Rigorous Results for the Ground States of the Spin-2 Bose-Hubbard Model

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We present rigorous and universal results for the ground states of the $f = 2$ spinor Bose-Hubbard model. The model includes three two-body on site interaction terms, two of which are spin dependent while the other one is spin independent. We prove that, depending only on the coefficients of the two spin dependent terms, the ground state exhibits maximum or minimum total spin or SU(5) ferromagnetism. Exact ground-state degeneracies and the forms of ground-state wave function are also determined in each case. All these results are valid regardless of dimension, lattice structure, or particle number. Our approach takes advantage of the symmetry of the Hamiltonian and employs mathematical tools including the Perron-Frobenius theorem and the Lie algebra so(5).

Introduction.—Ultracold atoms in optical lattices provide a unique playground for studying quantum many-body systems experimentally [1–4]. In particular, systems of bosonic alkali atoms with hyperfine spin $f$ have received considerable attention, as they can give rise to a variety of exotic phases [5–7]. Such systems are well described by the spinor Bose-Hubbard model [3, 8, 9], which is a discrete version of the model for condensates [10]. Most previous theoretical studies on lattice systems were based on a mean-field treatment of the original model [11–19] or a mapping to the effective spin model (perturbation on hopping) [9, 11, 20–23]. This is in contrast to the continuous case, where many results beyond mean-field have been obtained theoretically [24–29]. On the other hand, very few solid results are available for discrete lattice systems [30, 31]. In particular, almost nothing is known rigorously about the $f = 2$ case.

In this Letter, we prove universal theorems about the ground-state properties of the spin-$2$ Bose-Hubbard Hamiltonian. The model in Eq. (2) is characterized by the spin-dependent interaction constants $c_1$ and $c_2$. We precisely determine the total spin and the degeneracy of the ground states for the following three cases: (i) $c_1 < 0$ and $c_2 \geq 5c_1$, (ii) $c_1 = 0$ and $c_2 < 0$, and (iii) $c_1 = c_2 = 0$. In case (i), the system has SO(3) symmetry and the ground state exhibits saturated ferromagnetism. The following set of orthonormal states

$$|\Phi_m\rangle := \frac{1}{\sqrt{\prod_{i,\alpha} (n_{i,\alpha}!)} } \left\{ \prod_{i,\alpha} (a_{i,\alpha}^\dagger)^{n_{i,\alpha}} \right\} |\text{vac}\rangle \quad (1)$$

serves as a basis of the Hilbert space $\mathcal{H}$. Here, $|\text{vac}\rangle$ stands for the vacuum and $m = (n_{i,\alpha}) \in I$ is a set of non-negative integers, where $I$ is a set of $m$ that satisfies $\sum_{i,\alpha} n_{i,\alpha} = N$.

The Hamiltonian of the spin-$2$ Bose-Hubbard model [3, 24] is

$$\hat{H} = -\sum_{i \neq j, \alpha} t_{i,j} a_{i,\alpha}^\dagger a_{j,\alpha} + \sum_i V_i \hat{n}_i + \frac{c_0}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \frac{c_1}{2} \sum_i \left( (\hat{F}_i^x)^2 - 6\hat{n}_i \right) + \frac{2c_2}{5} \sum_i \hat{S}_{i,+} \hat{S}_{i,-} \quad (2)$$

Here $V_i \in \mathbb{R}$ is the single-particle potential at site $i$. The constants $c_0$, $c_1$, and $c_2$ are real coefficients for the two-body interactions, where the $c_1$ and $c_2$ terms are spin-dependent.
depended. The $c_2$ term favors (disfavors) singlet pairs when $c_2 > 0$ ($c_2 < 0$). We assume that $t_{i,j} = t_{j,i} \geq 0$ for all $i, j \in \Lambda$ and the whole lattice $\Lambda$ is connected via nonzero $t_{i,j}$.

