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Generalized valence bond state and solvable models for spin-$\frac{1}{2}$ systems with orbital degeneracy

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A spin-$\frac{1}{2}$ system with double orbital degeneracy may possess SU(4) symmetry. According to the group theory a global SU(4) singlet state can be expressed as a linear combination of all possible configurations consisting of four-site SU(4) singlets. Following Andersion's idea for spin-$\frac{1}{2}$ system, we propose that the ground state for the antiferromagnetic SU(4) model is an SU(4)-resonating valence-bond (RVB) state. A short-range SU(4)-RVB state is a spin and orbital liquid, and its elementary excitations has an energy gap. We construct a series of solvable models that ground states are short-range SU(4)-RVB states. The results are generalized to the antiferromagnetic SU(N) models.

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Electron configurations in transition metal oxides usually have an orbital degeneracy in additional to spin degeneracy. Strong Coulomb interaction in these systems may produce spin systems with orbital degeneracy (for an overview see Refs. 1, 2). Several coupled spin-orbital models arise for many kinds of relevant materials. At a symmetric point the models may possess higher symmetry, such as SU(4).[3–5] Systematic study of the symmetric models may help us to understand physical properties for realistic systems. SU(4) spin-orbital model is a good candidate to investigate coupled spin-orbital system. It can be solved exactly in one dimensional case by means of Bethe ansatz.[6] There are a lot of numerical and analytical calculations, and most are limited in one dimension or small clusters. Very few rigorous results for this system are known. Oppositely we have deep understanding on spin SU(2) systems. Some rigorous results and solvable models are established. For instance, it was proved that the spin-$\frac{1}{2}$ antiferromagnetic periodic chain of length L has a low-energy excitation of order $1/L$.[7] In the case of SU(2) system, Anderson proposed a resonating valence-bond (RVB) state as the ground state for a spin-$\frac{1}{2}$ antiferromagnet.[8] In each configuration all spins form spin-singlet pairs, and the RVB state is composed of all possible configurations. In fact the state is a completely general description for a global singlet state.[9] His idea was applied to explain unconventional properties of spin liquids. Some solvable models were constructed based on the idea.[10] In this paper we generalize Anderson's RVB idea to a coupled spin-orbital system. We first derive several identities for SU(4)-symmetric spin-orbital system, and then prove a rigorous statement on the SU(4) isotropic state. The state consists of SU(4) singlets, which can be regarded as a generalized SU(4)-RVB states. To illustrate the idea, we construct two types of solvable models and evaluate the ground-state energies. One ground state is a short-range SU(4)-RVB solid, and another one is highly degenerated.

We start with a Hamiltonian for a spin-$\frac{1}{2}$ system with double-fold orbital degeneracy, which was derived by Castellani *et al.*[3] By neglecting the Hund's-rule coupling between different on-site orbitals, the system possesses SU(4) symmetry. The symmetric spin-orbital Hamiltonian is expressed in terms of two sets of independent spin-$\frac{1}{2}$ operators,[4]

$$H=\sum_{ij} J_{ij}\left(2\mathbf{S}_i\cdot\mathbf{S}_j+\frac{1}{2}\right)\left(2\tau_i\cdot\tau_j+\frac{1}{2}\right)=\sum_{ij} J_{ij}P_{ij}. \quad (1)$$

The three operators for spin $\mathbf{S}_i^\alpha$, three operators for orbital τ_i^β, and nine operators for their direct multiplications $2\mathbf{S}_i^\alpha\tau_i^\beta$ $(\alpha,\beta=x,y,z)$ compose the fifteen generators for a SU(4) group,

$$\{T_i^m\}=\{2\mathbf{S}_i^\alpha,2\tau_i^\beta,4\mathbf{S}_i^\alpha\tau_i^\beta\} \quad (m=1,2,\ldots,15), \quad (2)$$

with $\Sigma_m T_i^m T_i^m=15$ and $P_{ij}=(\Sigma_m T_i^m T_j^m+1)/4$. To explore the physical meaning of P_{ij}, we define four-possible states $|i\mu\rangle$ on each lattice site according to the eigenvalues of $s^z=\pm 1/2$ and $\tau^z=\pm 1/2$, where $\mu=(s^z,\tau^z)$ or simply 1, 2, 3, and 4. Define the total SU(4) spin $T_{tot}=\Sigma_i T_i$. Due to the symmetry of the model we have $[H,T_{tot}]=0$. The total SU(4) spin T_{tot} is a good quantum number. The operator P_{ij} is in fact a permutation operator when it is applied on the state $|i\mu,j\nu\rangle$

