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Quantum criticality in the SO(5) bilinear-biquadratic Heisenberg chain

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The zero-temperature properties of the SO(5) bilinear-biquadratic Heisenberg chain are investigated by means of a low-energy approach and large-scale numerical calculations. In sharp contrast to the spin-1 SO(3) Heisenberg chain, we show that the SO(5) Heisenberg chain is dimerized with a twofold degenerate ground state. On top of this gapful phase, we find the emergence of a nondegenerate gapped phase with hidden $(Z_2 \times Z_2)^2$ symmetry and spin-3/2 edge states that can be understood from a SO(5) AKLT wave function. We derive a low-energy theory describing the quantum critical point which separates these two gapped phases. It is shown and confirmed numerically that this quantum critical point belongs to the $SO(5)_1$ universality class.

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One-dimensional (1D) quantum systems display a wealth of fascinating behaviors which have attracted much interest over the years. A paradigmatic example of an exotic phase stabilized by 1D quantum fluctuations is the Haldane phase of the spin-1 SU(2) Heisenberg chain.[1] On top of the existence of a gap, this phase displays remarkable properties like the existence of a hidden Néel antiferromagnetic order[2] or the emergence of fractional spin-1/2 edge states when the chain is doped by nonmagnetic impurities.[3] A simple way to grasp the main characteristics of the Haldane phase is provided by the seminal work of Affleck, Kennedy, Lieb, and Tasaki (AKLT),[4] where a fine-tuned biquadratic exchange interaction is introduced so that the ground state (GS) is made up solely of nearest-neighbor valence bonds. Due to the absence of a quantum phase transition upon switching on the biquadratic exchange from the Heisenberg model up to the AKLT point, all the exotic properties of the Haldane phase can be simply deduced from the AKLT wave function.[5]

In an interesting work, Tu *et al.*[6] have recently studied a generalization of the spin-1 bilinear-biquadratic Heisenberg chain to higher symmetry group $SO(2n+1)$, with Hamiltonian

$$\mathcal{H} = \cos\theta \sum_i \sum_{a<b} L_i^{ab} L_{i+1}^{ab} + \sin\theta \sum_i \left(\sum_{a<b} L_i^{ab} L_{i+1}^{ab} \right)^2, \quad (1)$$

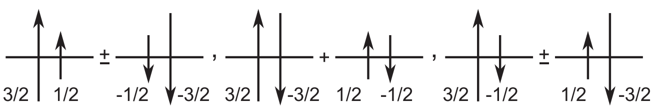
where L_{ab} $(1 \leqslant a < b \leqslant 2n+1)$ are the $n(2n+1)$ generators which transform in the vectorial representation ($n \times n$ matrices) of the $SO(2n+1)$ group. They are normalized such that the single-site Casimir operator is $\sum_{a<b}(L_i^{ab})^2 = 2n$. For $n=1$, this model is nothing but the spin-1 bilinear biquadratic Heisenberg chain. The phase diagram of the model (1) for general n has been conjectured in Ref. 6 based on the behavior at some special points. For $\theta = \tan^{-1} 1/(2n-1)$, the model is the $SU(2n+1)$ Sutherland model which displays a quantum critical behavior with $2n$ gapless modes.[7] There is a second $SU(2n+1)$ symmetric model for $\theta = \pm\pi/2$ with alternating fundamental and conjugate representations, where the GS is dimerized with a spontaneous breaking of translation symmetry.[8] For $\theta_{\mathrm{AKLT}} = \tan^{-1} 1/(2n+1)$, the GS is a $SO(2n+1)$ matrix product state which is the generalization of the SO(5) AKLT state introduced by Scalapino *et al.*[9] in the context of a SO(5) two-leg ladder. The resulting nondegenerate gapped phase is the $SO(2n+1)$ generalization of the Haldane phase with hidden antiferromagnetic ordering due to the breaking of a $(Z_2 \times Z_2)^n$ symmetry.[6] In open boundary geometry, the two edge states belong to the spinorial representation of $SO(2n+1)$ with dimension 2^n, so that the GS is 4^n-fold degenerate. Finally, the model with $\theta_R = \tan^{-1}(2n-3)/(2n-1)^2$ is exactly solvable[10] and is expected to have gapless excitations from general grounds.

