Effective field theory for the SO($n$) bilinear-biquadratic spin chain

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We present a low-energy effective field theory to describe the SO($n$) bilinear-biquadratic spin chain. We start with $n = 6$ and construct the effective theory by using six Majorana fermions. After determining various correlation functions we characterize the phases and establish the relation between the effective theories for SO(6) and SO(5). Together with the known results for $n = 3$ and 4, a reduction mechanism is proposed to understand the ground state for arbitrary SO($n$). Also, we provide a generalization of the Lieb-Schultz-Mattis theorem for SO($n$). The implications of our results for entanglement and correlation functions are discussed.

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Introduction.- The study of quantum spin chains dates back to the early days of quantum mechanics [1]. With seemingly simple Hamiltonians, quantum spin chains contain very rich physics and thus attract a considerable interest. A prominent example is the bilinear-biquadratic spin chain with SO($n$) symmetry,

$$H = \cos \theta \sum_{a<b} \sum_j L_j^{ab} L_{j+1}^{ab} + \sin \theta \sum_j \sum_{a<b} L_j^{ab} L_{j+1}^{ab}. \quad (1)$$

In the above expression $L_j^{ab} (1 \leq a < b \leq n)$ are the generators of SO($n$) in the $n$-dimensional vector representation, with the Casimir operator normalized at every site as $\sum_{a<b} (L_j^{ab})^2 = n - 1$. Thus, Eq. (1) represents a family of Hamiltonians parametrized by $\theta \in [-\pi, \pi]$ and $n$. As an example, the case of $n = 3$ corresponds to the well-known spin-1 bilinear-biquadratic model, of great relevance in the context of Haldane’s conjecture [2]. Also, for $n = 4$ the model is equivalent to a symmetrically coupled spin-orbital chain. Such spin-orbital models describe a family of transition metal oxide compounds, where orbital degeneracy plays an important role in the magnetic properties of the material [3]. Quite remarkably, the phase diagram of the model in Eq. (1) for these two cases has been established, and exhibits a rich variety of phases [4–6]. However, the properties for $n \geq 5$ remain mostly unclear yet. For instance, it is unknown whether the behavior in the large-$n$ limit is somehow similar to that of the models with smaller $n$ or not.

In this context, the main contributions of this Letter are (i) to provide a generalization of the Lieb-Schultz-Mattis theorem for SO($n$) and (ii) to present an effective field theory describing the low-energy physics of the model in Eq. (1) for arbitrary $n$ and $\theta \in [0, \theta_{\text{MPS}}]$, with $\theta_{\text{MPS}}$ a special point to be discussed later. This is relevant since it allows us to understand the low-energy physics of the system in the considered parameter regime in an exact way. To achieve this goal, we start with $n = 6$ and show that at a given phase transition point $\theta_R$ the system is critical and is described by the SO(6)$_1$ Wess-Zumino-Novikov-Witten model with central charge $c = 3$. This, in turn, allows us to determine various correlation functions characterizing the phases. Then, after establishing a relationship between the effective theories for SO(6) and for SO(5) [7] and gathering some known results for $n = 3$ and 4, we propose a reduction mechanism to understand the ground state of the SO($n$) Heisenberg chain and suggest an effective field theory for Eq. (1) in the considered parameter regime.

Known results for the general SO($n$) case.- Let us now comment briefly on what is known about the model in Eq. (1) for arbitrary $n$. In Ref. [8] a phase diagram was conjectured based on the existence of some exactly solvable points. For $n \geq 5$, this phase diagram exhibits two remarkable features between the SO($n$) Heisenberg model $\theta_H = 0$ and the integrable SU($n$) Uimin-Lai-Sutherland model $\theta_{\text{ULS}} = \tan^{-1} \frac{1}{\sqrt{n-2}}$ [9]. The first one is a parity effect in $n$; that is, the physical properties of the system are sharply different if $n$ is even or odd. This is best seen at the special point $\theta_{\text{MPS}} = \tan^{-1} \frac{1}{n}$, where the ground state of the model is exactly described by a matrix product state (MPS) [8, 10, 11]. This MPS is unique and translationally invariant for odd $n$, whereas it is twofold degenerate and breaks translational symmetry for even $n$.