In addition to the global ground states in the whole Hilbert space $H$, symmetry of the Hamiltonian enables us to discuss the local ground states in Hilbert subspaces. The Hamiltonian $\hat{H}$ is invariant under rotation in spin space, which implies that $\hat{H}$ has at least $\text{SO}(3)$ symmetry, yielding $[\hat{H}, F_{tot}^z] = 0$. Since $F_{tot}^z$ is conserved, $\hat{H}$ splits into subspaces labeled by $F_{tot}^z = M$. We shall show later that the symmetry is promoted to $\text{SO}(5)$ when $c_1 = 0$ and $c_2 \neq 0$. In this case, $\hat{H}$ splits into smaller subspaces labeled by two indices $P := N_1 - N_{-1}$ and $Q := N_2 - N_{-2}$.

Now we introduce some more notations. Define $H_A$ as a subspace of $H$ by $H_A := \{ |\psi\rangle \in H | \hat{A}|\psi\rangle = A|\psi\rangle \}$. Similarly, we have $H_B$ for $\hat{B}$. The intersection of $H_A$ and $H_B$ is denoted as $H_{A,B}$. Define $I_\Phi$ as a subset of $I$ by $I_\Phi := \{ m \in I | \hat{A}|\Phi_m\rangle = A|\Phi_m\rangle \}$. Operators $\hat{A}$ and $\hat{B}$ can be $M := F_{tot}^z$, $P := N_1 - N_{-1}$, $Q := N_2 - N_{-2}$, or $\Phi_m$ in the following.

Now we state our main theorems.

**Theorem 1.**—If $c_1 < 0$ and $c_2 \geq 5|c_1|$, the local ground state $|\Psi^G_M^S\rangle$ in $H_M$ is unique and can be written as

$$|\Psi^G_M^S\rangle = \sum_{m \in I_M} C_m|\Phi_m\rangle,$$

with $C_m > 0$, and has the maximum possible total spin $F_{tot} = 2N$ (saturated ferromagnetism). Each local ground state $|\Psi^G_M^S\rangle$ has energy independent of $M$ and hence is the global ground state in $H$ as well. Thus the ground-state degeneracy is $4N + 1$.

The following proposition is a special case of Theorem 1 where $|\Psi^G_M^S\rangle$ can be written more explicitly.

**Proposition 1.**—If $c_1 = -c_0/4 < 0$ and $c_2 \geq 0$, the ground state $|\Psi^G_M^S\rangle = 2N$ is unique and can be written as

$$|\Psi^G_M^S\rangle = \hat{b}_2^\dagger N|\text{vac}\rangle,$$

where $\hat{b}_2^\dagger = \sum_i \varphi(i)\hat{a}_i^\dagger$. Here, $\varphi(i) > 0$ ($i \in \Lambda$) is the hopping term and the on-site potential term. Clearly $|\Psi^G_M^S\rangle$ has the maximum total spin $F_{tot} = 2N$. Ground states in other subspaces can be obtained as $|\Psi^G_M^S\rangle = (F_{tot}^z)^{2N-M}|\Psi^G_M^S\rangle$.

**Theorem 2.**—If $c_1 = 0$ and $c_2 < 0$, the local ground state $|\Psi^G_P^Q\rangle$ in $H_{P,Q}$ is unique and can be written as

$$|\Psi^G_P^Q\rangle = \sum_{m \in I_{P,Q}} D_m (-1)^{(N_1 + N_{-1})/2}|\Phi_m\rangle,$$

with $D_m > 0$. The local ground-state energy in each $H_{P,Q}$ is a function only of $\Gamma := |P| + |Q|$. We denote this energy by $E_{P,Q}^G$. Their energy-level ordering is $E_{P,Q}^G < E_{P',Q'}^G$ if $N - \Gamma$ is even, $E_{P,Q}^G = E_{P',Q'}^G$ if $N - \Gamma$ is odd. Thus the global ground state has total spin $F_{tot} = 0$ and is unique if total particle number $N$ is even, while it has $F_{tot} = 2$ and is fivefold degenerate if $N$ is odd.