In this paper, we investigate part of the zero-temperature phase diagram between $\theta = 0$ and θ_{AKLT}, including the criticality of the SO(5) bilinear-biquadratic spin chain by means of complementary low-energy approach and several numerical calculations: exact diagonalization (ED) and density matrix renormalization group (DMRG).[11] We give further arguments supporting the phase diagram for $n=2$ conjectured in Ref. 6. In sharp contrast with the spin-1 Heisenberg chain, the AKLT point for $n=2$ is found *not* to capture the physics of the SO(5) Heisenberg chain. A quantum phase transition occurs at $\theta = \theta_R$ that we fully characterize and show to belong to the $SO(5)_1$ universality class with central charge $c = 5/2$.

Low-energy approach. In principle, a field-theory approach capturing the low-energy properties of the $SO(2n+1)$ Heisenberg chain can be derived from the solvable point at $\theta = \theta_R$. By exploiting the integrability of the model, one may determine the nature of the underlying conformal field theory (CFT) and investigate small deviations $|\theta - \theta_R| \ll 1$ in parallel to the Majorana fermion approach of Tsvelik for $n=1$.[12] Here we instead directly derive a low-energy description for the SO(5) Heisenberg chain by considering a spin-3/2 fermionic model which is SO(5) symmetric:[13,14]

$$\mathcal{H}_{SO(5)} = -t \sum_{i,\alpha} [c_{\alpha,i}^\dagger c_{\alpha,i+1} + \mathrm{H.c.}] - \mu \sum_i n_i + \frac{U}{2} \sum_i n_i^2 + V \sum_i P_{00,i}^\dagger P_{00,i}, \quad (2)$$

where $c^\dagger_{\alpha,i}$ denotes the fermionic creation operator with spin index $\alpha = \pm 3/2, \pm 1/2$, and $n_i = \sum_\alpha c^\dagger_{\alpha,i} c_{\alpha,i}$ is the density operator at site i. In Eq. (2), the singlet BCS pairing operator for spin-3/2 fermions is $P^\dagger_{00,i} = c^\dagger_{3/2,i} c^\dagger_{-3/2,i} - c^\dagger_{1/2,i} c^\dagger_{-1/2,i}$. As shown in Ref. 13, the spin-3/2 model (2) enjoys a $\mathrm{U}(1)_{\mathrm{charge}} \times \mathrm{SO}(5)_{\mathrm{spin}}$ continuous symmetry without any fine-tuning. When $U, V > 0$, the lowest states for $t = 0$ at half-filling are the quintet states:



A standard strong-coupling approach can then be applied when $U, V \gg t > 0$ and one finds the effective model to be a SO(5) Heisenberg chain: $\mathcal{H} = J \sum_i \sum_{a<b} L^{ab}_i L^{ab}_{i+1}$ with $J = 2t^2/3U$. Then, a low-energy description can be deduced for the latter model given the adiabatic continuity between weak and strong coupling regimes for the spin-3/2 model.[15] As derived in Ref. 15, the weak-coupling approach at half-filling is built from eight right- and left-moving Majorana fermions $\xi^A_{R,L}$ (with $A = 1, \ldots, 8$):

$$\mathcal{H}_{\mathrm{int}} = \frac{g_1}{2}\left(\sum_{a=1}^{5} \xi^a_R \xi^a_L\right)^2 + g_2\, \xi^6_R \xi^6_L \sum_{a=1}^{5} \xi^a_R \xi^a_L + \frac{g_3}{2}\left(\xi^7_R \xi^7_L + \xi^8_R \xi^8_L\right)^2 + \left(\xi^7_R \xi^7_L + \xi^8_R \xi^8_L\right)\left(g_4 \sum_{a=1}^{5} \xi^a_R \xi^a_L + g_5\, \xi^6_R \xi^6_L\right), \quad (3)$$