The second feature is the location of an integrable model at $\theta_H = \theta_{\text{ULS}} = \tan^{-1} \frac{1}{\sqrt{n-2}}$ [10], which sits between $\theta_H$ and $\theta_{\text{MPS}}$ for $n \geq 5$. This point turns out also to be critical for all $n$, which has important implications. For instance, the existence of this point implies that for $n \geq 5$ the MPS point $\theta_{\text{MPS}}$ no longer captures the physics of the SO($n$) Heisenberg chain. For $n = 5$ this feature is supported by an interesting recent work [11]. Thus, the model in Eq. (1) for $n \geq 5$ has a quite different phase diagram from the $n = 3$ case, where the Affleck-Kennedy-Lieb-Tasaki model at $\theta_{\text{MPS}}$ qualitatively describes the properties of the spin-1 Heisenberg chain [10].

Generalized Lieb-Schultz-Mattis theorem.- From a general perspective, the parity effect has its roots in the difference of the SO($n$) vector representation for odd and even $n$. More precisely, for even $n$, there exists an element $g \in \text{SO}(n)$ such that $\exp(i\pi g) = -I_{n \times n}$. The presence of this element enables a generalization of the Lieb-Schultz-Mattis theorem [13]: Assuming that $|\Psi\rangle$ is the unique ground state of the model in Eq. (1), the
“twisted” state $|\Psi_e\rangle = \exp(i \frac{\pi}{N} \sum_{j=1}^{N} j g_j) |\Psi\rangle$ is not only orthogonal to $|\Psi\rangle$ but also has a vanishing excitation energy in the thermodynamic limit $N \to \infty$. This implies that the model with even $n$ has either gapless excitations or degenerate gapped ground states with broken translational symmetry. On the contrary, the model with odd $n$ can have a unique gapped ground state.

Effective theory for $n = 6$. Let us consider now the model in Eq. (1) for $n = 6$, whose phase diagram is represented in Fig. 1. Since $SO(6) \simeq SU(4)$, this model is equivalent to the $SU(4)$ spin chain with self-conjugate representation 6 in Ref. [14]. For $\theta \in [0, \theta_{\text{MPS}}]$, the conjectured phase diagram in Ref. [14] is in agreement with Ref. [8] and the ground state at $\theta_{\text{MPS}}$ is identified as an extended valence-bond solid state with broken charge-conjugation symmetry. Moreover, an effective theory was derived in Ref. [14] by using non-Abelian bosonization techniques. Here, though, we use a different approach to obtain an effective theory, which makes a clear connection with the $SO(5)$ effective theory in Ref. [7] and enables a possible extension to general $n$. As expected, this effective theory recovers the results from Ref. [14].

Following Ref. [15], we derive the field theory for the $SO(6)$ Heisenberg chain by considering the $SU(4)$ Hubbard model in the strong coupling limit. Let us briefly review this approach to make the subsequent discussions self-contained and to introduce some necessary notations. The $SU(4)$ Hubbard model is written as

$$H_{\text{SU(4)}} = -t \sum_{j,\alpha} (c_{j\alpha}^\dagger c_{j+1,\alpha} + \text{H.c.}) + U \sum_j (n_j - 2)^2,$$  

(2)

where $c_{j\alpha}^\dagger$ is the fermion creation operator at site $j$ with color index $\alpha = 1, \ldots, 4$ and $n_j = \sum_\alpha c_{j\alpha}^\dagger c_{j\alpha}$ is the fermion number operator. Here we consider $U > 0$ and the case of a half-filled fermion energy band (two fermions per site). For $U \gg t$, charge excitations is strongly suppressed due to a Mott gap $\Delta_c \sim U$. Thus, two fermions frozen at each site constitute six states $c_{\alpha\beta}^\dagger c_{\gamma\delta}^\dagger |\text{0}\rangle$, which belong to the vector representation of $SO(6)$. In this limit, standard perturbation theory in $t/U$ yields an $SO(6)$ Heisenberg model [16]. With this correspondence in hand, the $SO(6)$ generators $L^{ab}$ are written as