$$P_{ij}|i\mu,j\nu\rangle=|i\nu,j\mu\rangle, \quad (3)$$

with $P_{ij}^2=1$, where we have used the standard relation for spin-$\frac{1}{2}$ system.[11] The two eigenvalues of P_{ij} is ± 1. This gives an upper and lower bound for energy per bond in Eq. (1), i.e., $-J_{ij}\leqslant J_{ij}\langle P_{ij}\rangle\leqslant J_{ij}$ for any state. For a two-site problem, there are six eigenstates for P_{ij} with eigenvalue -1, $(|i\mu,j\nu\rangle-|i\nu,j\mu\rangle)/\sqrt{2}$ where $\mu\neq\nu$. The total $(T_i+T_j)^2=20$, which indicates that a SU(4) singlet cannot be formed at two sites. The minimal number of lattice sites to form SU(4) singlet is four as shown by Li *et al.*[5] An SU(4) singlet is written as

$$su_4(i,j,k,l)=\sum_{\mu,\nu,\gamma,\delta}\Gamma_{\mu\nu\gamma\delta}|i\mu,j\nu,k\gamma,l\delta\rangle,$$

where Γ is an antisymmetric tensor. Alternatively, denote spin and orbital SU(2) singlets for sites i and j by $s(ij)$ and $\tau(ij)$, respectively. An SU(4) singlet can be expressed in terms of spin and orbital SU(2) singlets[12]

$$su_4(i,j,k,l)=\sqrt{\frac{2}{3}}[s(ij)s(kl)\tau(il)\tau(jk) - s(il)s(jk)\tau(ij)\tau(kl)]. \quad (4)$$

Exchange of the order of i, j, k, and l gives the same state. For any two sites i' and j' among i,j,k, and l, we have

$$P_{i'j'}su_4(i,j,k,l)=-su_4(i,j,k,l). \quad (5)$$

The exchange of the positions of four sites in the singlet keeps the singlet unchanged. Since -1 is the smallest eigenvalues of P_{ij}, for a four-site problem with all $J_{ij}\geqslant 0$, the lowest energy state is $su_4(1,2,3,4)$ with eigenvalues $-\Sigma_{ij}J_{ij}$. It is worth noting that the conclusion is independent of the values of the coupling J_{ij}. Furthermore, by using Eq. (5), it is not hard to check,

$$(T_i+T_j+T_k+T_l)^2su_4(i,j,k,l)=0. \quad (6)$$

This identity indicates that the total SU(4) $T_{tot}=\Sigma_i T_i$ is zero. There exists another important identity for two SU(4) singlets in eight sites when indices i_1 and j_1 in $P_{i_1j_1}$ belong to different singlets

$$P_{i_1j_1}su_4(i_1,i_2,i_3,i_4)su_4(j_1,j_2,j_3,j_4) = su_4(j_1,i_2,i_3,i_4)su_4(i_1,j_2,j_3,j_4). \quad (7)$$

To prove the identity we utilize the permutation properties of P as shown in Eq. (3). The resulting state is obtained by exchanging two positions of i_1 and j_1 in different singlets.

To proceed further we introduce a concept of generalized RVB state. An SU(4)-RVB state is composed of SU(4) singlets, instead of SU(2) singlet. In principle an SU(4)-RVB state consists of all possible configurations, which contain either the nearest-neighbor SU(4) singlets or the long-range SU(4) singlets. Depending on the Hamiltonian and the underlying lattice an SU(4)-RVB state as a ground state may have a different form. For instance in the example we shall present later the state is a short-range RVB state. The completeness of the RVB states as a basis for a global singlet state can be shown from the group theory. Take the direct product of $N_\Lambda(=4M)$ states $|i\mu\rangle$ as basis. Young Tableaux is used to represent the irreducible representation. If the irreducible representation is a singlet the Young tableaux must be of the form of a $4\times M$ rectangle. In each column it is antisymmetrized, and in each row it is symmetrized. In this way the Young tableaux represents a generalized RVB state, as in the case for SU(2) system.[9] Since the irreducible representation forms a complete set, a linear combination of a RVB state is another one. The number of the generalized RVB states are $(4M)!/(M!)$.[4] It is over complete and nonorthogonal. The Lanczos method can re-organize the states to form a complete and orthogonal set of basis. Thus, we have the following conclusion,

Given that the number of lattice sites $N_\Lambda=4M$ (M is an integer), the SU(4) isotropic state of the symmetric spin-orbital model that can be expressed as a linear combination of configurations consisting four-site SU(4) singlets, i.e., SU(4)-RVB state.