where the two Majorana fermions $\xi^{7,8}_{R,L}$ account for the U(1) charge symmetry, the five Majorana fermions $\xi^a_{R,L}$ (with $a = 1, \ldots, 5$) generate the SO(5) symmetry, and $\xi^6_{R,L}$ describes an internal discrete Z_2 symmetry. By integrating out the charge degrees of freedom which are fully gapped in the large U,V repulsive limit, one then obtains an effective Hamiltonian with leading part

$$\mathcal{H}_{\mathrm{eff}} = -\frac{iv}{2}\sum_{a=1}^{5}\left(\xi^a_R \partial_x \xi^a_R - \xi^a_L \partial_x \xi^a_L\right) - i m_s \sum_{a=1}^{5} \xi^a_R \xi^a_L, \quad (4)$$

describing five massive Majorana fermions with mass $m_s \sim U > 0$. In fact, after the integration of the charge degrees of freedom, $\xi^6_{R,L}$ is also a massive Majorana fermion, but with a higher mass $m_o > m_s$ so that its contribution can be neglected in the low-energy limit $E \ll m_0$. The effective low-energy approach of the SO(5) Heisenberg chain is thus given by model (4), a natural extension to SO(5) of Tsvelik's result (i.e., three massive Majorana fermions) for the spin-1 Heisenberg chain.[12] Since a 1D theory of massive Majorana accounts for the long-distance behavior of a 1D quantum Ising model, the low-energy properties of the SO(5) Heisenberg chain can be described in terms of five decoupled off-critical 1D quantum Ising models in their disordered phases ($m_s \sim T - T_c$).

To fully characterize the nature of the GS of the SO(5) Heisenberg chain, it is instructive to investigate the expectation value of the SO(5) dimerization operator $D_i = (-)^i \sum_{a<b} L^{ab}_i L^{ab}_{i+1}$. One can follow a similar strategy to derive a low-energy expression for this operator. In the low-energy limit $E \ll m_o$, we find that D is expressed in terms of the disorder operators μ_a of the underlying 1D quantum Ising degrees of freedom: $D \sim \prod_{a=1}^5 \mu_a$. Since the Ising models are locked in their disordered phases, we obtain that $\langle D \rangle \neq 0$. The GS of the SO(5) Heisenberg chain is thus twofold degenerate and spontaneously dimerized in sharp contrast with the Haldane phase of the spin-1 Heisenberg chain.

With this low-energy approach at hand, we can investigate the effect of the SO(5) biquadratic term in Eq. (1) in the vicinity of $\theta = 0$. The most relevant term consistent with the symmetries of the lattice model is the Majorana fermion mass term of Eq. (4). We thus deduce that the low-energy Hamiltonian of Eq. (1) is still given by (4) with a mass $m_s(\theta)$, a phenomenological parameter within our approach. The only possibility is that the mass m_s vanishes and changes sign to form a new gapful phase with the five effective 1D quantum Ising models entering their ordered phases. It is very tempting to identify the quantum critical point at $m_s = 0$ with the location of the integrable model at $\theta = \theta_R$ which is expected, on general grounds, to display a quantum critical behavior. This will be confirmed precisely numerically below. We thus conclude that the universality class of the integrable model for $\theta = \theta_R$ is the $\mathrm{SO}(5)_1$ CFT with central charge $c = 5/2$. In addition, our low-energy approach enables us to extract the leading asymptotics of the SO(5) spin-spin correlations which display a power-law decay with a universal exponent: $\langle L^{ab}_{i+x} L^{ab}_i \rangle \sim (-)^x x^{-5/4}$. The SO(5) dimerization operator vanishes at $\theta = \theta_R$ and has a power-law decaying correlation function with the same universal exponent. For $\theta > \theta_R$, a new gapful phase emerges with no spontaneous dimerization since $\langle \mu^a \rangle = 0$ for $m_s < 0$. This phase is the analog of the Haldane phase of the spin-1 Heisenberg chain. Each Ising model has a doubly degenerate GS which gives a 2^5 degeneracy. However, there is a redundancy in the Majorana fermion description since the transformation $\xi^a_{R,L} \to -\xi^a_{R,L}, \mu^a \to \mu^a, \sigma^a \to -\sigma^a$ leaves invariant the Hamiltonian and the physical operators. The correct hidden symmetry group is thus $(Z_2 \times Z_2)^2$ in full agreement with the description of the AKLT wave function for the SO(5) generalization of the Haldane phase.[6,9] As a consequence of this antiferromagnetic ordering, there are nontrivial edge states in this phase when a semi-infinite open chain is considered. Using the results of Ref. 16, we find the emergence of five localized Majorana fermion zero-mode states η^a inside the gap (mid-gap states). These five local fermionic states give rise to a local spin-3/2 operator $\vec{\mathcal{S}}$ since

