** of electrons.

- **1/S-fluctuations**: \( \Delta S_z = \pm 1 \)

- Bilinear exchange dominates

  \[
  \frac{t^2}{U} \vec{S}_i \cdot \vec{S}_j + \frac{t^4}{U^3} (\vec{S}_i \cdot \vec{S}_j)^2 + \ldots
  \]

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

Cold fermions: **large N**→ **enhanced fluctuations!**

- Large-hyperfine-spin as a whole object (no ionization).

\[ \Delta S_z = \pm 1, \pm 2, \ldots \pm S \]

- One step of super-exchange can completely overturn spin config.

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

\[ \vec{S}_i \cdot \vec{S}_j, (\vec{S}_i \cdot \vec{S}_j)^2, (\vec{S}_i \cdot \vec{S}_j)^3 \]
Two views of spin quartet (weight diagrams of Lie algebra)

Solid: SU(2) (1D lattice)

- $S_\pm$ $S_\pm$ $S_\pm$ $S_z$
- -3/2 -1/2 1/2 3/2

A high rank spinor Rep. of a small group.

Off-diagonal operator: (fluctuation) $S_\pm$

Cold fermions Sp(4) or SO(5) (2D lattice)

- $\pi_{1\pm}$ $m_2$
- $\pi_{2\pm}$ $\pi_{3\pm}$ $\pi_{4\pm}$ $m_1$

- The fundamental spinor Rep of a large group.

- Much more off-diagonal operators.

$\pi_{1\pm}$, $\pi_{2\pm}$, $\pi_{3\pm}$, $\pi_{4\pm}$
SU(2N), Sp(2N) (2N=2S+1)

• Alkaline-earth fermions: SU(2N), equivalent 2N components.
  
  fully filled electronics shells $\rightarrow$ spin-independent interaction

• Alkali fermions: broken SU(2N), spin-dependent interaction.

• Symplectic symmetry:

  SU(2N) $\rightarrow$ Sp(2N)

  Good properties under time-reversal transformation.
Outline

- **Introduction: what is large?** large \( N \) v.s. large \( S \)

- **Generic \( \text{Sp}(4) \) symmetry (spin-3/2).**

  Unification of antiferromagnetism, superconductivity, and charge-density-wave.

  [http://online.kitp.ucsb.edu/online/coldatoms07/wu2/](http://online.kitp.ucsb.edu/online/coldatoms07/wu2/)
The simplest case spin-3/2: **Hidden symmetry!**

- **Spin 3/2 atoms:** $^{132}\text{Cs}$, $^9\text{Be}$, $^{135}\text{Ba}$, $^{137}\text{Ba}$, $^{201}\text{Hg}$.

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

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

Spin-3/2 Hubbard model in optical lattices

\[ H = \sum_{\langle ij \rangle, \alpha} -t\{c_{i,\alpha}^+ c_{j,\alpha} + h.c.\} - \mu \sum_i c_{i,\alpha}^+ c_{i,\alpha} + U_0 \sum_i \eta^+(i) \eta(i) + U_2 \sum_{a=1 \sim 5} \chi_a^+(i) \chi_a(i) \]

- Fermi statistics: only \( F_{\text{tot}} = 0, 2 \) are allowed; \( F_{\text{tot}} = 1, 3 \) are forbidden.

**singlet:** \( \eta^+(i) = \sum_{\alpha\beta} \langle 00 | \frac{3}{2} \frac{3}{2} ; \alpha\beta \rangle c_{\alpha}(i) c_{\beta}(i) \)

**quintet:** \( \chi_a^+(i) = \sum_{\alpha\beta} \langle 2\alpha | \frac{3}{2} \frac{3}{2} ; \alpha\beta \rangle c_{\alpha}(i) c_{\beta}(i) \)

- For arbitrary values of \( t, \mu, U_0, U_2 \) and lattice geometry, there is an exact \( \text{Sp}(4) \), or \( \text{SO}(5) \) symmetry.
What is Sp(4)(SO(5)) group?

