Exact SO(5) Symmetry in spin 3/2 fermionic system

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The spin 3/2 fermion models with contact interactions have a generic SO(5) symmetry without any fine-tuning of parameters. Its physical consequences are discussed in both the continuum and lattice models. A Monte-Carlo algorithm free of the sign problem at any doping and lattice topology is designed when the singlet and quintet interactions satisfy $U_0 \leq U_2 \leq -\frac{2}{5}U_0$ ($U_0 \leq 0$), thus making it possible to study different competing orders with high numerical accuracy. This model can be accurately realized in ultra-cold atomic systems.

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With the rapid progress in ultra-cold atomic systems, many alkali fermions have been cooled below Fermi temperatures [1, 2, 3]. All of them except $^6$Li have spins higher than 1/2 in the lowest hyper-fine multiplets. The spin degrees of freedom become free in the optical traps, which has attracted interest in their effects on Cooper pair structures and collective modes [4, 5]. The proposal of the optical lattice [6] has led to a tremendous progress in studying the strongly correlated systems [7, 8, 9, 10, 11]. Recently, fermionic lattice systems have been verified in recent experiments [15].

In this article, we focus on the symmetry properties and corresponding consequences in the spin 3/2 system with contact interactions, including both the continuum and lattice Hubbard model with on-site interactions. For neutral atoms, these interactions are generally described by two parameters in the total spin $S_T = 0, 2$ channels as $g_{0,2} = 4\pi\hbar^2a_{0,2}/M$ in the continuum model with $a_{0,2}$ the corresponding s-wave scattering lengths and $M$ the atom mass; or $U_{0,2}$ in the lattice model. Interactions in the odd total spin ($S_T = 1, 3$) channels are forbidden by Pauli’s exclusion principle. Remarkably, in addition to the explicit spin SU(2) symmetry, an enlarged SO(5) symmetry is present without any fine tuning of parameters. In the continuum model, this symmetry has direct consequences on the collective modes and pairing structures. In the lattice model, exact phase boundaries of various competing phases can be determined directly from symmetries. Because of the time-reversal symmetry of the Kramers doublets, a Monte-Carlo algorithm free of the notorious sign problem is designed when $U_0 \leq U_2 \leq -3/5U_0$ ($U_0 \leq 0$) at any filling level and lattice topology.

We start with the standard form of the spin 3/2 Hamiltonian of the continuum model [12]

$$H = \int d^d r \left\{ \sum_{\alpha=\pm 3/2,\pm 1/2} \psi^\dagger_\alpha(r)(-\hbar^2/2m)\nabla^2 - \mu)\psi_\alpha(r) + g_0P_{0,0}(r)P_{0,0}(r) + g_2\sum_{m=\pm 2,\pm 1,0}P^1_{2,m}(r)P_{2,m}(r) \right\}, \quad (1)$$

with $d$ the space dimension, $\mu$ the chemical potential and $P^0_{0,0}, P^2_{2,m}$ the singlet ($S_T = 0$) and quintet ($S_T = 2$) pairing operators defined through the Clebsh-Gordan coefficients for two indistinguishable particles as $P^1_{F,m}(r) = \sum_{\alpha,\beta}\frac{3}{2}\frac{2}{2}\delta_{F,0}\delta_{m,0}\psi^\dagger_\alpha(r)\psi^\dagger_\beta(r)$, where $F = 0, 2$ and $m = -F, -F+1, ..., F$.

We first construct the SO(5) algebra by introducing the five Dirac $\Gamma^a (1 \leq a \leq 5)$ matrices

$$\Gamma^1 = \begin{pmatrix} 0 & iI \\ -iI & 0 \end{pmatrix}, \Gamma^{2,3,4} = \begin{pmatrix} \sigma & 0 \\ 0 & -\sigma \end{pmatrix}, \Gamma^5 = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix}.$$  

Then the ten SO(5) generators are defined as $\Gamma^{ab} = -\frac{1}{2}[\Gamma^a, \Gamma^b] (1 \leq a, b \leq 5)$, where $I$ and $\sigma$ are the 2x2 unit and Pauli matrices. The four-component spinor can be defined by $\psi(r) = (\psi^T_\uparrow(r), \psi^T_\downarrow(r), \psi_\uparrow(r), \psi_\downarrow(r))$. Furthermore, the bilinear operators can be classified according to their properties under the SO(5) transformations. The 16 bilinear operators in the particle-hole (p-h) channel can be classified as SO(5)’s scalar, vector, and anti-symmetric tensors (generators) as

$$n(r) = \psi^\dagger_\uparrow(r)\psi_\uparrow(r), \quad n_a(r) = \frac{1}{2}\psi^\dagger_\uparrow(r)\Gamma^a\psi_\uparrow(r), \quad L_{ab}(r) = \frac{1}{2}\psi^\dagger_\uparrow(r)\Gamma_{ab}\psi_\uparrow(r). \quad (2)$$