$$\mathcal{S}^x = -i\eta^1\eta^4 - i\eta^2\eta^5 - i\sqrt{3}\,\eta^2\eta^3,$$
$$\mathcal{S}^y = -i\eta^1\eta^5 + i\eta^2\eta^4 + i\sqrt{3}\,\eta^1\eta^3,$$
$$\mathcal{S}^z = -i\eta^1\eta^2 - 2i\eta^4\eta^5,$$

describe a local spin-3/2 operator thanks to the anticommutation relations of the Majorana fermions: $\{\eta^a, \eta^b\} = \delta^{ab}$. In the phase with $\theta > \theta_R$, we thus predict the occurrence of spin-3/2 boundary excitations at the edge of the chain, again in full agreement with the SO(5) AKLT wave function.[9]

Numerical results. We combine ED and DMRG calculations to clarify the phase diagram and the criticality of the phase transition. We use a spin-2 formulation of the model (1) using projectors,[6] which leads to

$$\mathcal{H} = \sum_{\langle ij\rangle} \cos\theta\left[-1-\frac{5}{6}\mathbf{S}_i\cdot\mathbf{S}_j+(\mathbf{S}_i\cdot\mathbf{S}_j)^2/9 + (\mathbf{S}_i\cdot\mathbf{S}_j)^3/18\right] + \sin\theta\left[1-5\mathbf{S}_i\cdot\mathbf{S}_j - \frac{17}{12}(\mathbf{S}_i\cdot\mathbf{S}_j)^2+\frac{1}{3}(\mathbf{S}_i\cdot\mathbf{S}_j)^3+\frac{1}{12}(\mathbf{S}_i\cdot\mathbf{S}_j)^4\right]. \quad (5)$$

First, we compute with ED the first singlet and magnetic excitations for various chains with periodic boundary conditions (PBCs). For $\theta < \theta_R$, the data (shown in Fig. 1) are compatible with a finite spin gap but a vanishing singlet gap (with momentum π), which suggests a singlet phase that breaks translation symmetry. It is remarkable that the extrapolation (using polynomial fit) of the crossing point of the first magnetic and nonmagnetic excitations gives $\theta_c = 6.34^\circ$ which is precisely the numerical value of θ_R.

The dimerized nature of the GS of the Heisenberg SO(5) chain at $\theta = 0$ is confirmed by computing the correlator $\langle \sum_{a<b} L_i^{ab} L_{i+1}^{ab}\rangle$ as a function of position i in an open chain. The DMRG data (see Fig. 2) obtained on a $L = 256$ chain with open boundary conditions (OBCs) in the range $0 \leqslant \theta \leqslant \theta_{\rm AKLT}$ clearly show a staggered pattern for $0 \leqslant \theta < \theta_R$, in contrast with the uniform values found for $\theta > \theta_R$, for instance at the AKLT point.

For $\theta \simeq \theta_{\rm AKLT}$, the lowest excitation is magnetic and has a finite gap. In fact, right at the AKLT point, ED *proves* the existence of a finite gap in the thermodynamic limit using an argument from Knabe:[17] The thermodynamic gap is bounded by the gap on a finite cluster with $L+1$ sites (OBC) as $\Delta_\infty > \frac{L}{L-1}(\Delta_L - \frac{1}{L})$. Using $L = 8$, we already obtain that the spin gap is finite and satisfies $\Delta_\infty > 0.185$.

