Rigorous Results for a Hierarchy of Generalized Heisenberg Models

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The Lieb-Schultz-Mattis theorem is extended to generalized Heisenberg models related to unexceptional Lie algebras. It is shown that there are no energy gaps above the ground states for SO(4), Sp(2), and SU(4) Heisenberg models; but gaps are suspected to occur in SO(5) and SO(6) models. The nondegenerate ground state for these models is rigorously proven.

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The study of the ground state and excitations for many-particle systems is of importance, being relevant to superconductivity as well as Mott transitions. Based on Marshall's rule [1], Lieb, Schultz, and Mattis proved [2] a remarkable theorem: the spin $1/2$ system with Heisenberg interaction favors an antiferromagnetic ordering; its ground state is nondegenerate and no energy gap exists above the ground state in its energy spectrum. Haldane pointed out [3] by means of a mapping into a nonlinear σ model that there will be a gap to the excited state for the system with integer spin. The Lieb-Schultz-Mattis (LSM) theorem was extended by Kolb [4] and by Affleck and Lieb [5] to arbitrary half-odd-integer spin, demonstrating a difference between integer spin and half-odd-integer spin, in agreement with Haldane's conjecture. Very recently, the LSM theorem was extended to the case with an applied external field [6]. It was also discussed [7] in a generalized single-band Hubbard model. Actually, Ref. [5] also made an extension to SU($2n$) model by placing self-conjugate representation on each lattice site. However, the case of fundamental representation which becomes very important nowadays due to the model study on the spin systems with orbital degeneracy [8] was not investigated. Additionally, a nondegenerate ground state has been proposed [5–7] but not rigorously proven for various models except in the original SU(2) model [2].

Since various symmetries, as in SO(5) model [9] for high T_c superconductivity and SU(4) model [8] for orbital physics [10] have been of interest lately, we consider general Heisenberg-type models related to the nonexceptional Lie algebras [11]. We explicitly study several cases by a procedure analogous to the LSM theorem. Some rigorous results on SO(4), Sp(2), SO(5), SU(4), and SO(6) Heisenberg models are given. The ground state of those models is rigorously proven to be nondegenerate. It is shown that there are gapless excitations in SO(4), Sp(2), and SU(4) models. For SO(5) and SO(6), however, an energy gap is expected to occur. In other words, the SO(4), Sp(2), and SU(4) models satisfy the sufficient condition for gapless excitation, but the SO(5) and SO(6) models obey the necessary condition for the existence of a gap.

We consider a generalized Heisenberg model:

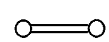
$$\mathcal{H} = \sum_{\substack{\langle x,x'\rangle \\ mn}} g^{mn} H_m(x) H_n(x') + \sum_{\substack{\langle x,x'\rangle \\ \alpha\in\Delta}} E_\alpha(x) E_{-\alpha}(x'), \quad (1)$$

where $\langle x, x'\rangle$ stands for nearest-neighbor pairing and Δ denotes the set of roots of some nonexceptional Lie algebra which will be specified in our discussion later on. $H_m(x)$ and $E_\alpha(x)$ are generators of the Lie algebra on site x in a lattice. The $\{H_m\}$ are the generators in the corresponding Cartan subalgebra. We adopt the following defining relations in our present paper,

$$\begin{gathered}[H_m, H_n] = 0, \qquad [E_{\alpha_m}, E_{-\alpha_m}] = 2H_m\,, \\ [E_\alpha, E_\beta] = E_{\alpha+\beta}, \quad \text{if } \alpha + \beta \in \Delta\,, \\ [H_m, E_\alpha] = (\alpha)_m E_\alpha\,,\end{gathered} \quad (2)$$

where $(\alpha)_m := \alpha \cdot \alpha_m$ is the mth *covariant component* of the root vector α in the nonorthogonal coordinates in which the simple roots $\{\alpha_m\}$ are chosen as the bases. We will adopt the standard terminology in group theory in order to avoid possible ambiguities. Meanwhile, we will give possible identifications in terms of the standard terminology in quantum mechanics when we deal with any concrete Lie algebra. We normalized the simple roots to unity so that the structure constant in Eq. (2) differs from the Cartan matrix in textbooks of group theory by a factor $1/2$.