Several remarks are in order.

(1) Following the Lanczos method we can re-construct the Hamiltonian in a tridiagonal form on a set of complete and orthogonal basis by utilizing Eqs. (5) and (7). Each of the basis can be expressed in a linear combination of SU(4)-RVB states.

(2) In one-dimensional chain with $4M$ site the short-range SU(4)-RVB state composed by M nearest-neighbor four-site SU(4) singlets has the energy per bond $-0.75J$, which is very close to the exact energy of Bethe ansatz $-0.82511J$.[6] This is a good starting point to calculate the ground-state energy. The two identities Eqs. (5) and (7) provide a possible way to evaluate the ground-state energy. In practice it is hard to include all possible SU(4) singlets. It is possible to construct the wave function by including some finite-size SU(4) singlets such that the average energy of the wave function is closer to the true ground state.

(3) On a SU(2) antiferromagnetic model on a hypercubic lattice, it was shown that the ground state is a spin singlet.[13] We postulate that this result is valid for SU(N) systems if the lattice can be decomposed into N sublattices. Numerical calculations for finite clusters supports this idea.

We now make use of the identities to construct two types of solvable models with SU(4) symmetry. The method we use here is that, if we can write the Hamiltonian in the form of the sum of semipositive operators, and find a state that has lowest eigenvalues for each semipositive operator, the state must be the ground state of the Hamiltonian. The method was used for spin-$\frac{1}{2}$ system by Majumdar and Ghosh.[14] The first type of solvable model is defined on a d-dimensional hypercubic lattice. Label the lattice site by $i\in\Lambda$. Each site contains four SU(4) spins. The SU(4) operators is denoted by $T_{i\gamma}$. ($\gamma=1,2,3,4$). Assume the number of lattice sites i is N. The total number of SU(4) spins is $4N$. The model Hamiltonian is

$$H=zJ'\sum_{i,\gamma\neq\gamma'}\left(2\mathbf{S}_{i\gamma}\cdot\mathbf{S}_{i\gamma'}+\frac{1}{2}\right)\left(2\tau_{i\gamma}\cdot\tau_{i\gamma'}+\frac{1}{2}\right) + J\sum_{\langle i,j\rangle,\gamma,\gamma'}\left(2\mathbf{S}_{i\gamma}\cdot\mathbf{S}_{j\gamma'}+\frac{1}{2}\right)\left(2\tau_{i\gamma}\cdot\tau_{j\gamma'}+\frac{1}{2}\right), \quad (8)$$

where the intrasite coupling is larger than the intersite coupling $J'=J(\alpha^2+1/\alpha^2)/2\geqslant J$, α is an arbitrary number, and z is the coordination number. To find the lowest-energy state, we rewrite the Hamiltonian in the form

$$H=\frac{J}{16}\sum_{ij}\left[\sum_{\gamma=1}^{4}\left(\frac{1}{\alpha}T_{i\gamma}+\alpha T_{j\gamma}\right)\right]^2-\sum_{\langle ij\rangle}(6/\alpha^2+6\alpha^2-4)J,$$

where $[\Sigma_{\gamma=1}^4(1/\alpha T_{i\gamma}+\alpha T_{j\gamma})]^2$ is semipositive definite. Its eigenvalues are always not less than zero. Thus, the Hamiltonian H is semipositive definite except for a constant. If we can find a state $|\Phi\rangle$ such that

$$\left[\sum_{\gamma=1}^{4}\left(\frac{1}{\alpha}T_{i\gamma}+\alpha T_{j\gamma}\right)\right]^2|\Phi\rangle=0,$$

for any nearest-neighbor pairs i and j, this state must be the ground state of the Hamiltonian H. Here we construct an SU(4)-valence bond (VB) state

$$|SVB\rangle = su_4(i_1 1, i_1 2, i_1 3, i_1 4) \times su_4(i_2 1, i_2 2, i_2 3, i_2 4) \cdots su_4(i_{N_\Lambda} 1, i_{N_\Lambda} 2, i_{N_\Lambda} 3, i_{N_\Lambda} 4).$$

