Exact spontaneous plaquette ground states for high-spin ladder models

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We study the exchange physics in high-spin Mott insulating systems with $S=3/2$ which is realizable in ultracold atomic systems. The high symmetry of $SO(5)$ or $SU(4)$ therein renders stronger quantum fluctuations than the usual spin-1/2 systems. A spontaneous plaquette ground state without any site and bond spin orders is rigorously proved in a ladder spin-3/2 model, whose topological excitations exhibit fractionalization behavior. The generalization to the $SU(N)$ plaquette state is also investigated.

There has been considerable interest recently in high-spin systems with enlarged symmetry among both condensed-matter and atomic physics.[1–6] With the rapid progress in the field of ultracold atomic physics,[7] optical traps and lattices open up possibilities of simulating and manipulating high-spin physics experimentally in a controlled way. For example, the high-spin fermionic ^{40}K gas has been produced in one-dimensional (1D) optical lattices.[8] On the other hand, as a paradigm in the low-dimensional magnetic systems, the spin chains and ladders have stimulated intense investigation recently of how to simulate them using cold atoms. Several schemes have been proposed to implement these quantum spin models in optical lattices.[3,9,10] So far most of these proposals are still concentrated in the spin-1/2 and spin-1 systems. Although most high-spin systems only exhibit the usual spin $SU(2)$ symmetry, a generic high symmetry of $SO(5)$, or isomorphic $Sp(4)$, has been rigorously proven in spin 3/2 systems.[1,2] They may be realized with several candidate atoms, such as ^{132}Cs, ^{9}Be, ^{135}Ba, and ^{137}Ba. This symmetry sets up a framework to unify many seemingly unrelated properties of Fermi liquid theory, Cooper pairs, and magnetic structures in such systems. Conventionally, a high-spin system is assumed in the large-S limit, and thus is considered as more classical-like than its low-spin counterpart. However, due to their high symmetry, the spin-3/2 systems are actually in the large-N limit. As a result, the quantum fluctuations are stronger than the usual spin-1/2 systems, which results in many unique properties.

In this work, a spin-3/2 exchange model with intrinsic $SO(5)$ symmetry is proposed by us, and it includes the $SU(4)$ model as its special case. We then study a class of solvable spin-3/2 ladder models which exhibit the exact spontaneous plaquette ground states without any site and bond spin orders, and the topological excitations are studied. The existence of a plaquette phase has been proposed and our results may provide a firm ground for understanding the plaquette phase.[4,11,12] The generalization of our theory to arbitrary spin systems with $SU(N)$ symmetry is also discussed.

We first derive the general $SO(5)$ exchange model from a spin-3/2 Hubbard model in the strong repulsive interaction limit $U_0, U_2 \gg t$, where $U_{0,2}$ are the on-site Hubbard repulsion in the singlet and quintet channels, respectively. The projection perturbation theory is employed to study the low-energy exchange process through virtual hopping at quarter-filling, i.e., one particle per site. For two neighboring sites, the total spin can be $S_{tot}=0,1,2,3$. Exchange energies in the singlet and quintet channels are $J_0=4t^2/U_0$ and $J_2=4t^2/U_2$ respectively. These two channels also form $Sp(4)$'s singlet and quintet. On the other hand, no exchange energies exist in the triplet and septet channels, which together form a ten-dimensional (10D) representation of the $Sp(4)$ group. The effective Hamiltonian can be expressed through the bond projection operators in the singlet channel $Q_0(ij)$ and quintet channel $Q_2(ij)$ as $H_{ex}=\Sigma_{\langle i,j \rangle}h_{ij}=-\Sigma_{\langle i,j \rangle}\{J_0Q_0(i,j)+J_2Q_2(i,j)\}$, or in an explicitly $Sp(4)$ invariant form as

$$H_{ex} = \sum_{\langle i,j \rangle} \left\{ \frac{1}{4}[c_1 A^{\gamma_1}(i)A^{\gamma_1}(j) + c_2 A^{\gamma_2}(i)A^{\gamma_2}(j)] - c_3 \right\}, \quad (1)$$

with $c_1=(J_0+J_2)/4$, $c_2=(3J_2-J_0)/4$ and $c_3=(J_0+5J_2)/16$, where $A^{\gamma_1}=2L_{ab}=c_\alpha^\dagger\Gamma_{\alpha\beta}^{ab}c_\beta$ $(\gamma_1=1,\ldots,10,1\leq a<b\leq 5)$ and $A^{\gamma_2}=2n_a=c_\alpha^\dagger\Gamma_{\alpha\beta}^a c_\beta$ $(\gamma_2=11,\ldots,15,1\leq a\leq 5)$ with the Dirac Γ matrices that can be found in Ref. 1. The n_a operators transform as a 5 vector under the $Sp(4)$ group and the L_{ab} operators form the ten generators of the $SO(5)$ group.