$L_{ab}$ and $n_a$ together form the SU(4), or isomorphically, the SO(6) generators. The spin SU(2) generators $J_{x,y,z}$ are expressed as $J_+ = J_+ + iJ_y = \sqrt{3}(-L_{34} + iL_{24}) + (L_{12} + iL_{25}) - i(L_{13} + iL_{35}), J_- = J_-^*, J_z = L_{15}$. $n$ and $n_a$ have spin 0 and 2, and $L_{ab}$ contains both the spin 1 and 3 parts. Pairing operators can also...
be organized as $SO(5)$ scalar and vectors through the matrix $R = \Gamma_1 \Gamma_3$

\[\eta^\dagger(r) = \text{Re} \eta + i \text{Im} \eta = \frac{1}{2} \psi^\dagger_\alpha(r) R_{\alpha \beta} \psi^\dagger_\beta(r),\]

\[\chi^\dagger_\alpha(r) = \text{Re} \chi_\alpha + i \text{Im} \chi_\alpha = \frac{i}{2} \psi^\dagger_\alpha(r) (\Gamma^a R)_{\alpha \beta} \psi^\dagger_\beta(r)\]

where $P^\dagger_{0,0} = -\eta^\dagger/\sqrt{2}$, and $P^\dagger_{0, \pm 2} = (-\chi^\dagger_3 \pm i \chi^\dagger_5)/2$, $P^\dagger_{2, \pm 1} = (-\chi^\dagger_3 \pm i \chi^\dagger_5)/2$, $P^\dagger_{2,0} = -i \chi^\dagger_1/\sqrt{2}$. That is, $\chi^\dagger_\alpha$ are polar combinations of $J_2$’s eigenvectors $P^\dagger_{2,m}$. The existence of the $R$ matrix is related to the pseudoreality of $SO(5)’s$ spinor representation. It satisfies $R^2 = -1$, $R^\dagger = R^{-1} = -R$ and $R \Gamma^a R = -\Gamma^a$, $R \Gamma^{ab} R = i \Gamma^{ab}$.

The anti-unitary time-reversal transformation can be expressed as $T = R\, C$, where $C$ denotes complex conjugation and $T^2 = -1$. $N$, $n_\alpha$, and $L_{ab}$ transform differently under the $T$ transformation

\[T n_{a} T^{-1} = n_{a}, \quad T L_{ab} T^{-1} = -L_{ab}.\] (4)

With the above preparation, the hidden $SO(5)$ symmetry becomes manifest. The kinetic energy part has an explicit $SU(4)$ symmetry which is the unitary transformation among four spin components. The singlet and quintet interactions are proportional to $\eta^\dagger(r)\eta(r)$ and $\chi^\dagger_\alpha(r)\chi_\alpha(r)$ respectively, thus reducing the symmetry group from $SU(4)$ to $SO(5)$. When $g_0 = g_2$, the $SU(4)$ symmetry is restored because $\chi^\dagger_\alpha, \eta^\dagger$ together form its 6 dimensional antisymmetrical tensor representation. In the continuum model, interactions in other even partial wave channels also keep the $SO(5)$ symmetry. The odd partial wave scattering include spin 1 and 3 channel interactions $g_1$ and $g_3$, which together could form the 10-d adjoint representation. of $SO(5)$, if and only if $g_1 = g_3$. However, to leading order, $p$-wave scattering is much weaker than the $s$-wave one for neutral atoms, and can thus be safely neglected.

The $SO(5)$ symmetry implies more degeneracies in the collective excitations in the spin 3/2 Landau fermi liquid theory, which generally requires four fermi liquid functions in total spin $S_T = 0, 1, 2, 3$ channels. The $SO(5)$ symmetry of the microscopic Hamiltonian reduces these to three independent sets, classified according to the $SO(5)$ scalar, vector, and tensor channels as

\[f_{a, \beta, \gamma, \delta}(p, p') = f_s(p, p') + f_s(p, p') (\Gamma^a / 2)_{\alpha \beta} (\Gamma^\gamma / 2)_{\gamma \delta} \]

\[+ f_i(p, p') (\Gamma^a / 2)_{\alpha \beta} (\Gamma^\gamma / 2)_{\gamma \delta}.\] (5)