It means that at each site i, four $T_{i\gamma}$ form an SU(4) singlet,

$$\sum_\gamma T_{i\gamma}|SVB\rangle = 0.$$

We can regard the state as an SU(4) singlet solid or VB solid at the lattice. Therefore we have

$$\left[\sum_{\gamma=1}^{4}\left(\frac{1}{\alpha}T_{i\gamma}+\alpha T_{j\gamma}\right)\right]^2|SVB\rangle = 0$$

for any pair of i and j. Alternatively,

$$\left[\sum_{\gamma\neq\gamma'}\left(\frac{1}{\alpha^2}P_{i\gamma i\gamma'}+\alpha^2 P_{j\gamma j\gamma'}\right)+\sum_{\gamma,\gamma'}P_{i\gamma j\gamma'}\right]|SVB\rangle = -(6/\alpha^2+6\alpha^2-4)|SVB\rangle.$$

Hence $|SVB\rangle$ is the ground state of the model [Eq. (8)]. The ground-state energy per bond is $(6/\alpha^2+6\alpha^2-4)J$. In this state there does not exist long-range correlation. The short-range RVB state is a typical quantum frustrated spin-orbital liquid. When we break an SU(4) singlet it will cost a finite energy. Thus the elementary excitation on this state has an energy gap.

The second type of solvable model is defined on a lattice that is decomposed into two sublattices. The sublattice A labeled by {j} has one SU(4) T on each site. A lattice site belonging to sublattice B (labeled by {i}) is located on the middle of two sites j. Each site i contains four $T_{i\gamma}$ ($\gamma=1,2,3,4$). The model Hamiltonian is defined as

$$H = 2J\sum_{i,\gamma\neq\gamma'}\left(2\mathbf{S}_{i\gamma}\cdot\mathbf{S}_{i\gamma'}+\frac{1}{2}\right)\left(2\tau_{i\gamma}\cdot\tau_{i\gamma'}+\frac{1}{2}\right) + J\delta\sum_{\langle i,j\rangle,\gamma}\left(2\mathbf{S}_{i\gamma}\cdot\mathbf{S}_{j}+\frac{1}{2}\right)\left(2\tau_{i\gamma}\cdot\tau_{j}+\frac{1}{2}\right), \quad (9)$$

with $0<\delta<1$. Similarly, the Hamiltonian can be rewritten as

$$H = \frac{J}{8}\sum_{\langle ij\rangle}\left[\sum_{\gamma=1}^{4}T_{i\gamma}+\delta T_j\right]^2 - \frac{J}{2}\sum_{\langle ij\rangle}\epsilon_0$$

with $\epsilon_0 = 12-2\delta+15\delta^2/4$. We can construct a state $|\Phi\rangle$ such that all four $T_{i\gamma}$ at site i form SU(4) singlets and T_j at site j are in any state. We have

$$\left[\sum_{\gamma=1}^{4}T_{i\gamma}+\delta T_j\right]^2|\Phi\rangle = 15\delta^2|\Phi\rangle. \quad (10)$$

The eigenvalue $15\delta^2$ is the lowest energy of the squared operator in Eq. (10) when $\delta<1$. The equation holds for any pair of i and j. Therefore the state is also the ground state of the second-type of solvable models (9). Its ground energy per bond is $E_g=(6-\delta)J$. The state is highly degenerated since each site j has fourfold degeneracy. The total degeneracy is 4^{N_j} where N_j is the number of lattice sites j. Among the degenerated states some are SU(4) singlets, which can be expressed as SU(4)-RVB states, and some are not.