It is obvious that an $SU(4)$ symmetry appears at $J_0=J_2$. Then Eq. (1) reduces into the $SU(4)$ symmetric form with the fundamental representations on every site where L_{ab} and n_a together (or A^γ with $\gamma=1,\ldots,15$) form the 15 generators of the $SU(4)$ group. In this case, the spin-3/2 Hamiltonian is equivalent to the well-known $SU(4)$ spin-orbital model up to a constant term.[4,11] Equation (1) can be expressed by the usual $SU(2)$ spin operators with biquadratic and bicubic terms as

$$H'_{ex} = \sum_{\langle i,j \rangle} a(\vec{S}_i \cdot \vec{S}_j) + b(\vec{S}_i \cdot \vec{S}_j)^2 + c(\vec{S}_i \cdot \vec{S}_j)^3, \quad (2)$$

with $a=-\frac{1}{96}(31J_0+23J_2)$, $b=\frac{1}{72}(5J_0+17J_2)$, and $c=\frac{1}{18}(J_0+J_2)$.

The magnetic structure of the one-dimensional spin-3/2 model (2) can be analyzed by bosonization methods combined with renormalization group methods via studying the corresponding Hubbard model at quarter-filling.[13] A spin gap opens with the appearance of the spin Peierls order at U_2
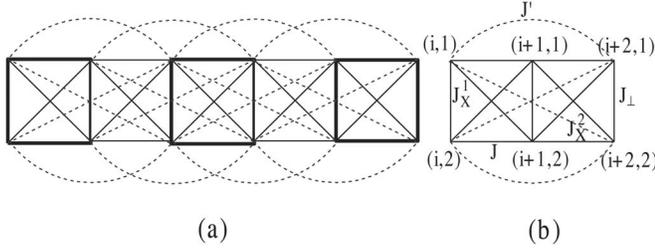
FIG. 1. (a) The spin ladder model. Plaquettes in bold lines represent the plaquette singlets. (b) The basic block to construct the spin ladder model.

$> U_0 > 0$, while it vanishes at $U_0 \geqslant U_2 > 0^2$, where $U_{0,2}$ are the on-site repulsions in the spin singlet and quintet channels respectively.

Now we construct a spin-3/2 ladder model exhibiting an exact plaquette ground state, which is an $SU(4)$ generalization of the valence bond state (VBS) as shown in Fig. 1. Different from the usual $SU(2)$ case where every bond is an $SU(2)$ singlet, here at least four sites, i.e., a plaquette, are needed to form an $SU(4)$ singlet, thus there is only plaquette order without any bond order in this state. As shown in Fig. 1(a), the model is described by the Hamiltonian

$$H_{lad} = J_\perp \sum_i h_{(i,1),(i,2)} + J \sum_{i,\alpha} h_{(i,\alpha),(i+1,\alpha)} + \sum_i \sum_{\delta=1}^2 J_\times^\delta [h_{(i,1),(i+\delta,2)}$$

$$+ h_{(i,2),(i+\delta,1)}] + J' \sum_{i,\alpha} h_{(i,\alpha),(i+2,\alpha)}, \tag{3}$$

where the site is labeled by its rung number i and chain index $\alpha = 1,2$ and $h_{ij} = \frac{1}{4}[c_1 A^{\gamma_1}(i) A^{\gamma_1}(j) + c_2 A^{\gamma_2}(i) A^{\gamma_2}(j)]$. Here we take $J_\perp$, J, $J_\times^1$, $J_\times^2$, and J' as positive constants in unit of J_0 and set $J = 1$. The regular railway-ladder model corresponds to $J_\times^1 = J_\times^2 = J' = 0$. To gain some intuition about the plaquette state, we first consider a four-site system with diagonal exchanges (a tetrahedron). For such a simple system with $SU(4)$ symmetry, the ground state (GS) is a plaquette singlet[4] defined as