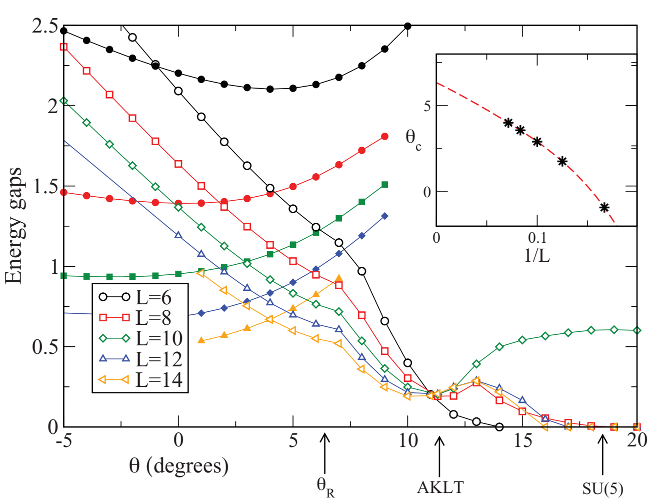


FIG. 1. (Color online) ED data showing the gap to the first singlet and magnetic excitations (solid and open symbols, respectively) vs θ for several chain lengths L. (Inset) The extrapolation of the crossing point.

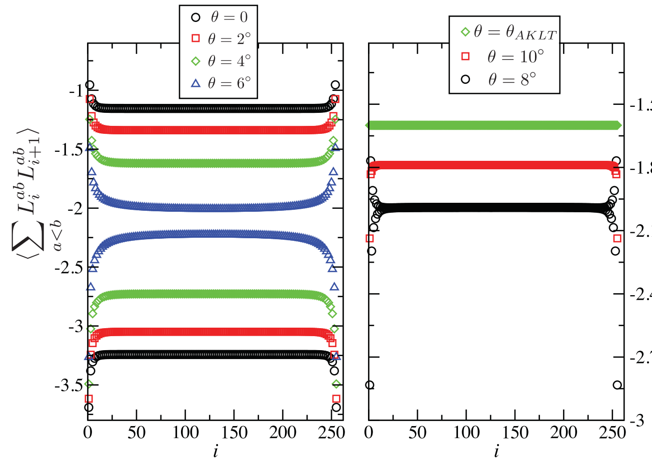


FIG. 2. (Color online) DMRG data of the dimerization $\langle \sum_{a<b} L_i^{ab} L_{i+1}^{ab}\rangle$ as a function of position i, induced in a $L = 256$ chain by the OBC in the ranges $\theta < \theta_R$ (left panel) and $\theta > \theta_R$ (right panel). At $\theta = 0$, the system is strongly dimerized.

For larger θ, data are also compatible with a SU(5) gapless phase but we observe strong finite-size effects due to incommensurate excitations, similar to the case of the spin-1 chain close to the SU(3) point.[18]

As argued in the low-energy section, the central charge of the critical point between the dimerized and SO(5) Haldane phases should be $c = 5/2$, corresponding to a $\mathrm{SO}(5)_1$ CFT. In Fig. 3(a), we show in log-linear scale the von Neumann entropy $S(x)$ of a block of x sites at θ_R as a function of the conformal distance $d(x) = L/\pi \sin(\pi x/L)$ for chains with PBC of sizes up to $L = 32$ with DMRG.[19] Fitting the data to the expected form for PBC $S(x) = c/3 \ln[d(x)] + K$ with K a constant (see Ref. 20), we obtain an estimate of the central charge $c = 2.53$. We can also obtain c using finite-size corrections of the GS energy per site: $e_0(L) = e_0 - (\pi v c)/6L^2$. Using ED data (not