- SU(2) (SO(3)) group.
  - 3-vector: \(x, y, z\); 3-generator: \(L_{12}, L_{23}, L_{31}\).
  - 2-spinor: \(|\uparrow\rangle, |\downarrow\rangle\)

- Sp(4)(SO(5)) group.
  - 5-vector: \(n_1, n_2, n_3, n_4, n_5\)
  - **10-generator**: \(L_{ab} \ (1 \leq a < b \leq 5)\)
  - 4-spinor: \(|\uparrow\rangle, |\uparrow \frac{3}{2}\rangle, |\uparrow \frac{1}{2}\rangle, |\downarrow \frac{1}{2}\rangle, |\downarrow \frac{3}{2}\rangle\)

- We will see what quantities correspond to these 5-vector and 10-generator.
spin-3/2 algebra \( \psi^+ M_{\alpha\beta} \psi \)

- Total degrees of freedom: \( 4^2 = 16 = 1 + 3 + 5 + 7 \).

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

- Rank: 0
  - 1, \( F_x, F_y, F_z \)
- \( M_{\alpha\beta} \) rank: 2
  - 2 \( \xi^a_{ij} F_i F_j \) (\( a = 1 \sim 5 \)):
  - \( F_x^2 - F_y^2, F_z^2 - \frac{5}{4} \),
  - \( \{ F_x, F_y \}, \{ F_y, F_z \}, \{ F_z, F_x \} \)
- 3 \( \xi^a_{ijk} F_i F_j F_k \) (\( a = 1 \sim 7 \))

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

\[
\Gamma^a = \xi^a_{ij} F_i F_j , \quad \{ \Gamma^a, \Gamma^b \} = 2 \delta_{ab} , \quad (1 \leq a, b \leq 5)
\]
Hidden conserved quantities: **spin-octupoles**

- Both $F_{x,y,z}$ and $\xi_{ijk} F_i F_j F_k$ commute with Hamiltonian $\to$
  10 SO(5) generators: $10 = 3 + 7$.

- **7 spin-octupole operators** are the hidden conserved quantities.

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

- 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 spin-octupole: $L_{ab} = \frac{1}{2} \psi^+ \Gamma^{ab} \psi$; odd
Unify AFM, SC, CDW with **exact** symmetries
(half-filled, bipartite lattice)

- SO(7): AFM (5-spin quadrupole) + SC (singlet).


- Large symmetry manifold--the adjoint rep. of SO(7). AFM(10-spin+spin octupole) + SC (10-quintet) + CDW.

\[ F : SO(7) \]
\[ U_0 = -3U_2 \]

\[ G : Sp(4) \otimes SU(2) \]
\[ U_0 = 5U_2 \]

\[ E : SU(4) \]
\[ U_0 = U_2 \]

\[ B : 5\text{-}AFM \]

\[ A : 10\text{-}AFM \]

\[ C : 2\text{-singlet SC} \]

\[ D : 1\text{-CDW} \]

\[ H : SO(7) \]
\[ U_0 = -3U_2 \]
Sign-problem free QMC algorithm away from half-filling

- An equivalent formulation:

\[
H = \sum_{\langle ij \rangle, \sigma} \left( -t \{ c_{i,\alpha}^+ c_{j,\alpha} + h.c. \} - \mu \sum_i c_{i,\alpha}^+ c_{i,\alpha} \right) - \sum_{i, 1 \leq a \leq 5} \left\{ V(n(i) - 2)^2 + Wn_a^2(i) \right\} \\
V = -\frac{3U_0 + 5U_2}{16}, \\
W = \frac{U_2 - U_0}{4}
\]

- Time-reversal invariant Hubbard-Stratonovich decomposition at \((V, W>0)\).