The cases of B_2 and C_2 Lie algebra.—As C_2 is isomorphic to B_2, we will only make our discussions on B_2 Lie algebra. From the Dynkin diagram:



which means that the α_1 and α_2 span an angle of 135°, we can write out the simple roots in the nonorthogonal coordinates, accordingly $\alpha_1 = (1, -1/2)$, $\alpha_2 = (-1, 1)$. The set of roots for B_2 is $\Delta = \{\pm\alpha_1, \pm\alpha_2, \pm(\alpha_1 + \alpha_2), \pm(2\alpha_1 + \alpha_2)\}$. The SO(5) Heisenberg chain is a chain with states on each site carrying a five-dimensional representation of B_2 Lie algebra. These five states ($|l\rangle, l = 1, 2, \ldots, 5$) are labeled by the eigenvalues of the Cartan subalgebra, which are two-dimensional vectors called the weight vectors in group theory, namely, $(0,1/2)$, $(1,-1/2)$, $(0,0)$, $(-1,1/2)$, and $(0,-1/2)$. For example, $(H_1,H_2)|2\rangle = (1,-1/2)|2\rangle$. If placing the states that carry the spinor representation of B_2 (meanwhile the fundamental representation of C_2) Lie algebra at each site, we will have a Sp(2) Heisenberg chain. It is a four dimensional representation labeled by weight vectors $(1/2,0)$, $(-1/2,1/2)$, $(1/2,-1/2)$, and $(-1/2,0)$, respectively.

Let us investigate the nature of the ground state of those systems. We will extend the strategy of [2] to show the ground state of present models on bipartite lattice $L = A \cup B$ is nondegenerate. By making use of a unitary transformation,

$$U = \exp\left[-i\pi \sum_{y\in B}\left[H_1(y) + \frac{1}{2}\right]\right], \tag{3}$$

that rotates each state on the sublattice B, the original Hamiltonian (1) is mapped to the following form:

$$\begin{aligned}\widetilde{\mathcal{H}} = &\sum_{\substack{x,x'\\ mn}} g^{mn} H_m(x)H_n(x') \\ &- \sum_{\langle xx'\rangle}\Bigg[\sum_{\tilde{\alpha}} E_{\tilde{\alpha}}(x)E_{-\tilde{\alpha}}(x') \\ &\qquad - E_\beta(x)E_{-\beta}(x') - E_{-\beta}(x)E_\beta(x')\Bigg],\end{aligned} \tag{4}$$

where $\tilde{\alpha} \in \{\pm\alpha_1, \pm\alpha_2, \pm(2\alpha_1 + \alpha_2)\}$ and $\beta = \alpha_1 + \alpha_2$. It is easy to show, after some algebra, that this transformation is also a canonical transformation. The application of canonical transformation to the traditional SU(2) Heisenberg model can turn out an overall negative sign in the second sum of Eq. (1), but it is not possible in the present case. Nevertheless, we will see that this does not affect the proving of the nondegenerate ground state, although several authors had not succeeded.

As we consider $N = 2n$ (bipartite lattice), the group theory concludes that there always exists one state of any multiplet lying in the subspace of zero weight $(0,0)$, i.e., zero eigenvalues of $H_m^{\rm tot} = \sum_x H_m(x)$, $m = 1,2$. This guarantees the eigenvalues determined within the subspace cover the whole spectrum of the model. A complete set of states in the subspace consists of all possible configurations that can be constructed in the following way. As for Sp(2), there are n_1 sites labeled by $(1/2,0)$ and the same number of sites labeled by $(-1/2,0)$, additionally n_2 sites labeled by $(-1/2,1/2)$ and the same number of sites labeled by $(1/2,-1/2)$ for any partition $n = n_1 + n_2$. For SO(5), however, we should consider arbitrary partitions $n = n_0 + n_1 + n_2$. The possible states in the subspace consists of $2n_0$ sites labeled by $(0,0)$, n_1 labeled by $(0,1/2)$ and the same number of sites labeled by $(0,-1/2)$, and n_2 sites labeled by $(1,-1/2)$ and the same number of sites labeled by $(-1,1/2)$.