$$su_4(1234) = \sum_{\mu\nu\gamma\delta} \frac{1}{\sqrt{24}} \Gamma_{\mu\nu\gamma\delta} |1_\mu 2_\nu 3_\gamma 4_\delta\rangle,$$

where $\Gamma_{\mu\nu\gamma\delta}$ is an antisymmetric tensor and $\mu, \nu, \gamma, \delta = \pm\frac{3}{2}, \pm\frac{1}{2}$. Such a $SU(4)$ singlet is rotationally invariant under any of the 15 generators A^i of a $SU(4)$ group with $i = 1, \ldots, 15$. For a tetrahedron with $SO(5)$ symmetry, the $SU(4)$ singlet is no doubt an eigenstate with the eigenenergy $e_\boxtimes = -5c_1 - \frac{5}{2}c_2$. Furthermore, it is easily verified that the $SU(4)$ singlet is the ground state of the four-site $SO(5)$ exchange model for $c_2 \geqslant 0$.

We now focus on the $SU(4)$ ladder described by Eq. (3) with $c_2 = c_1$. It turns out that the exact ground state of the $SU(4)$ ladder model is a doubly degenerate singlet provided the relation

$$J_\perp = \frac{3}{2}J = \frac{3}{2}J_\times^1 = 3J_\times^2 = 3J' \tag{4}$$

is fulfilled. The degenerate GSs are composed of products of nearest-neighboring plaquette singlets. Explicitly, for a ladder with length M, the two degenerate ground states are given by

$$|P_1\rangle = \prod_{i=1}^{M/2} su_4[(2i,1),(2i,2),(2i+1,1),(2i+1,2)]$$

$$|P_2\rangle = \prod_{i=1}^{M/2} su_4[(2i-1,1),(2i-1,2),(2i,1),(2i,2)],$$

with the corresponding ground energy

$$E = -M\frac{35}{8}c_1, \tag{5}$$

where periodic boundary condition is assumed $M+1 \equiv 1$.

The proof of the above conclusion can be understood through two steps. First, one observes that the plaquette singlet product is no doubt an eigenstate of the global Hamiltonian because any generator of the $SU(4)$ aside from the plaquette acting on the plaquette singlet is zero, i.e.,

$$A_5^\gamma[A_1^\gamma + A_2^\gamma + A_3^\gamma + A_4^\gamma]su_4(1234)|5\nu\rangle = 0,$$

where $\gamma = 1, \ldots, 15$. Secondly, we prove that such an eigenstate is the ground state of the global Hamiltonian. In order to prove it, we utilize the Rayleigh-Ritz variational principle

$$\langle\Psi|\sum_{i=1}^M h(B_i)|\Psi\rangle \geqslant E_{\text{g.s.}} \geqslant \sum_{i=1}^M e_{\text{g.s.}}(B_i), \tag{6}$$

which implies that an eigenstate $|\Psi\rangle$ is the ground state of a global Hamiltonian if it is simultaneously the ground state of each local sub-Hamiltonian.[14] Here $E_{\text{g.s.}}$ is the ground state energy of the global Hamiltonian, which is represented as a sum of M sub-Hamiltonians, say, $H = \sum_{i=1}^M h(B_i)$, and $e_{\text{g.s.}}(B_i)$ represents the ground state energy of a sub-Hamiltonian $h(B_i)$.

Now we apply the above general principle to study our model given by Eq. (3). Explicitly, as long as Eq. (4) holds true, we can decompose Eq. (3) as

$$H = \sum_{i=1}^M h(B_i), \tag{7}$$

where $h(B_i) = J' \sum_{\langle ij \rangle} h_{ij}$ denotes the Hamiltonian of a six-site block as shown in Fig. 1(b) and $\langle ij \rangle$ represents all the available bonds in the block of B_i. For convenience, we use the rung index on the left side of a six-site block to label the block. For such a six-site cluster with 15 equivalent bonds, the local Hamiltonian can be represented as a Casimir operator and the representation with smallest Casimir corresponds to the Young diagram $[2^2 1^2]$. It follows that eigenstates given by

$$|B_i\rangle_1 = su_4[(i,1),(i,2),(i+1,1),(i+1,2)] \otimes d_{i+2},$$

$$|B_i\rangle_2 = d_i \otimes su_4[(i+1,1),(i+1,2),(i+2,1),(i+2,2)]$$

are two of the degenerate ground states of the six-site block B_i with the ground energy $e_g(B_i) = -J'\left(\frac{15}{2}c_1 + \frac{5}{4}c_1\right)$, where d_i represents a dimer on the ith rung