Note that $H_{P,Q} \subset H_{M-P+2Q}$. When $c_0 = 0$ and $c_2 < 0$, due to the $\text{SO}(5)$ symmetry of the $c_2$ term (to be shown in the Proof of Theorem 2), the Hamiltonian conserves two quantities $P = N_1 - N_{-1}$ and $Q = N_2 - N_{-2}$. Nevertheless, the energy-level ordering is determined by only one quantum number $\Gamma$. The fact that the ground state tends to be a singlet is consistent with what one would expect from the $c_2 > 0$ term which favors singlet pairs.

**Theorem 3.**—If $c_1 = c_2 = 0$, the local ground state $|\Psi^G_\Lambda_{N_2,...,N_{-2}}\rangle$ in $H_{N_2,...,N_{-2}} := \bigcap_{a=-2}^2 H_{N_a}$ is unique and can be written as

$$|\Psi^G_\Lambda_{N_2,...,N_{-2}}\rangle = \sum_{m \in I_{N_2,...,N_{-2}}} G_m|\Phi_m\rangle,$$

with $G_m > 0$. The local ground-state energy is independent of $N_2, \ldots, N_{-2}$. Thus each $|\Psi^G_\Lambda_{N_2,...,N_{-2}}\rangle$ is also the global ground state in $H$, and the ground-state degeneracy is $\binom{N+4}{N+2} = (N + 4)!/(N/4)!$.

Note that $H_{N_2,...,N_{-2}} \subset H_{M=2(N_2 - N_{-2}) + N_1 - N_{-1}}$. Because of the absence of the spin-dependent interaction, the Hamiltonian in this case has $\text{SU}(5)$ symmetry and conserves the particle number of each spin state. We can say that the ground states exhibit “$\text{SU}(5)$ fermagnetism”.

The above three theorems concern the ground-state magnetic properties and degeneracies. In Fig. 1, the regions of these three theorems are shown together with the mean-field phase diagram of spin-2 condensates.

**Proofs.**—It is worth noting that, if $\hat{H}$ is expanded in terms of bosonic operators $\hat{a}^\dagger$ and $\hat{a}$, the coefficient of each term implies the matrix element $\langle \Phi_m | \hat{H} | \Phi_m \rangle$. As a simple example, the hopping term always results in nonpositive off-diagonal matrix elements because $-t_{i,j} \leq 0$.

**Proof of Theorem 1.**—We first consider a single-site model in which $N$ particles sit on the same site $q \in \Lambda$ [35]. The Hamiltonian of the model can be obtained by taking $t_{i,j} = 0$ for all $i, j$ in Eq. (2). Let us first prove the following lemma.

**Lemma.**—Every local ground state $|\Psi^G_M^S\rangle$ of the single-site model has a total spin $F_{tot} = 2N$.

**Proof of Lemma.**—Recall the $\text{SO}(3)$ symmetry of the Hamiltonian. Without hopping, we then see that all terms in the Hamiltonian commute with each other, which allows us to explicitly write down the energy eigenvalues of the system (see [24–26] or Supplemental Mater-
where \( v \) is the number of bosons that do not form (two-particle) singlets. To minimize \( E \) in \( \mathcal{H}_M \), note that \( c_1 < 0 \) and \( 0 \leq F_{\text{tot}} = F_q \leq 2v \). A simple analysis yields \( F_{\text{tot}} = 2v = 2N \) for every local ground state \( \tilde{\Psi}_M^{\text{GS}} \).

Theorem 1 can now be proved in two separate regions.

(1) \( \{c_1 < 0,5c_1 < c_2 \leq 0\} \): By directly expanding \( \tilde{H} \) in terms of \( \hat{a} \) and \( \hat{a}^\dagger \)'s, one can easily find that \( \forall \mathbf{m} \neq \mathbf{m}' \), \( \langle \Phi_m | \tilde{H} | \Phi_{m'} \rangle \leq 0 \) is always true. Because of the SO(3) symmetry, in the basis \( \{ | \Phi_m \rangle \} \), the matrix of \( \tilde{H} \) is real symmetric and block diagonal with respect to \( M \). Within each \( \mathcal{H}_M \), all possible configurations (distributions of particles on \( \Lambda \), regardless of their spins) are connected via hopping, and all possible spin states are connected via spin-dependent interactions \( c_1 \) and \( c_2 \) terms. Therefore, for each block of \( \tilde{H} \), we can apply the Perron-Frobenius theorem [37], which implies that the local ground state \( | \Psi_M^{\text{GS}} \rangle \) in \( \mathcal{H}_M \) is unique and can be written as Eq. (3).