In other words, the effective interaction functions in the $S_T = 1, 3$ channels are exactly identical in all orders in perturbation theory. Furthermore, within the $s$-wave scattering approximation, the interaction functions become constants, and are given as $f_s = (g_0 + 5g_2)/16$, $f_i = (g_0 - 3g_2)/4$, $f_t = -(g_0 + g_2)/4$. Experiments in the fermi liquid regime can determine the four fermi liquid constants in the $S_T = 0, 1, 2, 3$ channels separately and verify the degeneracy between spin 1 and 3 channels. This degeneracy appears to be accidental in Ref.

\[\text{It is in fact exact and protected by the generic $SO(5)$ symmetry.}\]

The $SO(5)$ symmetry also enriches the Cooper pair structures. Ref. showed that, in addition to the singlet pairing when $g_0 < 0$, the spin 3/2 system energetically favors the polar pairing state in the quintet channel when $g_2 < 0$ with the order parameter $\Delta_{\text{real}} = \xi_1 P_{2,0} + \xi_2 (P_{2,0} + 2 P_{2,2}) \propto \xi_1 \lambda^4 + \xi_2 \lambda^5$ ($\xi_1$ are real). We understand that this is only a special case of the general pairing structures spanned by all the $\chi^\dagger_1, \ldots, \lambda$. The polar pairing states break the $SO(5) \otimes U(1)$ (charge) symmetry to $SO(4) \otimes Z_2$, and thus the Goldstone (GS) manifold is the quotient space [$SO(5) \otimes U(1)])/[SO(4) \otimes Z_2] = [S^4 \otimes U(1)])/Z_2$. Its dimension, 5, is the number of GS modes. When both $g_0, g_2$ are positive, $s$-wave pairing is not favorable. However, similarly to the spin fluctuation exchange mediated $p$-wave pairing in $^3$He \[\text{\textit{It is in fact exact and protected by the generic $SO(5)$ symmetry.}}\]

Now we consider the more interesting case of spin 3/2 fermions in the optical lattice. The periodic potential is $V(x, y, z) = V_0 (\sin^2(kx) + \sin^2(ky) + \sin^2(kz))$ with $V_0$ the potential depth, $k = \pi/l_0$ the wavevector, and $l_0$ the lattice constant. The hopping integral $t$ between neighboring sites decreases exponentially with increasing $V_0$. Within the harmonic approximation, the parameter $U/\Delta E \approx (\pi^2/2)(a_s/l_0)(V_0/E_\text{r})^{1/4}$, with $U$ the repulsion of two fermions on one site, $\Delta E$ the gap between the lowest and first excited single particle state in one site, $a_s$ the $s$-wave scattering length in the corresponding channel, and $E_\text{r} = \hbar^2k^2/2M$ the recoil energy. With the typical estimate of $a_s \sim 100a_B$ ( $a_B$ the Bohr radius), $l_0 \sim 5000\text{Å}$, and $(V_0/E_\text{r})^{1/4} \sim 1 \sim 2$, we arrive at $U/\Delta E < 0.1$. Thus this system can be approximated by the one-band Hubbard model

\[H = -t \sum_{(i,j), \sigma} \{ c^\dagger_{i \sigma} c_{j \sigma} + h.c. \} - \mu \sum_{i \sigma} c^\dagger_{i \sigma} c_{i \sigma} \]

\[+ U_0 \sum_{i} P^\dagger_{0,0}(i) P_{0,0}(i) + U_2 \sum_{i, m = \pm 2, \pm 1, 0} \sum_{i} \xi_{i, \sigma} P^\dagger_{2, m}(i) P_{2, m}(i).\] (6)

for particle density $n \leq 4$. At half-filling on a bipartite lattice, $\mu$ is given by $\mu_0 = (U_0 + 5U_2)/4$ to ensure the particle-hole (p-h) symmetry under the transformation $c_{i, \sigma} \rightarrow (-)^i c_{i, \sigma}$. The lattice fermion operators and their continuum counterparts are related by $\psi_\alpha(r) = c_{\alpha}(i)/(l_0)^{d/2}$. We use the same symbols for bilinear fermion operators as in the continuum model.