Denoting those states by $|\mu\rangle$, we can expand any eigenstate of $\widetilde{\mathcal{H}}$ in this subspace as $|\psi\rangle = \sum\langle\mu|\psi\rangle|\mu\rangle$. The Schrödinger equation $\widetilde{\mathcal{H}}|\psi\rangle = E|\psi\rangle$ in this representation gives rise to

$$\sum_{\langle xx'\rangle} \eta(p_{xx'})\langle p_{xx'}(\mu)|\psi\rangle = (\epsilon_\mu - E)\langle\mu|\psi\rangle, \tag{5}$$

where $\epsilon_\mu|\mu\rangle = \sum g^{mn}H_m(x)H_n(x')|\mu\rangle$ and $p_{xx'}$ stands for an exchange of the states on adjacent sites x and x'. For Sp(2), $\eta(p_{xx'}) = -1$ if the exchange occurs either between $(1/2,0)$ and $(1/2,-1/2)$, or between $(-1/2,1/2)$ and $(0,-1/2)$; $\eta(p_{xx'}) = 1$ if for the other exchanges. For convenience in the following discussions, we call the former the mutable exchange, and the later the immutable exchange. For SO(5) the mutable exchanges occur between $(0,1/2)$ and $(0,0)$, or between $(0,0)$ and $(0,-1/2)$.

First we will show that all the coefficients $a_\mu = \langle\mu|\psi_0\rangle$ are nonvanishing for any ground state $|\psi_0\rangle = \sum a_\mu|\mu\rangle$. To prove this, we suppose some of them being zero, saying $a_{\bar{\mu}} = 0$, and consider a trial state (wave function) $|\psi'\rangle = \sum \eta(\mu)|a_\mu||\mu\rangle$ with $\eta(\mu) = \pm 1$. The $\eta(\mu)$ is defined in the following way. Given one state $|\mu_0\rangle$ for each aforementioned partition in the subspace of null weight, any others of the whole states in the subspace can always be obtained by a sequence of adjacent permutations. We define $\eta(\mu) = 1$ if an even number of mutable exchange is involved in achieving the desired state $|\mu\rangle$. Otherwise, if an odd number of that is involved, we define $\eta(\mu) = -1$. Now it is easy to calculate that

$$\begin{aligned}\langle\psi'|\widetilde{\mathcal{H}}|\psi'\rangle &= \sum_\mu a_\mu^2 - \sum_\mu\sum_{\langle xx'\rangle}|a_\mu||a_{p_{xx'}(\mu)}|, \\ \langle\psi_0|\widetilde{\mathcal{H}}|\psi_0\rangle &= \sum_\mu a_\mu^2 - \sum_\mu\sum_{\langle xx'\rangle}\eta(p_{xx'})a_\mu a_{p_{xx'}(\mu)},\end{aligned} \tag{6}$$

which concludes that

$$\langle\psi'|\widetilde{\mathcal{H}}|\psi'\rangle \le \langle\psi_0|\widetilde{\mathcal{H}}|\psi_0\rangle. \tag{7}$$

Because $|a_{\bar{\mu}}| = 0$ but $\sum|a_{p_{xx'}(\bar{\mu})}| \neq 0$, $|\psi'\rangle$ is not an eigenstate. According to variational principle we will have $\langle\psi'|\widetilde{\mathcal{H}}|\psi'\rangle > \langle\psi_0|\widetilde{\mathcal{H}}|\psi_0\rangle$ that contrasts with Eq. (7). This contradiction proves that $a_{\bar{\mu}} = 0$ is not possible for a ground state.