Since \( (\tilde{F}_{\text{tot}})^2 \) commutes with both \( \tilde{H} \) and \( \mathcal{H}_M \), each \( | \Psi_M^{\text{GS}} \rangle \) must be an eigenstate of \( (\tilde{F}_{\text{tot}})^2 \). To determine the total spin of \( | \Psi_M^{\text{GS}} \rangle \), consider the overlap between \( | \Psi_M^{\text{GS}} \rangle \) and \( | \tilde{\Psi}_M^{\text{GS}} \rangle \). Since the Perron-Frobenius theorem also applies to the single-site model and implies that the ground state \( | \tilde{\Psi}_M^{\text{GS}} \rangle \) has an expansion similar to Eq. (3) with \( C_m \geq 0 \), we have \( \langle \tilde{\Psi}_M^{\text{GS}} | \Psi_M^{\text{GS}} \rangle \neq 0 \). This means that the total spin of \( | \tilde{\Psi}_M^{\text{GS}} \rangle \) is the same as that of \( | \tilde{\Psi}_M^{\text{GS}} \rangle \). It then follows from the Lemma that \( | \Psi_M^{\text{GS}} \rangle \) has the total spin \( F_{\text{tot}} = 2N \).

(2) \( \{c_1 < 0, c_2 > 0\} \): In this region, we cannot apply the Perron-Frobenius theorem in the basis Eq. (1), because the off-diagonal matrix elements of \( \tilde{H} \) take both positive and negative values. Instead, we use the min-max theorem [38]. Define \( \tilde{H}_a := \tilde{H} (c_1 < 0, 5c_1 < c_2 \leq 0) \) and \( \tilde{H}_b := \tilde{H} (c_1 < 0, c_2 > 0) \). Also in each \( \mathcal{H}_M \), define \( E_{a,0} \) and \( E_{a,1} \) as the energies of the local ground state and the first local excited state of \( \tilde{H}_a \), respectively. Similarly, we have \( E_{b,0} \) and \( E_{b,1} \). (If there is degeneracy in the ground state, then \( E_{b,1} = E_{b,0} \)). The local ground state of \( \tilde{H}_a \), as proved above, is a ferromagnetic state which is a zero-energy state of the \( c_2 \) term, as it does not contain any spin singlets. Therefore, Eq. (3) is an eigenstate of \( \tilde{H}_b \). Since \( \tilde{S}_{i,+}, \tilde{S}_{i,-} \) is positive semidefinite, we have \( H_a \leq \tilde{H}_b \). Then the min-max theorem implies that \( E_{a,0} = E_{b,0} \) and \( E_{a,1} \leq E_{b,1} \). Recalling that \( E_{a,0} < E_{a,1} \), we get \( E_{b,0} < E_{b,1} \). This proves that the local ground state in the case \( c_1 < 0 \) and \( c_2 > 0 \) is also unique.

**Proof of Proposition 1.**—Under the conditions of Proposition 1, the Hamiltonian in Eq. (2) becomes \( \tilde{H}' = -\sum_{i\neq j,\alpha} a_{i,j}^\dagger a_{i,j}^\dagger \alpha a_{j,i} - \sum_{i} 2n_{i} + (c_2/8) \sum_{i}[2n_i(2n_i+1) - (\tilde{F}_i)^2] + (c_2/5) \sum_{i} \tilde{S}_{i,+}\tilde{S}_{i,-} \). We seek states (if any) that minimize all terms in \( \tilde{H}' \) simultaneously. The last two terms in \( \tilde{H}' \) are now positive semidefinite. According to Theorem 1, the ground states must have \( F_{\text{tot}} = 2N \), which clearly makes the last two terms zero. As for the hopping term, according to the Perron-Frobenius theorem, its single-particle ground state \( \varphi_{\theta} \) is unique and satisfies \( \varphi_{\theta}(i) > 0 \). Thus it is obvious that \( (\tilde{b}_i)^N \langle \text{vac} | \tilde{F}_{\text{tot}} \rangle \). According to Eq. (4), the ground state in \( \mathcal{H}_{M=2N} \) gives the unique ground state in \( \mathcal{H}_{M=2N} \). The uniqueness of local ground states then implies \( | \Psi_M^{\text{GS}} \rangle \propto (\tilde{F}_{\text{tot}})^{2N-M} | \Psi_M^{\text{GS}} \rangle \).

