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

Congjun Wu,[1] Jiang-ping Hu,[2] and Shou-cheng Zhang[1]

[1]Department of Physics, McCullough Building, Stanford University, Stanford California 94305-4045, USA

[2]Department of Physics and Astronomy, University of California, Los Angels, California 90095-1547, USA

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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 $U_0 \le U_2 \le -\frac{3}{5}U_0$ ($U_0 \le 0$), thus making it possible to study different competing orders with high numerical accuracy. This model can be accurately realized in ultracold atomic systems.

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With the rapid progress in ultracold atomic systems, many alkali fermions have been cooled below Fermi temperatures [1–3]. All of them except ^{6}Li have spins higher than 1/2 in the lowest hyperfine 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 bosonic lattice systems [7–11]. Recently, fermionic lattice systems are also exciting. For example, the degenerate ^{40}K gas has been prepared in a one-dimensional optical lattice [12].

Comprehensive analysis of symmetries is helpful in understanding the physics in strongly correlated systems. For example, the SO(5) theory [13] of high-T_c cuprates unifies the d-wave superconductivity (SC) and antiferromagnetism orders, leading to many experimental consequences. The sharp neutron scattering mode can be interpreted as the pseudo Goldstone (GS) mode [13]. The prediction of the antiferromagnetic vortex core [14] has also 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 model with s-wave scattering and the generalized 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 $g_{0,2} = 4\pi\hbar^2 a_{0,2}/M$ 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 $U_0 \le U_2 \le -3/5U_0$ ($U_0 \le 0$) at any filling level and lattice topology.

We start with the standard form of the spin-3/2 Hamiltonian of the continuum model [4,5]

$$H = \int d^d\mathbf{r} \Big\{ \sum_{\alpha=\pm 3/2,\pm 1/2} \psi^\dagger_\alpha(\mathbf{r}) \Big(\frac{-\hbar^2}{2m}\nabla^2 - \mu \Big) \psi_\alpha(\mathbf{r}) + g_0 P^\dagger_{0,0}(\mathbf{r}) P_{0,0}(\mathbf{r}) + g_2 \sum_{m=\pm 2,\pm 1,0} P^\dagger_{2,m}(\mathbf{r}) P_{2,m}(\mathbf{r}) \Big\}, \quad (1)$$

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

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

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

Then the ten SO(5) generators are defined as $\Gamma^{ab} = -\frac{i}{2}[\Gamma^a, \Gamma^b]$ ($1 \le a, b \le 5$), where I and $\vec\sigma$ are the 2×2 unit and Pauli matrices. The four-component spinor can be defined by $\psi(\mathbf{r}) = [\psi_{3/2}(\mathbf{r}), \psi_{1/2}(\mathbf{r}), \psi_{-1/2}(\mathbf{r}), \psi_{-3/2}(\mathbf{r})]^T$. 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 antisymmetric tensors (generators) as

$$n(\mathbf{r}) = \psi^\dagger_\alpha(\mathbf{r})\psi_\alpha(\mathbf{r}), \qquad n_a(\mathbf{r}) = \frac{1}{2}\psi^\dagger_\alpha(\mathbf{r})\Gamma^a_{\alpha\beta}\psi_\beta(\mathbf{r}),$$
$$L_{ab}(\mathbf{r}) = -\frac{1}{2}\psi^\dagger_\alpha(\mathbf{r})\Gamma^{ab}_{\alpha\beta}\psi_\beta(\mathbf{r}). \quad (2)$$

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 $J_+ = J_x + iJ_y = \sqrt{3}(-L_{34} + iL_{24}) + (L_{12} + iL_{25}) - i(L_{13} + iL_{35})$, $J_- = J_+^\dagger$, and $J_z = -L_{23} + 2L_{15}$. 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 $R = \Gamma_1\Gamma_3$,

$$\begin{aligned}\eta^\dagger(\mathbf{r}) &= \mathrm{Re}\eta + i\mathrm{Im}\eta = \frac{1}{2}\psi_\alpha^\dagger(\mathbf{r})R_{\alpha\beta}\psi_\beta^\dagger(\mathbf{r}),\\ \chi_a^\dagger(\mathbf{r}) &= \mathrm{Re}\chi_a + i\mathrm{Im}\chi_a = -\frac{i}{2}\psi_\alpha^\dagger(\mathbf{r})(\Gamma^a R)_{\alpha\beta}\psi_\beta^\dagger(\mathbf{r}),\end{aligned} \tag{3}$$