The proof of $SO(5)$ invariance in the continuum model applies equally well in the lattice model at any lattice topology and at any filling level. Eq. \[\text{\textit{It is in fact exact and protected by the generic $SO(5)$ symmetry.}}\] can be conveniently rewritten in another manifestly $SO(5)$ invariant form as

\[H_0 = -t \sum_{(i,j)} \{ \psi^\dagger(i) \psi(j) + h.c. \}.\] (7)
where the SU(4) symmetry appears at $U_0 = U_2$ as before.

\[ H_I = \sum_{i, 1 \leq a \leq 5} \left\{ \frac{3U_0 + 5U_2}{16} (n(i) - 2)^2 - \frac{U_2 - U_0}{4} n_a^2(i) \right\} - (\mu - \mu_0) \sum_i n(i), \]  

(8)

The lattice Hamiltonian, Eq. 6 contains even higher symmetries under certain conditions. One can construct the largest SO(8) algebra using all the independent fermionic bilinear operators. Its generators $M_{ab} (0 \leq a < b \leq 7)$ including $L_{ab} (1 \leq a < b \leq 5)$ as its SO(5) sub-algebra, are denoted as

\[ M_{ab} = \begin{pmatrix} 0 \Re \chi_1 & \Re \chi_5 & N & \Re \eta & \Im \chi_1 & n_1 & \Im L_{ab} & n_5 & 0 & - \Im \eta \\ \Re \chi_1 & 0 & \Im \chi_5 & n_5 & 0 & 0 & \X 0 & \X 0 & \X 0 \end{pmatrix}. \]

with $N = (n - 2)/2$. Its Casimir is a constant $C_{so8} = \sum_{0 \leq a < b \leq 7} M_{ab}^2 = 7$. The global SO(8) generators are defined to be uniform in the p-h channel as $M_{ab} = \sum_{i} M_{ab}(i)$ and staggered in the p-p channel as $M_{ab} = \sum_{(i)} (-)^i M_{ab}(i)$ on the bipartite lattice. These global generators commute with the hopping term $[M_{ab}, H_0] = 0$. On the other hand, order parameters transformed under the SO(8) group should be staggered (uniform) in the p-h (p-p) channel respectively. The SO(8) symmetry is always broken by the interaction, but its subgroup symmetry, the SO(5)$\otimes$SU(2) and SO(7) symmetries, appear under special conditions as shown below.

At $U_0 = 5$, $U_2$, $H_I$ can be rewritten as $H_I = \sum_{i, 1 \leq a \leq 5} \left\{ -U_2 L_{ab}^2(i) - (\mu - \mu_0) n(i) \right\}$, using the Fierz identity $\sum_{1 \leq a \leq 5} L_{ab}^2(i) + \sum_{1 \leq a \leq 5} n_a^2(i) + 5N^2(i) = 5$. As a generalization of the pseudospin algebra in the usual Hubbard model [21], we construct them as $\eta^a$, $\eta^b$, $N$. The symmetry at half-filling is SO(5)$\otimes$SU(2), which unifies the charge density wave (CDW) and the singlet pairing (SP) order parameters. Away from half-filling, this symmetry is broken but $\eta, \eta'$ are still eigen-operators since $[H, \eta^a] = - (\mu - \mu_0) S^a$ and $[H, \eta^b] = (\mu - \mu_0) \eta^b$.

The above symmetry structures guide the mean field (MF) analysis of the phase diagram. In the weak coupling limit, the complete MF decoupling is performed in the direct, exchange, and pairing channels. We take the MF ansatz on the 2d square lattice

\[ \langle n_a(i) \rangle = \langle \eta^a \rangle, \quad \langle N(i) \rangle = \langle \eta^b \rangle, \quad \langle L_{ab}(i) \rangle = \langle \eta^b \rangle, \quad \langle \chi_a(i) \rangle = \langle \chi_a \rangle. \]

and solve it self-consistently at half-filling to obtain the phase diagram shown in Fig. 1. Higher symmetry lines E, F, G, H separate phases A, B, C, D as first order phase transition boundaries where order parameters smoothly rotate from one phase to another. Symmetries on lines E, F, G, H and the order parameters are SU(4)(adjoint Rep), SO(7)(vector Rep), SO(5)$\otimes$SU(2) (scalar $\otimes$ vector Rep), SO(7) (adjoint Rep) as discussed before. Phases A and B spontaneously break the SO(5) symmetry in the

![FIG. 1: The mean-field phase diagram at half-filling on a bipartite lattice. A) and B): staggered phases of the SO(5) adjoint and vector Reps; C): the singlet superconductivity; D): CDW; E), F), G) and H): exact phase boundaries with higher symmetries. Between the dashed lines ($U_0 \leq U_2 \leq -3/5 U_2$), a Monte-Carlo algorithm free of the minus sign problem at any filling level and lattice topology is possible.](image)
adjoint and vector Rep channels respectively. Phases C and D have singlet pairing SC and CDW as order parameters, respectively. Order parameters in each phase and corresponding GS modes are summarized in Table 1. The effective theory is generally given by a quantum non-linear σ model defined on the GS manifold.