**Proof of Proposition 2.**—There exists a new set of bosonic operators \( d^\dagger \) and \( d \) defined in the Supplemental Material [36], such that the singlet creation operator can be written as \( \tilde{S}_{i,+} = (\sum_{\mu=1}^{5} d_{\mu}^\dagger d_{\mu}^\dagger) / 2 \). The form of \( \tilde{S}_{i,+} \) now remains unchanged when \( d_{\mu}^\dagger \)'s are subject to SO(5) transformations. Thus the \( c_2 \) term has a manifest SO(5) symmetry. In the Cartan-Weyl basis, ten generators of SO(5) are

\[
\tilde{E}_{i,\alpha\beta} = (-1)^\alpha \hat{a}_{i,\alpha}^\dagger \hat{a}_{i,-\beta} - (-1)^\beta \hat{a}_{i,\beta}^\dagger \hat{a}_{i,-\alpha},
\]

where \( -2 \leq \beta < \alpha \leq 2 \). Taking \( \alpha = -\beta \), we get a basis of the Cartan subalgebra: \( \tilde{P}_i := \tilde{E}_{i,-i-1} = \tilde{n}_{i,1} - \tilde{n}_{i,-1} \) and \( \tilde{Q}_i := \tilde{E}_{i,1,-2} = \tilde{n}_{i,2} - \tilde{n}_{i,-2} \). Indices \( (\alpha, \beta) \) of the other eight generators are roots in the root system \( \mathbb{B}_2 \).

Because of the SO(5) symmetry of the Hamiltonian, we have \( \{ \tilde{P}, \tilde{H} \} = \{ \tilde{Q}, \tilde{H} \} = 0 \), which shows that \( \tilde{H} \) conserves \( P = \tilde{N}_{1} - \tilde{N}_{-1} \) and \( Q = \tilde{N}_{2} - \tilde{N}_{-2} \) and splits into blocks with respect to these two quantum numbers. Besides the
hopping term, off-diagonal matrix elements appear only in the $c_2$ term. By applying the following $U(1)$ transformation for every $i$: $\hat{a}^\dagger_{i,1} = i\hat{a}^\dagger_{i,1}$, $\hat{a}^\dagger_{i,2} = \hat{a}^\dagger_{i,2}$ and $\hat{a}_{i,0} = \hat{a}_{i,0}^\dagger$, one can verify that all the off-diagonal matrix elements of $\hat{H}$ in this basis become nonpositive. Furthermore, connectivity of configurations and that of spin states are guaranteed by the hopping term and the $c_2$ term, respectively. The Perron-Frobenius theorem is thus applicable and asserts that the local ground state $\ket{\Psi^{GS}_{P,Q}}$ in $\mathcal{H}_{P,Q}$ is unique and can be written as Eq. (5).