where $P_{0,0}^\dagger = -\eta^\dagger/\sqrt{2}$, and $P_{2,\pm2}^\dagger = (\mp\chi_1^\dagger + i\chi_5^\dagger)/2$, $P_{2,\pm1}^\dagger = (-\chi_3^\dagger \pm i\chi_2^\dagger)/2$, $P_{2,0}^\dagger = -i\chi_4^\dagger/\sqrt{2}$. That is, $\chi_a^\dagger$ are polar combinations of J_z's eigenoperators $P_{2,m}^\dagger$. The existence of the R matrix is related to the pseudoreality of SO(5)'s spinor representation. It satisfies $R^2 = -1$, $R^\dagger = R^{-1} = {}^tR = -R$, and $R\Gamma^a R = -{}^t\Gamma^a$, $R\Gamma^{ab}R = {}^t\Gamma^{ab}$ [16]. The antiunitary time-reversal transformation can be expressed as $T = RC$, where C denotes complex conjugation and $T^2 = -1$. N, n_a, and L_{ab} transform differently under the T transformation

$$TnT^{-1} = n, \qquad Tn_aT^{-1} = n_a, \qquad TL_{ab}T^{-1} = -L_{ab}. \tag{4}$$

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 $\eta^\dagger(\mathbf{r})\eta(\mathbf{r})$ and $\chi_a^\dagger(\mathbf{r})\chi_a(\mathbf{r})$, respectively, thus reducing the symmetry group from SU(4) to SO(5). When $g_0 = g_2$, the SU(4) symmetry is restored because $\chi_a^\dagger$, $\eta^\dagger$ together form its six-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 10D adjoint representation of SO(5) at $g_1 = g_3$. However, to the leading order, p-wave scattering is weak 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 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

$$\begin{aligned}f_{\alpha\beta,\gamma\delta}(p,p') &= f_s(p,p') + f_v(p,p')(\Gamma^a/2)_{\alpha\beta}(\Gamma^a/2)_{\gamma\delta}\\ &\quad + f_t(p,p')(\Gamma^{ab}/2)_{\alpha\beta}(\Gamma^{ab}/2)_{\gamma\delta}.\end{aligned} \tag{5}$$

In other words, the effective interaction functions in the $S_T = 1, 3$ channels are exactly identical in all orders in perturbation theory. Within the s-wave scattering approximation, the interaction functions become constants, and are given as $f_s = (g_0 + 5g_2)/16$, $f_v = (g_0 - 3g_2)/4$, $f_t = -(g_0 + g_2)/4$. 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. [5]. It is in fact exact and protected by the generic SO(5) symmetry.

The SO(5) symmetry also enriches the Cooper pair structures. Reference [4] showed that the quintent pairing state at $g_2 < 0$ energetically favors the polar state with the order parameter $\Delta_{\mathrm{real}}^\dagger = \xi_1 P_{2,0}^\dagger + \xi_2(P_{2,2}^\dagger + P_{2,-2}^\dagger) \propto \xi_1\chi_4^\dagger + \xi_2\chi_5^\dagger$ ($\xi_{1,2}$ are real). We understand that this is only a special case of the general pairing structures spanned by all the $\chi_{1-5}^\dagger$. The polar pairing states break the SO(5) ⊗ U(1) (charge) symmetry to SO(4) ⊗ Z_2, and thus the Goldstone manifold is the quotient space $[\mathrm{SO}(5)\otimes \mathrm{U}(1)]/[\mathrm{SO}(4)\otimes Z_2] = [S^4 \otimes \mathrm{U}(1)]/Z_2$. Its dimension, 5, is the number of GS modes. When both $g_{0,2}$ are positive, s-wave pairing is not favorable. However, similarly to the ^{3}He system [17,18], the spin fluctuations in the tensor channel can induce effective attractions between two atoms with total spin 1 and 3. This may lead to p-wave pairing where the spin part forms the 10D adjoint representation of SO(5).

Now we consider the 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 wave vector, and l_0 the lattice constant. The hopping integral t decreases exponentially with increasing V_0. Within the harmonic approximation, parameter $U/\Delta E \approx (\pi^2/2)(a_s/l_0) \times (V_0/E_r)^{1/4}$, with U the repulsion of two fermions on one site, ΔE 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 $E_r = \hbar^2k^2/2M$ the recoil energy. With the typical estimation of $a_s \sim 100a_B$ (a_B the Bohr radius), $l_0 \sim 5000$ A, and $(V_0/E_r)^{1/4} \approx 1$–2, we arrive at $U/\Delta E < 0.1$. Thus this system can be approximated by the one-band Hubbard model

$$\begin{aligned}H &= -t\sum_{\langle ij\rangle,\sigma}\{c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{H.c.}\} - \mu\sum_{i\sigma}c_{i\sigma}^\dagger c_{i\sigma}\\ &\quad + U_0\sum_i P_{0,0}^\dagger(i)P_{0,0}(i) + U_2\sum_{i,m=\pm2,\pm1,0}P_{2,m}^\dagger(i)P_{2,m}(i),\end{aligned} \tag{6}$$