- Fermion determinant remains positive-definite at any filling.

\[
U_0 < U_2 < -\frac{3}{5} U_0
\]

- Sign problem free region includes Superconductivity, CDW, AFM.
“Grand-unifications” – elegancy and power of the group theory

- Pseudo-spin SO(3=2+1) unifies SC (singlet) + CDW


  41mev neutron resonance mode in the high Tc SC state: pseudo-Goldstone mode ($\pi$-mode)

- Exact SO(7=2+5) symm. unifies SC + AFM (5-spin quadrupole).

\[
\begin{align*}
\left[\chi^+_a, \Delta\right] &= AF_{a,qd} \\
\left[H, \chi^\pm_a\right] &= \mp (\mu - \mu_0) \chi^\pm_a \\
H(\chi^+_a \mid G_{SC}) &= \left[ E_G + (\mu - \mu_0) \right] \langle \chi^+_a \mid G_{SC} \rangle \\
5-\chi \text{ models: rotate SC} \leftrightarrow \text{AF.} \\
\text{Analogy to the } \pi \text{-modes in high Tc.}
\end{align*}
\]
Non-abelian statistics – Alice vortex loop/particle
(SO(4) Cheshire charge)

• Quintet pairing \((S=2) \rightarrow \) half-quantum vortex loop carrying spin quantum number.

\[
|\text{init}\rangle = \left| \frac{3}{2} \rightangle_p \otimes |\text{zero charge}\rangle_{\text{vort}}
\]

\[
|\text{final}\rangle = \left| \frac{1}{2} \rightangle_p \otimes |S_z = 1\rangle_{\text{vort}} - \left| \frac{-1}{2} \rightangle_p \otimes |S_z = 2\rangle_{\text{vort}}
\]

\[
|00;00\rangle_{vt} \otimes \left| \frac{1}{2} \rightangle_{q_p},
\]

\[
\left| \frac{1}{2} \frac{-1}{2} \right\rangle_{vt} \otimes |00;\frac{1}{2}\frac{1}{2}\rangle_{q_p} - \left| \frac{1}{2} \frac{-1}{2} \right\rangle_{vt} \otimes |00;\frac{1}{2}\frac{-1}{2}\rangle_{q_p}.
\]

More details

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

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Outline

- **Introduction: what is large?**  large N v.s. large S

- **Generic Sp(4) symmetry (spin-\(\frac{3}{2}\)).**
  
  Unification of antiferromagnetism, superconductivity, and charge-density-wave.  
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- **Slater v.s. Mott: quantum phase transition at SU(6) -- QMC**
  
  Interplay between charge and spin degrees of freedom
SU(2): Slater V. S. Mott (half-filling)

- Fermi surface nesting (small $U/t$): divergent AFM susceptibility; strong charge fluctuations.

\[ \vec{Q} \rightarrow \vec{\sigma} \rightarrow \vec{\sigma} - \vec{Q} \]

\[ m \propto t e^{-\frac{\sqrt{t}}{U}} \]

\[ \vec{Q} = (\pi, \pi) \]

- Local moments (Large $U/t$): charge fluctuation suppressed; AFM super-exchange.

\[ H = J \sum_i (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}) \]
SU(2): no phase transition

• SU(2): smooth cross-over from Slater to Mott region.


Projector determinant QMC + pinning field.

Neel moment
Half-filled SU(2N) Hubbard model (local moment limit)

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

\[ n_i = \sum_{\sigma=1}^{2N} n_{i,\sigma} \]

• SU(4) as an example. In the atomic limit, \( t=0 \).

\[ \Delta E = U \]

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

SU(4)  
one step of exchange  
two steps of exchanges
Enhancement of spin fluctuations

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

\[ \Delta E = -2zN \frac{t^2}{U} \]

![classic-Neel bond SU(2N) singlet]

• Bond dimer state consists of $\left( \frac{2^N}{N} \right)$ resonating configurations.