$$L^{ab} = \frac{1}{2} \sum_{\alpha,\beta} c_{\alpha}^\dagger T^{ab}_{\alpha\beta} c_{\beta},$$

where the $4 \times 4$ $SU(4)$ matrices $T_{ab}$ are normalized as $\text{Tr}(T_{ab} T_{cd}) = 4 \delta_{ac} \delta_{bd}$. Since $SO(6)$ is a rank-3 algebra, we choose three diagonal Cartan generators $L^{12}, L^{34},$ and $L^{56}$ with $T^{12} = \sigma^x \otimes \sigma^z, T^{34} = \sigma^y \otimes \sigma^0, T^{56} = \sigma^z \otimes \sigma^y$, where $\sigma^0$ and $\sigma^z$ are $2 \times 2$ identity and Pauli matrices, respectively.

The field theory for the $SO(6)$ Heisenberg chain can be derived by applying Abelian bosonization techniques to the $SU(4)$ Hubbard model (2) [15]. After linearizing the spectra around two Fermi points $k_F = \pm 2 \pi/\alpha_0$, the fermion operators are decomposed into left-moving and right-moving components as $c_{\alpha} \rightarrow \sqrt{\alpha_0} (\psi_{R\alpha} e^{ik_F x} + \psi_{L\alpha} e^{-ik_F x})$, where $\alpha_0$ is the lattice spacing. These chiral fermions are related to boson fields as $\psi_{R(L),\alpha} = (2\pi/\alpha_0)^{-1/2} \zeta_\alpha \exp[\pm i \sqrt{\pi} (\Theta_{\alpha} \mp \Theta_{\beta})]$, where $\zeta_\alpha$ are Klein factors. The boson fields for $U(1)$ charge and $SO(6)$ spin channels are just linear combinations of $\phi_{\alpha}$, defined by $\phi_{c,s1} = (\phi_1 \pm \phi_2 + \phi_3 \mp \phi_4)/2$ and $\phi_{s2,s3} = (\phi_1 \pm \phi_2 - \phi_3 \mp \phi_4)/2$ [6, 17], respectively. Similar equations hold for their dual fields. The bosonized Hamiltonian density $H = H_0 + H_{\text{int}}$ contains the usual free part $H_0 = \frac{\pi}{2} \sum_{K,s} (K_s (\partial_\theta \Theta_{s})^2 + \frac{1}{K_s} (\partial_\phi \phi_{s})^2)$ with velocities $v_{c,s1}$ and Luttinger parameters $K_{c,s1}$. The interaction part is $H_{\text{int}} = g_\nu \sum_{s \neq \pi} \cos \sqrt{4\pi} \phi_{s\nu} \cos \sqrt{4\pi} \phi_{s\nu}^* - g_{sc} \cos \sqrt{4\pi} \phi_{s\nu} \sum_{s \neq \pi} \cos \sqrt{4\pi} \phi_{s\nu}^*$, where $g_\nu, g_{sc} > 0$ and the spin-charge coupling term comes from the $4k_F$ umklapp scattering presence at half filling. Because of the large Mott gap, the charge boson can be safely integrated out. By introducing six Majorana fermions to refermionize the boson fields $\phi_s$, for instance $(\xi^1 + i \xi^2)(R,L) \sim \exp[i \sqrt{4\pi} \phi_{s1,R(L)}]$, the low-energy effective Hamiltonian density describing the $SO(6)$ spin sector reads [15]

$$H_{\text{eff}} = -\frac{iv}{2} \sum_{\nu=1}^{6} (\xi_{i\nu} \partial_\xi \xi_{i\nu}^* - \xi_{i\nu}^* \partial_\xi^* \xi_{i\nu}) - im \sum_{\nu=1}^{6} \xi_{i\nu}^* \xi_{i\nu}$$

$$-G_s \sum_{1 \leq \nu < \mu \leq 6} \xi_{Ri\nu}^* \xi_{Ri\mu} \xi_{Li\mu}^* \xi_{Li\nu},$$

(3)

with $m > 0$ and $G_s > 0$. Equation (3) predicts a gapped ground state with spin-Peierls order for the $SO(6)$ Heisenberg chain [15], which was confirmed numerically [16].
term is marginal [18]. Other terms are either irrelevant, which play no role in the low-energy limit, or break the SO(6) symmetry, which is forbidden since the effective theory must preserve the symmetry of the original model.