$$d_i = [(i,1),(i,2)] = \frac{1}{\sqrt{2}}\Gamma_{\mu\nu}|(i,1)_\mu(i,2)_\nu\rangle,$$

with $\Gamma_{\mu\nu}$ denoting an antisymmetric tensor. A global eigenstate can be constructed by a combination of local eigenstates $|B_i\rangle_1$ or $|B_i\rangle_2$ because the dimers on the side of the block are free in the sense that they can form plaquette singlets with other sites belonging to the neighboring blocks. Now it is obvious that the eigenstates $|P_1\rangle$ and $|P_2\rangle$ are the ground state of each sub-Hamiltonian $h(B_i)$, and therefore the degenerate GSs of the global Hamiltonian with the GS energy given by Eq. (5). In fact, the constraint relation Eq. (4) can be further released to

$$J_\perp \geqslant \frac{3}{2}J = \frac{3}{2}J_\times^1 = 3J_\times^2 = 3J', \qquad (8)$$

which means that the degenerate plaquette products are the GSs even in the strong rung limit $J_\perp \gg J$. Furthermore, we note that $|P_1\rangle$ and $|P_2\rangle$ are the eigenstate of the $SU(4)$ ladder model even for arbitrary $J_\perp$, but not necessarily the GS.

This plaquette-product state is a spin-gapped state with only short-range spin correlations. The two GSs are spontaneously tetramerized and thus break translational symmetry. The elementary excitation above the GS is produced by breaking a plaquette singlet with a finite energy cost, thus leading to an energy gap. Two kinds of excitations are possible, either a magnonlike excitation or a spinon-like excitation. The gap size of a magnonlike excitation is approximately equivalent to the energy spacing level between the GS and the first excited state of a local tetrahedron. For the model (8), the first two excited states above the plaquette singlet are represented by the Young diagrams $[2^1 1^2]$ and $[2^2]$ and the corresponding gap sizes are $\Delta_m = 4c_1$ and $\Delta_s = 6c_1$ respectively. The spinonlike excitation is made up of a pair of rung dimers which propagate along the leg to further lower the energy, and thus the excitation spectrum is a two-particle continuum. The propagating dimer pairs behave like domain-wall solitons (kink and antikink) connecting two spontaneously tetramerized ground state. We represent an excited state with a kink at site $2m-1$ and an antikink at site $2n$ as $\Psi(m,n)$, so the corresponding momentum-space wave function is

$$\Psi(k_1, k_2) = \sum_{1 \leqslant m \leqslant n \leqslant M} e^{i(2m-1)k_1 + i2nk_2}\Psi(m,n).$$

The excited energy can be calculated directly by using the above variational wave fuction.[14] For a spontaneously tetramerized ladder system, it is reasonable to assume that the kink and antikink are well separated because there exists no intrinsic mechanism binding them together to form a bound state, and we therefore treat kink and antikink separately. Since the state $\Psi(m)$ is not orthogonal with the inner product given by $\langle \Psi(m')\|\Psi(m)\rangle = \left(\frac{1}{6}\right)^{|m'-m|}$, thus $\Psi(k_1, k_2)$ has a non-
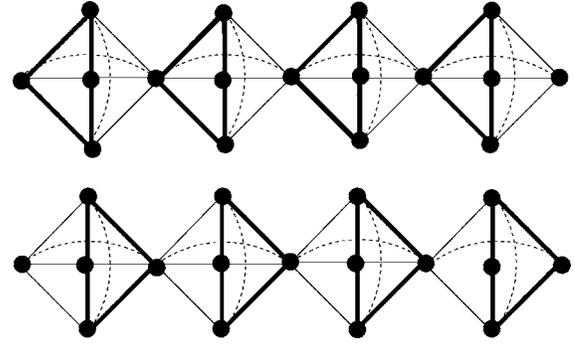

FIG. 2. Twofold degenerate ground state of the $SU(4)$ diamond-chain model. The Heisenberg exchange is defined on every linked bond with the equal magnitude.