• As $N > z$ (coordination number), valence bond dimerization is favored (Sachdev + Read).
Projector QMC with the pinning field

• Usual methods to identify long-range-order in simulations:

1) 2-point correlation function:
\[
\lim_{r \to \infty} <S\left(\frac{L}{2}\right)S(0)> \neq 0
\]

2) Structure factor:
\[
\frac{1}{L^2} \sum <S(r)S(0)> e^{iQr} \neq 0
\]

• The pinning field method (sensitive to weak ordering):

add external field at central sites to explicitly break the symmetry

\[
H_{pin,n} = h\{m_{i_0} - m_{j_0}\}
\]

\[
m_Q(L) = \frac{1}{L^d} \sum \langle S(r) \rangle e^{iQr} \quad L \to \infty
\]

QMC with pinning field: sensitive

\[ m_Q(L) = \frac{1}{L^d} \sum \langle S(r) \rangle e^{iQr} \]

\[ S_Q(L) = \sum \langle S(r) S(0) \rangle e^{iQr} \]

Pinning field

Structure factor

SU(6), U=4

\[ h_{ij} = 1 \]
\[ h_{ij} = 2 \]

\[ \text{U=4} \]
\[ \text{U=10} \]
QMC with pinning field: NOT over-sensitive

- 1D Hubbard model:
  
  SU(2): critical behavior
  
  SU(4): no Neel order

---

\[ m(L) \text{ vs. } (\log L)^{1/4}/L^{1/2} \]

\[ m(L) \text{ vs. } 1/L \]
SU(6): Slater and Mott are different phases

- SU(4) and SU(6): non-monotonic behavior of Neel moment.
- Complete suppression of AFM for SU(6).

Mott gap: short-range charge fluctuations

- Single particle gap extracted from Green’s function.

\[ G(i, i, \tau) = \left\langle G \left| c_\alpha^+(i, \tau)c_\alpha(i,0) \right| G \right\rangle \]
\[ \Rightarrow e^{-\Delta_c \tau} \]

- Mott insulating states do not mean that charge does not move! Charge localization length.

\[ \xi_c / a_0 \approx t / \Delta_c \]

- Enhancing charge fluctuations as N increases! It is NOT legitimate to neglect charge degree of freedom.
Estimation of the single particle gap v.s N (large U)

- Charge gap decreases due to the enhanced number of hopping processes of charge excitations.

\[ \Delta_c = \frac{U}{2} \quad \Delta_c = \frac{(U-W)}{2} \]

\[ W \propto Nt \]

\( SU(2) \)

\( SU(4) \)
Rapid increase of Mott gap around $U \sim 10$ (SU(6))

$U / t = 8$

$U / t = 12$

$\Delta_c / t \approx 0.2 \quad \Delta_c / t \approx 1.26$
Thermodynamics: Pomeranchuk effect

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

- Pomeranchuk effect is more efficient in large spin systems due to the enhanced entropy capability.

Pomeranchuk effect (SU(6), half-filling)

- Iso-entropy curve (three-particle per site).

\[ S_{su(2N)} = \frac{S}{(NL^2)} \]

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

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

\[ J = \frac{4t^2}{U} \]

Sample size \( 10 \times 10 \)

Probability of onsite occupation (SU(4))

\[ P(0) = \prod_{\alpha=1}^{4} (1 - n_i^\alpha); \]
\[ P(1) = \sum_{\alpha=1}^{4} n_i^\alpha \prod_{\beta \neq \alpha} (1 - n_i^\beta); \]
\[ P(2) = \sum_{\alpha \neq \beta} n_i^\alpha n_i^\beta \prod_{\gamma \neq \alpha \beta} (1 - n_i^\gamma). \]
Digression: itinerant FM based on the Hubbard model

• Fails of the Stoner mechanism: exchange included but correlation neglected!

• A sufficient condition itinerant FM – a rigorous result as a reference point.

  Hund’s rule + quasi 1D band + strong correlation \(\rightarrow\) itinerant FM


• Non-perturbative QMC study on Cure-Weiss metals and magnetic transitions.

• Cold atom p-orbital systems and SrTiO\(_3\)/LaAlO\(_3\) interface.

Conclusion

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

• Elegancy of unification (group theory based on $Sp(4)$):
  AFM, SC and CDW phases/ Non-abelian Alice/Cheshire physics

• SU(6) Mott-ness: competition between Fermi surface (Slater) and local moments (Mott).
  Quantum phase transitions inside the insulating regime.

• Pomeranchuk effect of 2D SU(6) Hubbard model.