More evidence for this effective theory comes from the integrable point \( \theta_R = \tan^{-1} \frac{1}{2} \) for \( n = 6 \). The Bethe ansatz solution of this model, as shown by Minahan and Zarembo [19], indicates that there are three branches of gapless excitations above the SO(6) singlet ground state. In the low-energy limit, these excitations have the same linear dispersion \( \varepsilon(p) \approx v_L p \). This is in full agreement with the effective theory (3) with a vanishing Majorana mass, which becomes the SO(6) \(_1\) Wess-Zumino-Novikov-Witten theory (possibly perturbed by marginally irrelevant terms) with central charge \( c \).

Furthermore, in Ref. [14], a dimerization operator (possibly perturbed by marginally irrelevant terms) with central charge \( c \) and \( \theta < \theta_R \), centralizes the Majorana mass is expected to be decreasing when \( \theta \) increases from 0 to \( \theta_R \). For \( \theta > \theta_R \), it changes sign \((m < 0)\) and an energy gap reopens.

Let us now derive the correlation functions. First, we note that the effective theory in Eq. (3) is equivalent to six decoupled Ising models and the Majorana mass is \( m \sim (T - T_c)/T_c \), with \( T_c \) the Ising critical temperature [20]. For \( \theta < \theta_R \), the model in Eq. (1) is in the Ising disordered phase with \((\mu_\nu) \neq 0 \) \((\nu = 1, 2, \ldots, 6)\), while for \( \theta > \theta_R \) it is in the Ising ordered phase with \((\sigma_\nu) \neq 0 \) \((\nu = 1, \ldots, 6)\) and \( m = \sigma_\nu \). The Ising variables are expressed as \( J_{iL}^{\mu \nu} = J_{iR}^{\mu \nu} + \sigma_\mu \sigma_\nu \mu_\nu \), where the slowly varying SO(6) Kac-Moody currents \( J_{iL}^{\mu \nu} \) and the staggered components \( n^{ab} \) have critical dimensions 1 and 3/4, respectively. The \( n^{ab} \)'s associated with the Cartan generators are fixed by the model (2), and the staggered components \( n^{ab} \) have critical dimensions 1 and 3/4, respectively. Any two-point correlator \( \langle L_{ij}^{ab} L_{ij+1}^{ab} \rangle \) decays exponentially in both Ising disordered and ordered phases, while at the critical point \( \theta_R \) it decays algebraically as

\[
\langle L_{ij}^{ab} L_{ij+1}^{ab} \rangle \sim C_1 \frac{1}{r^2} + (-1)^i \frac{C_2}{r^{3/2}},
\]

where \( C_1 \) and \( C_2 \) are nonuniversal constants. Furthermore, in Ref. [14], a dimerization operator \( D_j = (-1)^j \sum_{a<b} D_{ij} L_{ij+1}^{ab} L_{ij+2}^{ab} \) and an operator \( C_j = \sum_{a<b} D_{ij} L_{ij+1}^{ab} L_{ij+2}^{ab} \) characterizing the staggered charge-conjugation order were suggested to distinguish between the two phases. Remarkably, in the continuum limit we find that \( D \sim \mu_1 \mu_2 \mu_3 \mu_4 \mu_5 \mu_6 \) and \( C \sim \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \sigma_6 \), satisfying \( \langle D_i \rangle \neq 0 \), \( \langle C_i \rangle = 0 \) for \( \theta < \theta_R \) and \( \langle D_i \rangle = 0 \), \( \langle C_i \rangle \neq 0 \) for \( \theta > \theta_R \), which indeed characterizes the two different phases. At the critical point \( \theta_R \) these competing orders have the same critical exponents and we have \( D_j \sim 1/r^{1/2} \) and \( C_j \sim 1/r^{3/2} \). Therefore, the critical ground state at \( \theta_R \) is an algebraic spin liquid unifying the dimerization order, the staggered charge-conjugation order, and the Néel order.