One major difficulty of Monte-Carlo simulations in fermionic systems, the sign problem [21], is absent in the spin 3/2 model when $U_0 \leq U_2 \leq -3/5 U_0$. By the Hubbard-Stratonovich (HS) transformation, the partition function can be written as below when $V = -(3U_0 + 5U_2)/8 > 0$ and $W = (U_2 - U_0)/2 > 0$, or equivalently $U_0 \leq U_2 \leq -3/5 U_0$,

$$Z = \int Dn \int Dn^a \exp \left\{ -\frac{V}{2} \int_0^\beta d\tau \sum_i n(i, \tau)^2 \right. - \frac{W}{2} \int_0^\beta d\tau \sum_{i,a} n^2_i (i, \tau) \left. \right\} \det \{ I + B \},$$

where $B = T e^{-\int_0^\beta d\tau H_0 + H_1(\tau)}$ and $T$ is the time order operator. Its discrete version is

$$B = e^{\Delta \tau H_0} e^{\Delta \tau H_1(\tau _1)} \ldots e^{\Delta \tau H_0} e^{\Delta \tau H_1(\tau _2)} e^{\Delta \tau H_0} e^{\Delta \tau H_1(\tau _1)},$$

$$H_1(\tau) = -\sum_i \psi^\dagger \psi \left( V (n(i, \tau) - 2) + (\mu - \mu_0) \right) -W \sum_{i,a} \psi^\dagger \psi \Gamma_{a\beta} \psi \quad n^a(i, \tau),$$

where $\Delta \tau = \beta/L$. $I + B$ is invariant under the time-reversal transformation: $T(I + B)T^{-1} = I + B$. If $\lambda$ is an eigenvalue of $I + B$ with the eigenvector $|\phi\rangle$, then $\lambda^*$ is also an eigenvalue with the eigenvector $T|\phi\rangle$. From $T^2 = -1$, it follows that $T|\phi\rangle = T^2|\phi\rangle = 0$, i.e. $|\phi\rangle$ and $T|\phi\rangle$ are orthogonal. Thus although $I + B$ may not be Hermitian because of the $T$ operator, its determinant, a product of $\lambda^* \lambda$, is always positive-definite. Our proof is equally valid in the practical sampling with the discrete HS transformation as in Ref. [22], and has been confirmed numerically [24]. We emphasize that this proof is valid for any filling and lattice topology. A similar model has recently been introduced in Ref. [29], where the sign problem is also introduced. However, their model keeps only the diagonal $n^2_i$ interaction and is not spin rotationally invariant. The valid region for the above algorithm (see Fig. 1) includes the 5-vector phases B, SP phase C and their SO(7) boundary, which are analogs of the competitions between antiferromagnetism and superconductivity in the high $T_c$ context. It would be interesting to study the doping effect, the frustration on the triangular lattice, etc, which are difficult at low temperatures for previous Monte-Carlo works. Extensive numerical simulations are currently being carried out [24].

Besides the alkali atoms, the trapping and cooling of the alkaline-earth atoms are also exciting recently [23,28]. Among these two families, $^{132}$Cs, $^9$Be, $^{135}$Ba and $^{137}$Ba are spin 3/2 atoms. $^{132}$Cs is unstable and the $2s^2 \rightarrow 2s^22p^1$ resonance of Be lies in the ultraviolet region, making them difficult for experimental use. The resonances of the last two Ba atoms are $6s^2 \rightarrow 6s^16p^1$ at 553.7 nm [27], thus they are possible candidates. Their scattering lengths are not available now, but that of $^{138}$Ba (spin 0) was estimated as $-41a_B$ [22]. Because the 6s shell of Ba is full-filled, both the $a_0$, $a_2$ of $^{135}$Ba and $^{137}$Ba should have the similar value. Considering the rapid development in this field, we expect more and more spin 3/2 systems will be realized experimentally, allowing us to explore the full phase diagram.

In summary, we found an exact and generic SO(5) symmetry in spin 3/2 models with local interactions. This model can be accurately realized in cold atom systems and the theoretical predictions can be tested experimentally by the exact reaction among the Landau fermi liquid parameters, spin wave functions of the Cooper pairs, exact boundaries of quantum phase transitions among various competing states and the number of the collective modes. In the regime where accurate Monte Carlo simulations can be carried out without the sign problem, detailed quantitative comparisons with experiments are possible, including the quantum phase transition from the AF to the SC phases as a function of doping.

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