Clearly, if $|\psi_0\rangle$ is a ground state, only the equal sign in Eq. (7) is possible. This implies that the coefficients of two configurations/states should have opposite signs if they are related by an odd number of mutable exchanges of adjacent sites, otherwise they should have the same sign. It is obviously not possible to get two states with the mentioned restrictions on the coefficients to be orthogonal to each other. Therefore there can be only one ground state. Now we complete our proof that the ground states of Sp(2) and SO(5) Heisenberg models on bipartite lattice have nondegenerate ground states.

We are now in the position to observe the features of energy excitations above the nondegenerate ground state. Introduce a slowly varying twist operator

$$V(\theta) = \exp\left[-i\theta \sum_{x=1}^{N} xK(x)\right], \tag{8}$$

with $K(x) = H_1(x)$. In order to guarantee the periodic boundary condition, we must let $\theta = 2\pi\nu/N$ (ν is any integer number). Since the ground state $|\psi_0\rangle$ is nondegenerate and the Hamiltonian is invariant under translation, we have $T|\psi_0\rangle = e^{-i\delta}|\psi_0\rangle$ where T denotes the operator of translation by one site. Following Lieb, Schulz, and Mattis [2], we construct a state $|\psi_\nu\rangle = V(2\pi\nu/N)\,|\psi_0\rangle$. Noting the fact that $\sum_x H_1(x)\,|\psi_0\rangle = 0$, we get

$$\begin{aligned}\langle\psi_0|\psi_\nu\rangle &= \langle\psi_0|TVT^{-1}|\psi_0\rangle \\ &= \langle\psi_0|V\exp[i2\pi\nu K(1)]\,|\psi_0\rangle.\end{aligned} \tag{9}$$

Obviously, $\langle\psi_0|\psi_\nu\rangle = -\langle\psi_0|\psi_\nu\rangle$ for an odd ν in the Sp(2) case, but $\langle\psi_0|\psi_\nu\rangle = \langle\psi_0|\psi_\nu\rangle$ for any ν in the SO(5) case. So the state $|\psi_\nu\rangle$ of odd ν is orthogonal to the ground state $|\psi_0\rangle$, and hence is an excited state for the Sp(2) model, but is not for the SO(5) one.

From the commutation relation Eq. (2) for B_2 Lie algebra, we get

$$\begin{aligned} e^{i\theta H_1}E_{\pm\alpha_m}e^{-i\theta H_1} &= e^{\mp i(-1)^m\theta}E_{\pm\alpha_m}, \qquad m = 1,2, \\ e^{i\theta H_1}E_{\pm(\alpha_1+\alpha_2)}e^{-i\theta H_1} &= E_{\pm(\alpha_1+\alpha_2)}, \\ e^{i\theta H_1}E_{\pm(2\alpha_1+\alpha_2)}e^{-i\theta H_1} &= e^{\pm i\theta}E_{\pm(2\alpha_1+\alpha_2)}. \end{aligned}$$

With the help of these relations, we obtain after some algebra that

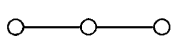
$$\begin{aligned} V^\dagger \mathcal{H} V - \mathcal{H} &= i\sin(2\pi\nu/N)\left[\sum_x xH_1(x), \mathcal{H}\right] \\ &\quad - 2\sin^2(\pi\nu/N)\sum_x\sum_{\tilde\alpha} E_{\tilde\alpha}(x)E_{-\tilde\alpha}(x+1), \end{aligned} \tag{10}$$

where $\tilde\alpha \in \{\pm\alpha_1, \pm\alpha_2, \pm(2\alpha_1 + \alpha_2)\}$ and the term corresponding to $\alpha_1 + \alpha_2$ is absent in the summation. Then the excitation energy is evaluated,

$$\langle\psi_\nu|\mathcal{H}|\psi_\nu\rangle - \langle\psi_0|\mathcal{H}|\psi_0\rangle \le \frac{2\pi^2}{N}\,\nu. \tag{11}$$

Thus there is no energy gap in the Sp(2) Heisenberg model. For SO(5), however, the possibility of existence of the energy gap could not be ruled out.