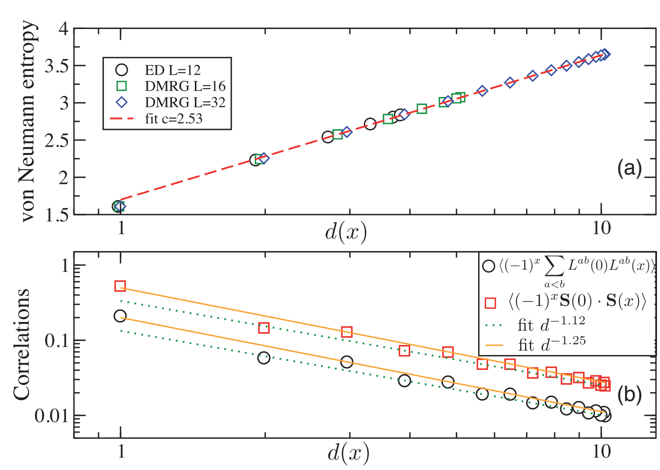


FIG. 3. (Color online) At θ_R and as a function of conformal distance $d(x) = L/\pi \sin(x\pi/L)$ for systems with PBC: (a) von Neumann entropy of a block of size x (log-lin scale), (b) spin $\langle(-)^x \mathbf{S}_0 \cdot \mathbf{S}_x\rangle$ and SO(5) generators $\langle (-)^x \sum_{a<b} L_0^{ab} L_x^{ab}\rangle$ correlators (log-log scale). Correlators are translation-invariant due to the PBC and are normalized to 1 at their onsite values.

shown) for both the energy and finite-size velocity $v(L) = E_0(k = 2\pi/L) - E_0(k = 0)$, we obtain the same estimate $c = 2.53$, in excellent agreement with a $SO(5)_1$ quantum criticality.

At the critical point θ_R, the low-energy approach predicts the leading behavior of two-point correlations: $\langle L_i^{ab} L_{i+x}^{ab} \rangle \sim (-)^x x^{-5/4}$ (the same dependence is expected for spin correlations $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+x} \rangle$). These correlators, plotted in Fig. 3(b) for a $L = 32$ chain with PBC, exhibit an even/odd effect besides the $(-)^x$ factor. Fits of the two sets of points, respectively, lead to power-law exponents of 1.25 and 1.12, equal or close to the theoretical prediction 5/4 for both correlators. We expect that all correlators decay with the same exponent 5/4 in the thermodynamic limit and that the even/odd effect (and the corresponding different exponents) is caused by subleading correlations, which can be important for the moderate system size $L = 32$ that can be reached in the DMRG simulations.

Conclusion. Using complementary techniques, we confirm the phase diagram that has been proposed phenomenologically in Ref. 6. In particular, we derive a low-energy approach in terms of five massive Majorana fermions which makes it possible to determine that (i) the GS at $\theta = 0$ is spontaneously dimerized and (ii) it is separated from the SO(5) generalization of the Haldane phase by a quantum critical point described by a $SO(5)_1$ CFT with central charge $c = 5/2$. All these predictions are quantitatively confirmed using extensive numerical simulations. In sharp contrast to the $n = 1$ case, the SO(5) AKLT point does not share the same physics with the Heisenberg point $\theta = 0$. This property should be a general feature of the model with $n > 1$.[6] In this respect, the $n = 1$ case is very special and *not* representative of the generic situation.

To give some perspective, let us mention that the low-energy approach presented here is directly relevant to the quantum critical behavior of the spin-2 model interpolating between two topologically distinct AKLT states.[21–23] In particular, the quantum phase transition between the SO(5) AKLT state and the spin-2 dimerized phase found in Refs. 21 and 23 can be shown to be described by the effective Hamiltonian (4) and thus belongs to the $SO(5)_1$ universality class. However, our approach does not capture the direct topological quantum phase transition between the spin-2 AKLT state with spin-1 edge states and the SO(5) AKLT state put forward in Refs. 21–23. It will be interesting to understand how it can be extended to explain the emergence of $SO(5)_1$ criticality recently observed numerically for this transition.[23]

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