For the solvable point \( \theta_{\text{MPS}} \), it was shown in Ref. [8] that the MPS has a hidden antiferromagnetic order quantified by a generalized den Nijs-Rommelse string order parameter (SOP) [21] \( O_{ab} = \lim_{|k-j| \to \infty} \langle L_j^{ab} \prod_{\ell=1}^{k-j} \exp(i \pi L_\ell^{ab}) \rangle_{ab} \). Because of the unbroken SO(6) symmetry, all these SOPs are equal and it is sufficient to consider the SOPs for the Cartan generators. We find that they are related to the Ising variables as

\[
O^{12} \sim \langle \sigma_1 \rangle \langle \sigma_2 \rangle, \quad O^{34} \sim \langle \sigma_3 \rangle \langle \sigma_4 \rangle, \quad O^{56} \sim \langle \sigma_5 \rangle \langle \sigma_6 \rangle
\]

These SOPs have nonzero values in the Ising ordered phase for \( \theta > \theta_R \) and vanish in the disordered phase for \( \theta < \theta_R \). Therefore, they are also proper order parameters for the phase with staggered charge-conjugation order and their utility goes beyond the solvable point \( \theta_{\text{MPS}} \).

Reduction from \( n = 6 \) to \( n = 5 \). In the following we establish a relationship between the effective field theories for SO(6) and for SO(5) [7]. Let us go back to the SU(4) Hubbard model in Eq. (2) and interpret the fermion color index as spin-$\frac{3}{2}$ quantum numbers \((\alpha = \pm \frac{1}{2}, \pm \frac{1}{2})\). Then, the SO(6) vector representation at each site unifies the spin-2 quintet states and the spin-0 singlet state formed by two spin-$\frac{3}{2}$ fermions. If an on-site spin-dependent interaction \( V \sum_j \mathbf{S}_j^2 \) is added to the model (2), then the singlet and quintet sectors pick up different energies and the SU(4) symmetry of the Hamiltonian is broken down to SO(5) [22], with an energy difference \( \Delta_s \sim V \) between the two sectors. For \( V < 0 \) the quintet states, forming SO(5) vector representation, have lower energy and the effective exchange Hamiltonian in the Mott regime is an SO(5) Heisenberg model [22, 23]. In the field theory treatment [7], the quintet and singlet degrees of freedom are described by Majorana fermions \( \xi^{\sigma} \) \((\sigma = 1, 2)\) and \( \xi^6 \), respectively. In Eq. (3), the energy difference \( \Delta_s \) is formally accounted for by giving \( \xi^6 \) a large mass \( m_6 \gg m_q > 0 \), while \( m_q \) is the mass of the other five Majorana fermions. In the low-energy limit, integration over \( \xi^6 \) yields five massive Majorana fermions with a renormalized mass \( m_q' > 0 \). Although the five remaining Majorana fermions have a smaller mass \( m_q' < m_q \), the SO(5) Heisenberg chain is still in the Ising disordered phase, corresponding to dimerized ground states [7].

Thanks to this mechanism, we can now study the correlation functions of the SO(5) model. This is accomplished by simply replacing the Ising variables \( \mu_6 \) and \( \sigma_q \) in the expressions for SO(6) by their expectation values \( \langle \mu_6 \rangle \neq 0 \) and \( \langle \sigma_q \rangle = 0 \), respectively. In the SO(5) Ising ordered phase, unlike the SO(6) case, translational symmetry is preserved and all two-point correlation functions decay exponentially. For example, it is easy to show that for SO(5) the operator \( C \) has a vanishing expectation value. However, according to Eq. (5), the nonlocal SOPs
are still nonzero and thus are valid order parameters in this phase.