The case of A_3 Lie algebra.—From its Dynkin diagram



we write out the simple roots in the nonorthogonal coordinates, $\alpha_1 = (1, -1/2, 0)$, $\alpha_2 = (-1/2, 1, 1/2)$, and $\alpha_3 = (0, -1/2, 1)$. In SU(4) Heisenberg model the states at each site carry out the fundamental representation of A_3 Lie algebra. The weight vectors of the four states are $(1/2, 0, 0)$, $(-1/2, 1/2, 0)$, $(0, -1/2, 1/2)$, and $(0, 0, -1/2)$. In the SO(6) model the six states at each site are labeled by weight vectors $(0, 1/2, 0)$, $(1/2, -1/2, 1/2)$, $(-1/2, 0, 1/2)$, $(1/2, 0, -1/2)$ $(-1/2, 1/2, -1/2)$, and $(0, -1/2, 0)$, respectively. These states carry out the six-dimensional representation of A_3 Lie algebra.

In Ref. [5], the assumption of the unique ground state was made for investigating the excitations; here we can prove the nondegenerate ground state rigorously. Analogous to our previous discussion on the models of B_2 Lie algebra, we consider again the model of bipartite lattice and employ the following canonical transformation,

$$U = \exp\left[-i\pi\sum_{y\in B} K(y)\right]; \tag{12}$$

here $K(y) = H_1(y) + H_3(y)$. This transformation maps the Hamiltonian into

$$\begin{aligned} \widetilde{\mathcal{H}} &= \sum_{\substack{\langle xx'\rangle \\ mn}} g^{mn}H_m(x)H_n(x') \\ &\quad - \sum_{\langle xx'\rangle}\left[\sum_{\tilde\alpha} E_{\tilde\alpha}(x)E_{-\tilde\alpha}(x') - \sum_{\beta} E_\beta(x)E_{-\beta}(x')\right], \end{aligned} \tag{13}$$

where $\tilde\alpha \in \{\pm\alpha_1, \pm\alpha_2, \pm\alpha_3 \pm (\alpha_1 + \alpha_2 + \alpha_3)\}$ and $\beta \in \{\pm(\alpha_1 \pm \alpha_2), \pm(\alpha_2 + \alpha_3)\}$.

Because we discuss the fundamental representation of A_3 Lie algebra (instead of self-conjugate representation considered in [5]), we need to consider $N = 4n$. In this case, any multiplet of the system will always have a state within the subspace of zero weight $(0, 0, 0)$. Any eigenstate of the $\widetilde{\mathcal{H}}$ in Eq. (13) can be expanded by $|\mu\rangle$ $\mu = 1, 2, \ldots, (4n)!/(n!)^4$. The Schrödinger equation in this representation is formally the same as Eq. (5). The only difference is that the mutable exchanges occur between the states of either $(1/2, 0, 0)$ and $(0, -1/2, 1/2)$ or $(-1/2, 1/2, 0)$ and $(0, 0, -1/2)$. The formulations up to Eq. (6) are almost the same as the previous formulation except that $\eta(\mu)$ is defined according to the mutable exchange of present A_3 representation. Actually, we can also choose either $K = H_3 - H_1$ or $K = H_1 + 2H_2 + H_3$ (the set of $\tilde\alpha$ and β variants, correspondingly) to achieve the same conclusion that the ground states of SU(4) Heisenberg model and SO(6) one are nondegenerate.

Concerning the features of energy excitations above the nondegenerate ground state, we should introduce a slowly varying twist operators such as (8) with $K = H_1 + H_3$. Repeating the similar calculation we got formally the same relation such as Eq. (9) because the operator $H_1 + H_3$ acting on all the SU(4) states will always yield an eigenvalue of $1/2$, but acting on all the SO(6) states will get 0 or 1. Then the state constructed by the twist operator V is orthogonal to the ground state in the SU(4) case, but is not in the SO(6) case. By means of the commutation relations (2) for A_3 Lie algebra, we obtain again Eq. (11) after careful calculation. We therefore conclude that there are gapless excitations above the nondegenerate ground state for the SU(4) Heisenberg model and suspect an energy gap opens up in the SO(6) Heisenberg model. It is worthwhile to point out that the above formulation can be extended to the fundamental representation for any SU(M) straightforwardly as long as the number of the site is $N = nM$.