Now we extract some useful information from the aforementioned single-site model. We claim that states written in the form $\ket{\langle \alpha, \beta \rangle; N, v} := \hat{E}_{q,\alpha,\beta} \cdots \hat{E}_{q,\alpha_1,\beta_1} (\hat{S}_q^+)^{N-v}/(2^{a_{q,+2}^2})\ket{\text{vac}}$ are eigenstates of $\hat{S}_q^+ + \hat{S}_q^-$ with eigenvalues $(N^2 + 3N - 2v^2 - 3v)/4$ [36]. Since $c_2 < 0$, the smaller $v$, the lower energy. Define $\Gamma := \ket{P} + \ket{Q}$ and note that $v \geq \Gamma > 0$. Since $v$ is the number of particles that do not form singlets, for a ground state of the single-site model $\ket{\Psi^{GS}_{P,Q}}$, $v$ takes the minimum possible value, which is $v_{\text{min}} = \Gamma$ if $N - \Gamma$ is even, while $v_{\text{min}} = \Gamma + 1$ if $N - \Gamma$ is odd. The Casimir operator for the model on the total lattice $\Lambda$ is defined as $\tilde{C}_{\text{tot}}^2 = \sum_{\alpha, \beta} (\hat{E}_{\alpha, \beta}^2 - \alpha \beta \hat{E}_{\alpha, \beta})/2$, where $E_{\alpha, \beta} := \sum_q \hat{E}_{\alpha, \beta}$. It is easy to see that $\tilde{C}_{\text{tot}}^2 \ket{\Psi^{GS}_{P,Q}} = \tilde{C}_{\text{tot}}^2 \ket{\Psi^{GS}_{P,Q}} = v_{\text{min}}(v_{\text{min}} + 3)\ket{\Psi^{GS}_{P,Q}}$. Since the Perron-Frobenius theorem again applies to the single-site model, we have $\langle \Psi^{GS}_{P,Q} | \Psi^{GS}_{P,Q} \rangle = 0$, which implies

$$\tilde{C}_{\text{tot}}^2 \ket{\Psi^{GS}_{P,Q}} = v_{\text{min}}(v_{\text{min}} + 3)\ket{\Psi^{GS}_{P,Q}}.$$ (9)

We are now ready to prove the energy-level ordering. Let $E_{P,Q}^{GS}$ be the energy of the local ground state $\ket{\Psi^{GS}_{P,Q}}$. We first note that $E^{GS}_{P,Q} = E^{GS}_{|P,Q|}$ because under the transformation $\hat{a}_{i,2} \leftrightarrow \hat{a}_{i,1}$ or $\alpha_{i,1} \leftrightarrow \alpha_{i,2}$, the Hamiltonian remains unchanged but $P$ or $Q$ gets a minus sign. Thus it suffices to consider the case $P, Q \geq 0$. Next, we prove that all $E^{GS}_{P,Q}$'s with the same $\Gamma$ are the same. Define $\ket{\Psi_{\alpha}} = \hat{E}_{-1,0} \ket{\Psi^{GS}_{P+1,0,1}} \in \mathcal{H}_{P,Q}$ (assume $Q \geq 1$). Apparently energy eigenvalue of $\ket{\Psi_{\alpha}}$ should be the same as $\ket{\Psi^{GS}_{P+1,0,1}}$, which is $E^{GS}_{P+1,0,1}$. So we have $E^{GS}_{P,Q} \leq E^{GS}_{P+1,0,1}$. Define $\ket{\Psi_0} = \hat{E}_{0,0} \ket{\Psi^{GS}_{P+1,0,1}} \in \mathcal{H}_{P+1,0,1}$ (assume $Q \geq 1$), and similarly we get $E^{GS}_{P+1,1} \leq E^{GS}_{P,Q}$. Thus, we have $E^{GS}_{P+1,0,1} = E^{GS}_{P+1,1}$, which means that $E^{GS}_{P,Q}$ is only a function of $\Gamma = \ket{P} + \ket{Q}$, denoted as $E^\Gamma_{\Gamma}$. Now we show the ordering of $E^\Gamma_{\Gamma}$. Construct $\ket{\Psi_0} = \hat{E}_{0,0} \ket{\Psi^{GS}_{P+1,0,1}} \in \mathcal{H}_{P,Q}$ and then get $E^{\Gamma}_{\Gamma} \leq E^{\Gamma_{\Gamma}}_{\Gamma+1}$. When $N - \Gamma$ is even, $\ket{\Psi_0}$ and $\ket{\Psi^{GS}_{P,Q}}$ have different $C^\Gamma_{\Gamma}$, and hence are orthogonal. The uniqueness of each local ground state then yields $E^{\Gamma} < E^{\Gamma_{\Gamma}}_{\Gamma+1}$. When $N - \Gamma$ is odd, construct $\ket{\Psi_0} = \hat{E}_{1,0} \ket{\Psi^{GS}_{P,Q}} \in \mathcal{H}_{P+1,0,0}$, and similarly we have $E^{\Gamma} \geq E^{\Gamma_{\Gamma}}_{\Gamma+1}$, which finally gives $E^{GS}_{\Gamma+1} = E^{GS}_{\Gamma+1}$. We thus obtain the desired energy-level ordering stated in Theorem 2. Consequently, the global ground state is unique and lies in the subspace $\mathcal{H}_{N=0}$ when $N$ is even, while it is five-fold degenerate and lies in $\mathcal{H}_{N=0} \otimes \mathcal{H}_{N=1}$ when $N$ is odd. Then it follows from $[\hat{H}, (\hat{F}_{\text{tot}})^2] = 0$ that the global ground state has $F_{\text{tot}} = 0$ ($F_{\text{tot}} = 2$) when $N$ is even (odd).