trivial norm. After considerable but straightforward algebra, we get

$$\varepsilon(k_1, k_2) = \frac{37}{35}\Delta - \frac{6}{35}(\cos 2k_1 + \cos 2k_2)\Delta,$$

where $\Delta = 5c_1$ is the energy level spacing between the GS and the excited state where a local plaquette is broken into two rung singlets. Since the $SU(4)$ spin-3/2 model can be mapped into the spin-orbital model, our above results can be directly applied to the corresponding spin-orbital ladder model. For an $SU(4)$ spin-orbital railway-ladder model, we noticed that it has similar degenerate GSs composed of $SU(4)$ singlets from the work of vanden Bossche *et al.* based on the exact diagonalization method and analytical analysis in strong coupling limits.[12]

For the $SO(5)$ ladder (3) with $c_2 > 0$, one might expect that the degenerate plaquette states are the GSs in the parameter regime (8), such as in the case of the $SU(4)$ ladder. Unfortunately, one can check that those plaquette states are no longer the eigenstates and therefore not the exact GSs. Nevertheless, we can prove that $|P_1\rangle$ and $|P_2\rangle$ are degenerate eigenstates of the global Hamiltonian if $J_\perp = J = J_\times^1 = 2J_\times^2 = 2J'$.

Next we turn to a solvable diamond-chain model as shown in Fig. 2, where the spin-3/2 Heisenberg model is defined on the linked bonds with the same exchange energy $H = J\Sigma_{\langle ij \rangle}h_{ij}$. For an $SU(4)$ model, the Hamiltonian can be written as a sum of the Casimir of the total spin in each five-site cluster. Thus we conclude that the GSs are doubly degenerate plaquette singlets because among the possible representations composed by five sites, the above ground state configurations provide the smallest Casimir. By the same reasoning as above, this conclusion holds true for the $SO(5)$ case with $c_2 > 0$. The excitation is composed of a spinon and a three-site bound state as a result of a plaquette singlet breaking up to a $1+3$ pattern, which bears some similarity to the above spin ladder model where symmetric spinonlike excitations correspond to a plaquette singlet breaking up to a $2+2$ pattern.

The exact plaquette GS discussed above can be straightforwardly generalized to the $SU(N)$ case. The $SU(2)$ case corresponds to the celebrated spin-1/2 Majumdar-Ghosh
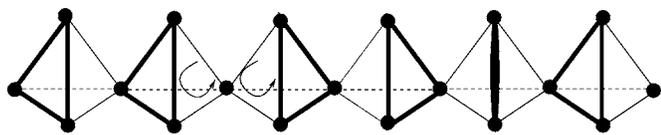
FIG. 3. Excitations in the $SU(3)$ model as the nearest-neighbor Heisenberg model defined on the 1D corner-shared tetrahedrons.

model.[15,16] The $SU(3)$ case as shown in Fig. 3 is particularly interesting. It is defined in a 1D correspondence of the pyrochlore lattice where only the nearest-neighbour bond interaction is involved. The Hamiltonian is

$$H = J\sum_{\langle ij \rangle} \sum_{\gamma=1}^{8} A^\gamma(i) A^\gamma(j), \qquad (9)$$

where A's are the eight $SU(3)$ generators in the fundamental representations, and $\langle ij \rangle$ means the sum over the nearest neighbors. It can also be written as the spin-1 representation as $H = J\Sigma_{\langle ij \rangle} \vec{S}(i) \cdot \vec{S}(j) + a(\vec{S}(i) \cdot \vec{S}(j))^2$, where the $SU(3)$ point is located at $a = 1$. The Hamiltonian can be written as a sum of the Casimir of the total spin in each tetrahedra. We know that the representations with the smallest Casimir made out of four sites in the fundamental representations is three dimensional. The excitations also have a gap and are fractionalized as in the 1D polymer systems. The three-site singlet (quark) is broken up to a $1+2$ pattern as one monomer in the fundamental representation, and the other two form an antifundamental (antiquark) representation. Thus the quark and antiquark pair states are 3×3-fold degenerate. The singlet site monomer can hop around in the two faces without breaking more singlets. The detail will be the subject of a future publication.

In summary, we derived and studied the effective $SO(5)$ spin-3/2 exchange model as well as the spin-ladder models with exact twofold degenerate plaquette GS. Our results indicate the formation of spontaneously tetramerized GS for a translational invariant spin-ladder system. Quantitative results for the elementary excitation spectrum of the $SU(4)$ spin-orbital ladder are also obtained. Due to the existence of an intrinsic $SO(5)$ symmetry, we expect that the plaquette phase of the spin-3/2 models can be observed in optical lattices in the future experiment. The generalization of our theory to the system with $SU(3)$ or even $SU(N)$ symmetry is also addressed.

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