The physics implications of those models.—Up to now, we adopted mathematical terminology so as to keep the discussions rigorous. It is worthwhile to exhibit the physics implications of those models. We know the SU(4) Heisenberg model [8] describes the spin system with twofold orbital degeneracy, which is an effective model of doubly degenerate electrons at quarter filling [12] in the limit of strong on-site coupling. At half filling, moreover, it reduces to a SO(6) Heisenberg model [12] in the strong coupling limit. The gapless nature of the SU(4) model was also confirmed in Ref. [8] on the basis of Bethe-ansatz solution.

The Sp(2) and SO(5) Heisenberg models are discussed separately. Consider the state on each site being double occupancy of electrons, spin up, spin down, and empty. It is not difficult to verify that the four states $|1\rangle = |\uparrow\downarrow\rangle$, $|2\rangle = |\uparrow\rangle$, $|3\rangle = |\downarrow\rangle$, and $|4\rangle = |0\rangle$ carry out the fundamental representation of C_2 Lie algebra. The Chevalley basis of the C_2 Lie algebra is realized by $H_1 = S^z$, $H_2 = C_\downarrow^\dagger C_\downarrow - 1/2$, $E_{\alpha_1} = S^+$, and $E_{\alpha_2} = C_\downarrow^\dagger$, where $C_\downarrow^\dagger$ denotes the operator that creates an electron of spin down. This gives us a Sp(2) system.

The SO(5) system can be realized by pseudospin one particles. Excluding the double occupancy of parallel pseudospins, we can define $|1\rangle = |\Uparrow\Downarrow\rangle$, $|2\rangle = |\Uparrow\rangle$, $|3\rangle = |\Rightarrow\rangle$, $|4\rangle = |\Downarrow\rangle$, and $|5\rangle = |0\rangle$ to carry out a five-dimensional representation of B_2 Lie algebra. The generators $H_1 = J^z$, $H_2 = C_\Rightarrow C_\Rightarrow^\dagger (C_\Downarrow^\dagger C_\Downarrow - 1/2)$, $E_{\alpha_1} = J^+$, and $E_{\alpha_2} = C_\Downarrow^\dagger C_\Rightarrow C_\Rightarrow^\dagger$, where $C_\Downarrow^\dagger$ and $C_\Rightarrow^\dagger$ create the state $|\Downarrow\rangle$ and $|\Rightarrow\rangle$, respectively, so that $J^z|\Downarrow\rangle = -|\Downarrow\rangle$ and $J^z|\Rightarrow\rangle = 0$. Here the creation/annihilation operators are required to obey anticommutation relations so as to realize commutation relations of the B_2 Lie algebra. Five states related two d-wave superconducting order parameters and three antiferromagnetic order parameters were suggested to constitute the bases of a SO(5) theory [9] for a phenomenological understanding of the phase diagram of high T_c superconductive materials.

In summary, we extended the Lieb-Schultz-Mattis theorem to a hierarchy of generalized Heisenberg models related to nonexceptional Lie algebras. The nondegenerate ground state in these models is rigorously proven by means of a procedure analogous to the original LSM theorem for the SU(2) model. The main sketch of the proof consists of the following steps. Since the canonical transformation does not change the spectrum of a system, as a first step, we find a useful canonical transformation which maps the original Hamiltonian into what can be analyzed by the method invented in [2]. To confirm the nondegenerate ground state, we have proven that it is impossible to construct a second state which possesses the lowest energy, in the meanwhile keeping orthogonal to the given ground state. As the standard literature employed by many authors [2,5–7], we separately introduced slowly varying twist operators for those models. The twist operator will create a gapless excitation mode from the nondegenerate ground state, as long as the created state is orthogonal to the original ground state. Otherwise, the possibility of existence of an energy gap cannot be ruled out. Our investigation has shown that there is no energy gap above the ground states in SO(4), Sp(2), and SU(4) Heisenberg models, but gaps are suspected to open in SO(5) and SO(6) models.

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