Proof of Theorem 3.—Applying the Perron-Frobenius theorem to the hopping term proves the theorem. The proof is essentially the same as that of Theorem 3 in [30] (see the Supplemental Material [36] for details).

Discussion.—In conclusion, we have established the basic ground-state properties of the spin-2 Bose-Hubbard model, as stated in the main theorems. Symmetry plays an important role in our proofs. In particular, the SO(5) symmetry is essential in the case $\{c_1 = 0, c_2 < 0\}$. Although the Cartan subalgebra of so(5) is two-dimensional, we found that the energy-level ordering is effectively “one-dimensional”, as it is characterized only by the quantum number $v$.

In the presence of an external magnetic field in the $z$ direction, one should add linear and quadratic Zeeman terms $\sum_{i,a} (-p_i \alpha \hat{n}_{i,a} + q_i \alpha^2 \hat{n}_{i,a})$ to $\hat{H}$ [25, 39]. In this case, the total Hamiltonian no longer has SO(3) symmetry. However, since the Zeeman terms are diagonal in the basis Eq. (1), the uniqueness of the ground state within each subspace as well as Eqs. (3)–(6) still holds in each respective parameter region.

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[31] Supplemental Material of “Rigorous Results for the Ground States of the Spin-2 Bose-Hubbard Model”

SO(5) SYMMETRY OF SINGLET-CREATION OPERATOR

Here we show how to express the singlet-creation operator in the form with explicit SO(5) symmetry. In the so-called $d$-orbital basis that is obtained by the following unitary transformation

$$
\begin{pmatrix}
\hat{a}^+_i,1 \\
\hat{a}^+_i,2 \\
\hat{a}^+_i,3 \\
\hat{a}^+_i,4 \\
\hat{a}^+_i,5 \\
\end{pmatrix}
= \frac{1}{\sqrt{2}}
\begin{pmatrix}
i & 0 & 0 & 0 & -i \\
0 & i & 0 & i & 0 \\
0 & 0 & \sqrt{2} & 0 & 0 \\
0 & 1 & 0 & -1 & 0 \\
1 & 0 & 0 & 0 & 1 \\
\end{pmatrix}
\begin{pmatrix}
\hat{a}^+_i,2 \\
\hat{a}^+_i,1 \\
\hat{a}^+_i,0 \\
\hat{a}^+_i,1 \\
\hat{a}^+_i,2 \\
\end{pmatrix},
$$

(S1)
singlet creation operator can be written as

\[ S_{i,+} = \frac{1}{2} \sum_{\alpha=-2}^{2} (-1)^{\alpha} a_{i,\alpha}^\dagger a_{i,-\alpha}^\dagger = \frac{1}{2} \sum_{\mu=1}^{5} d_{i,\mu}^\dagger d_{i,\mu}^\dagger. \] (S2)

The SO(5) symmetry now becomes clear in d-orbital basis.