Reduction and effective theory for arbitrary $n$. Motivated by the above discussions, we now propose a reduction mechanism to understand the ground state of the $SO(n)$ Heisenberg model. As we have seen, the $SO(n)$ Heisenberg models for $n = 6$ and $5$ are both described by $n$ massive Majorana fermions with mass $m > 0$ and marginally irrelevant terms. Formally speaking, one can say that we go from an effective theory for $SO(n)$ to an effective theory for $SO(n - 1)$ by giving a large mass to the Majorana fermion $\xi^n$ and integrating it out. Because of the marginally irrelevant couplings in the $SO(n)$ effective theory, the elimination of the large-mass Majorana fermion induces a negative contribution to the mass of the $n - 1$ remaining Majorana fermions. Usually, the exact values of the parameters in these effective theories are not known. However, the sublety here is that the $SO(4)$ Heisenberg chain lies exactly at the critical point $\theta_R$. Since $SO(4) \cong SU(2) \times SU(2)$, the $SO(4)$ Heisenberg chain is equivalent to two decoupled spin-$\frac{1}{2}$ Heisenberg chains, whose effective theory contains four massless Majorana fermions [24]. Thus, if one wishes to construct this theory from the effective theory for $SO(5)$, the only possibility to obtain the zero mass of the four Majorana fermions is the miraculous exact cancellation of their original mass [in the $SO(5)$ theory] and the negative contribution that comes from integrating over the large-mass Majorana fermion $\xi^5$. We can proceed further from this massless $SO(4)$ theory on to an $SO(3)$ theory, where three massive Majoranas with $m < 0$ are obtained and which recovers Tsvelik’s theory for the spin-1 Heisenberg chain [25].

What about the effective field theory for general $n$? By combining the results for $n = 3, \ldots, 6$ and applying the reduction mechanism in the reverse direction, we can argue that at the integrable point $\theta_R$ the $SO(n)$ spin chain in Eq. (1) is described by an $SO(n_1)$ Wess-Zumino-Novikov-Witten model with $n$ massless Majorana fermions perturbed by marginally irrelevant terms. This theory has central charge $c = n \times \frac{1}{2}$, and thus the entanglement entropy of a block increases linearly with $n$ for the ground state of the system close to and at $\theta_R$ [26]. For $n \geq 5$, the isolated critical point $\theta_R$ separates the region $\theta \in [0, \theta_{\text{MPS}}]$ into and Ising disordered phase for $\theta < \theta_R$ and an ordered phase for $\theta > \theta_R$. By using the results in Ref. [27], $n$ zero-energy Majorana modes $\eta^a$ ($a = 1 \sim n$) localized at the boundary are obtained from the $SO(n)$ effective theory for $m < 0$ in a semi-infinite chain and form $SO(n)$ generators $\Gamma^{ab} = i\eta^a \eta^b$ in spinor representation. Note that the $SO(n)$ spinor is irreducible for odd $n$ but reducible for even $n$ and contains two subspaces. This explains the appearance of $SO(n)$ spinor edge states at $\theta_{\text{MPS}}$ and their crucial differences for even and odd $n$ [8]. Another interesting prediction of our theory is the two-point correlator $\langle L^{ab}_j L^{ab}_{j+r} \rangle$ at the critical point $\theta_R$. In the continuum limit, the $SO(n)$ generators $L^{ab}$ are a sum of uniform $SO(n)$ currents with critical dimension 1 and staggered components with critical dimension $n/8$ ($n$ Ising variables). For $3 < n < 7$, the contribution from the staggered components is dominant in the correlator and we have $\langle L^{ab}_j L^{ab}_{j+r} \rangle \sim (-1)^r/r^{n/4}$. However, for $n > 8$, the contribution from uniform $SO(n)$ currents becomes dominant and in this case $\langle L^{ab}_j L^{ab}_{j+r} \rangle \sim 1/r^2$.

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