for particle density $n \le 4$. At half-filling on a bipartite lattice, μ is given by $\mu_0 = (U_0 + 5U_2)/4$ to ensure the particle-hole symmetry. The lattice fermion operators and their continuum counterparts are related by $\psi_\alpha(\mathbf{r}) = c_\alpha(i)/(l_0)^{d/2}$. The same symbols are used for bilinear 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. Equation (6) can be rewritten in another manifestly SO(5) invariant form as

$$H_0 = -t\sum_{\langle i,j\rangle}\{\psi^\dagger(i)\psi(j) + \text{H.c.}\}, \qquad (7)$$

$$H_I = \sum_{i,1\le a\le 5}\Big\{\frac{3U_0+5U_2}{16}[n(i)-2]^2 - \frac{U_2-U_0}{4}n_a^2(i)\Big\} - (\mu-\mu_0)\sum_i n(i), \qquad (8)$$

where the SU(4) symmetry appears at $U_0 = U_2$ as before.

Equation (6) contains even higher symmetries under certain conditions. One can construct the largest SO(8) [19] algebra using all the independent fermionic bilinear operators. Its generators M_{ab} $(0 \le a < b \le 7)$ including L_{ab} $(1 \le a < b \le 5)$ as its SO(5) subalgebra are

$$M_{ab} = \begin{pmatrix} 0 & \text{Re}\chi_1 \sim \text{Re}\chi_5 & N & \text{Re}\eta \\ & & \text{Im}\chi_1 & n_1 \\ & L_{ab} & \sim & \sim \\ & & \text{Im}\chi_5 & n_5 \\ & & 0 & -\text{Im}\eta \\ & & & 0 \end{pmatrix},$$

with $N = (n-2)/2$. Its Casimir operator is a constant $C_{\text{SO}(8)} = \sum_{0\le a<b\le 7} M_{ab}^2(i) = 7$. 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 SO(5) ⊗ SU(2) and SO(7) can appear as shown below.

At $U_0 = 5U_2$, H_I can be rewritten as $H_I = \sum_{i,1\le a,b\le 5}\{-U_2 L_{ab}^2(i) - (\mu-\mu_0)n(i)\}$, using the Fierz identity $\sum_{1\le a\le 5} L_{ab}^2(i) + \sum_{1\le a\le 5} n_a^2(i) + 5N^2(i) = 5$. As a generalization of the pseudospin algebra in the usual Hubbard model [20], we construct them as $\eta^\dagger$, η, N. The symmetry at half-filling is SO(5) ⊗ 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 η, $\eta^\dagger$ are still eigenoperators since $[H, \eta^\dagger] = -(\mu-\mu_0)\eta^\dagger$, and $[H, \eta] = (\mu-\mu_0)\eta$.

The p-h channel SO(5) ⊗ U(1) symmetry can also be extended to SO(7) at $U_0 = -3U_2$ where H_I can be rewritten as $\sum_{i,0\le a<b\le 6}\{\frac{2}{3}U_2 M_{ab}(i)^2 - (\mu-\mu_0)n(i)\}$. The SO(7) symmetry is exact at half-filling. Its 7D vector representation unifies the staggered five-vector and SP order parameters. Its 21D adjoint representation unifies the staggered SO(5) adjoint representation order parameters, CDW, and quintet pairing (QP) order parameters.

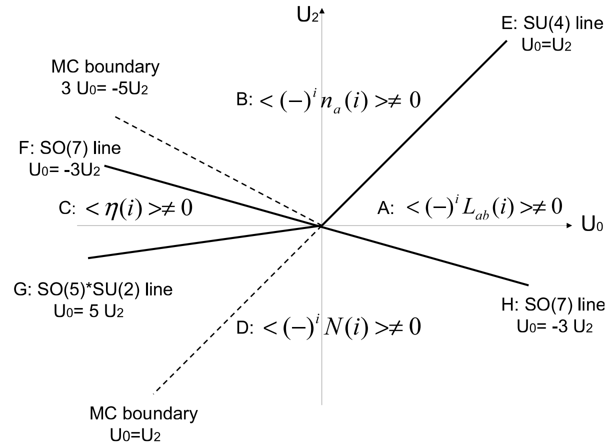

FIG. 1. The MF phase diagram at half-filling on a bipartite lattice. (A) and (B): staggered phases of the SO(5) adjoint and vector representations; (C): the singlet superconductivity; (D): CDW; (E), (F), (G), and (H): exact phase boundaries with higher symmetries. Between the dashed lines ($U_0 \le U_2 \le -3/5U_0$), a Monte Carlo algorithm free of the sign problem is possible.