**EIGENSTATES OF \( S_{q,+} S_{q,-} \) FROM HIGHEST-WEIGHT REPRESENTATION OF \( so(5) \)**

In this section we discuss how to find all the eigenstates and eigenvalues of \( S_{q,+} S_{q,-} \) using the highest-weight representation of \( so(5) \). The Cartan-Weyl basis of \( so(5) \) algebra at site \( q \) is

\[ \hat{E}_{q,\alpha\beta} = (-1)^{\alpha} a_{q,\alpha}^\dagger a_{q,-\beta} - (-1)^{\beta} a_{q,\beta}^\dagger a_{q,-\alpha} \] (S3)

with \( (\alpha, \beta) \in B_2 \). Two simple roots in \( B_2 \) are \( \Delta = \{(2,-1),(1,0)\} \). A highest weight state of \( so(5) \) algebra at site \( q \) may be any non-negative integer as long as \( \Delta = \{(2,-1),(0,1)\} \) and \( m \) can be any non-negative integer as long as \( \Delta = \{(2,-1),(0,1)\} \). We claim that \( (\alpha, \beta); N, v \rangle \) is an eigenstate of \( \hat{E}_{q,\alpha\beta} \) with eigenvalue

\[ (\alpha, \beta); N, v \rangle \equiv (\hat{S}_{q,+} \hat{S}_{q,-}) (\alpha, \beta); N, v \rangle = \frac{1}{4} (N^2 + 3N - v^2 - 3v) \langle (\alpha, \beta); N, v \rangle. \] (S6)

To prove it, recall that the SO(5) symmetry leads to \( \hat{E}_{q,\alpha\beta} \hat{S}_{q,+} = 0 \), and the desired result then follows from an iterated application of the identity: \( \hat{S}_{q,-} \hat{S}_{q,+} = (2N+5)/2 \). Note that for a given \( (\alpha, \beta) \), the eigenstate \( (\alpha, \beta); N, v \rangle \) can be labeled by quantum numbers \( (N, v, P_q, Q_q) \). The state is, however, not necessarily an eigenstate of \( \hat{F}_q^2 \), which is in contrast to the eigenstates constructed in [25], labeled by \((N, v, F_q, F_q^2)\).

Now we are going to show that all the eigenstates have been found by the construction of Eq. (S5). With fixed \((N, v), [N, v] := \text{span}(\{(\alpha, \beta); N, v \}) \) forms a highest-weight representation space (module) of \( so(5) \) [40]. For \( N \) spin-2 bosons on the same site \( q \), the Hilbert space must be symmetric. This symmetric space can be decomposed as

\[ \mathcal{H}^S \otimes \mathcal{H}^S \otimes \cdots \otimes \mathcal{H}^S \rangle_{\text{sym}} = [N, v = N] \oplus [N, v = N - 2] \oplus \cdots \oplus [N, v = 1] \text{ or } [N, v = 0], \] (S7)

where \( \mathcal{H}^S \) is the five-dimensional Hilbert space of a single spin-2 particle. Each subspace denoted by \([N, v]\) corresponds to an eigenspace of \( \hat{S}_{q,+} \hat{S}_{q,-} \). We thus have already found all eigenstates of \( \hat{S}_{q,+} \hat{S}_{q,-} \), i.e., all eigenstates can be expressed as linear combinations of the states \( [(\alpha, \beta); N, v] \). This decomposition is nothing but a way of constructing irreducible representation of SO(5) group [41].

**ON THE PROOF OF THEOREM 3**

Proof of Theorem 3 is rather straightforward. However, readers who may need further details may refer to the following. In the case of Theorem 3, it suffices to consider the subspace labeled by \( \{N_\alpha\}_{\alpha=1}^5 \). It is easy to see that all possible states in each subspace are connected via the off-diagonal elements \( \langle \Phi_m | \hat{H} | \Phi_{m'} \rangle \leq 0 \) \((m \neq m')\), which result from the hopping term. Then the Perron-Frobenius theorem guarantees that the ground state within each \( \mathcal{H}_{N_1, \ldots, N_5} \) is unique and is written as Eq. (6). The ground-state degeneracy is exactly the same as the number of subspaces.