For the SU(4) symmetric spin-orbital model, mathematically, we can write the Hamiltonian in terms of the generators of SU(4) groups in the fermion representation. It provides us a routine to generalize the main results in this paper to the systems with the SU(N) symmetry.[15] For a SU(N) group there are N^2 generators S_m^n with a constraint $\Sigma_{m=1}^{N}S_m^m=1$. On each site there are N-possible states $|m\rangle$ ($m=1,2,\ldots,N$). In the fermion representation, we introduce N species of fermions $f_{i\mu}$, and the SU(N) generators can be expressed as $S_{im}^n=f_{im}^\dagger f_{in}$ with a constraint $\Sigma_{m=1}^{N}f_{im}^\dagger f_{im}=1$. In this way we generalize the SU(4) model to the SU(N) one

$$H = \sum_{ij}J_{ij}S_m^n(i)S_n^m(j) \equiv \sum_{ij}J_{ij}P_{ij}(N). \quad (11)$$

The operator $P_{ij}(N)$ is a permutation operator as shown in the case of SU(4). An SU(N) singlet can be defined as

$$su_N(i_1,i_2,\ldots,i_N) = c_N\sum f_{j_1 1}^\dagger f_{j_2 2}^\dagger,\ldots,f_{j_N N}^\dagger|0\rangle,$$

where the sum runs over all of the permutation of N sites $(j_1,j_2,\ldots j_N)=(i_1,i_2,\ldots,i_N)$. $c_N=1/\sqrt{N!}$ is a normalized constant. The SU(N) singlet is the eigenstate for the permutation operator

$$P_{ij}(N)su_N(i_1,i_2,\ldots,i_N) = -su_N(i_1,i_2,\ldots,i_N),$$

if i and j belong to $i_1,i_2,\ldots,i_N$, and

$$P_{i_2 j_1}(N)su_N(i_1,i_2,\ldots,i_N)su_N(j_1,j_2,\ldots,j_N) = su_N(i_1,j_1,\ldots,i_N)su_N(i_2,j_2,\ldots,j_N),$$

for any two sites in different singlets. Due to the SU(N) symmetry in the model Hamiltonian, we can generalize the main result to the SU(N) system:

Given that the lattice is connected by the hopping matrix, and all $J_{ij}\geq 0$ and $N_\Lambda=Nm$ (m is an integer), the SU(N) isotropic state of the SU(N) model (11) can be expressed as a linear combination of configurations consisting N-site SU(N) singlets, SU(N)-RVB state.

When $N=2$, this result is reduced to the usual spin-$\frac{1}{2}$ SU(2) antiferromagnetic Heisenberg model. In this sense our main result can be regarded as a generalization of Anderson's RVB idea to SU(N) system. The solvable models are simply modified in this way: the site i contains N SU(N) spins. On the ground state the SU(N) spins at the N site form a SU(N) singlet. Hence we construct the two types of solvable SU(N)

models. The coupling coefficients should be modified slightly according to the structures of different lattices.

In summary, we propose a generalized SU(4)-RVB picture for spin-orbital model. A state with global SU(4) singlet can be expressed as a SU(4)-RVB state. The idea is also generalized to systems with SU(N) symmetry. We construct two types of solvable models, and evaluate the ground-state energies. One ground state is a SU(4)-RVB solid, and another one is a spin-orbital liquid.

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[1] K. I. Kugel and D. I. Khomskii, Usp. Fiz. Nauk **136**, 621 (1982) [Sov. Phys. Usp. **25**, 231 (1982)].
[2] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).
[3] C. Castellani, C. R. Natoli, and J. Ranninger, Phys. Rev. B **18**, 4945 (1978).
[4] T. M. Rice, in *Spectroscopy of Mott Insulators and Correlated Metals*, edited by A. Fujimori and Y. Tokura (Springer, Berlin, 1995).
[5] Y. Q. Li, M. Ma, D. N. Shi, and F. C. Zhang, Phys. Rev. Lett. **81**, 3527 (1998).
[6] B. Sutherland, Phys. Rev. B **12**, 3795 (1975).
[7] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[8] P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973); Science **235**, 1196 (1987).
[9] M. Ma, Phys. Rev. B **38**, 6813 (1988).
[10] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
[11] L. Hulthen, Ark. Mat., Astron. Fys. **26A**, 11 (1938).
[12] M. van den Bossche, F. C. Zhang, and F. Mila, Eur. Phys. J. B **17**, 367 (2000).
[13] W. Marshall, Proc. R. Soc. London, Ser. A **232**, 28 (1955); E. H. Lieb and D. C. Mattis, J. Math. Phys. **34**, 891 (1993). For an overview, see S. Q. Shen, Int. J. Mod. Phys. B **12**, 709 (1998).
[14] C. K. Majumdar and D. K. Ghosh, J. Math. Phys. **10**, 1388 (1969).
[15] I. Affleck, Phys. Rev. Lett. **54**, 966 (1985); Nucl. Phys. B **265**, 409 (1986).