Away from half-filling, QP operators are spin-2 quasi Goldstone operators $[H, \chi_a^\dagger(\chi_a)] = \mp(\mu-\mu_0)\chi_a^\dagger(\chi_a)$. These χ modes are just the analogs of the π modes in the high-T_c context [13].

In the weak coupling limit, the complete mean-field (MF) decoupling is performed in the direct, exchange, and pairing channels. We take the MF ansatz on the 2D square lattice $\langle n_a(i)\rangle = (-)^i\overline{n}_a$, $\langle N(i)\rangle = (-)^i\overline{N}$, $\langle L_{ab}(i)\rangle = (-)^i\overline{L}_{ab}$, $\langle\eta(i)\rangle = \overline{\eta}$, and $\langle\chi_a(i)\rangle = \overline{\chi}_a$. Then we 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 representation), SO(7) (vector representation), SO(5) ⊗ SU(2) (scalar ⊗ vector representation), SO(7) (adjoint representation) as discussed before. Phases A and B spontaneously break the SO(5) symmetry in the adjoint and vector representation 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 I. The effective theory is generally given by a quantum nonlinear σ model defined on the GS manifold.

One major difficulty of Monte Carlo simulations in fermionic systems, the sign problem [21], can be absent in the spin-3/2 model. 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 $U_0 \le U_2 \le -3/5U_0$,

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

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

TABLE I. Order parameters, the corresponding Goldstone manifolds, and the number of Goldstone modes in each phase on the bipartite lattice at half-filling.

Phase	Order parameters	GS manifold	GS modes
A	$(-)^i L_{ab}(i)$	SO(5)/[SO(3) ⊗ SO(2)]	6
B	$(-)^i n_a(i)$	SO(5)/SO(4) ≡ S^4	4
C	$\eta(i)$	$U(1)$	1
D	CDW		
E	$(-)^i n_a(i), (-)^i L_{ab}(i)$	U(4)/[U(2) ⊗ U(2)]	8
F	$(-)^i n_a(i)$, $\eta(i)$	SO(7)/SO(6) ≡ S^6	6
G	CDW, $\eta(i)$	SO(3)/SO(2) ≡ S^2	2
H	CDW, $\chi_a(i), (-)^i L_{ab}(i)$	SO(7)/[SO(5) × SO(2)]	10

$$B = e^{\Delta\tau H_0} e^{\Delta\tau H_I(\tau_L)} \cdots e^{\Delta\tau H_0} e^{\Delta\tau H_I(\tau_2)} e^{\Delta\tau H_0} e^{\Delta\tau H_I(\tau_1)},$$
$$H_I(\tau) = -\sum_i \psi_\alpha^\dagger(i)\psi_\alpha(i)\{V(n(i,\tau) - 2) + (\mu - \mu_0)\} \quad (9)$$
$$- W\sum_{i,a} \psi_\alpha^\dagger(i)\Gamma^a_{\alpha\beta}\psi_\beta(i) n^a(i,\tau),$$

where $\Delta\tau = \beta/L$. $I + B$ is invariant under the time-reversal transformation: $T(I + B)T^{-1} = I + B$. If λ is an eigenvalue of $I + B$ with the eigenvector $|\phi\rangle$, then λ^* is also an eigenvalue with the eigenvector $T|\phi\rangle$. From $T^2 = -1$, it follows that $\langle\phi|T\phi\rangle = \langle T^2\phi|T\phi\rangle = 0$, i.e., $|\phi\rangle$ and $T|\phi\rangle$ are orthogonal. Thus, although $I + B$ may not be Hermitian because of the $\mathcal{T}$ operator, its determinant, a product of $\lambda^*\lambda$, is always positive semidefinite. Our proof is equally valid in the practical sampling with the discrete HS transformation as in Ref. [22], and has been confirmed numerically [23]. We emphasize that this proof is valid for any filling and lattice topology. A similar model without the sign problem has recently been introduced in Ref. [24], which only keeps the diagonal n_4^2 interaction. The valid region for the above algorithm (see Fig. 1) includes the five-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 [23].

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 $6s^2 \rightarrow 6s^1 6p^1$ 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.

In summary, we found an exact and generic SO(5) symmetry in spin-3/2 models with local interactions, which can be realized in cold atomic systems. This hidden symmetry can be tested experimentally by the structures of Fermi liquid parameters and Cooper pairs, boundaries of various competing quantum phases, and numbers of the collective modes. In the regime where Monte Carlo simulations are free of the sign problem, quantitative comparisons with experiments are possible to study different competing phases with high accuracy.

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