Critical behavior of the spin-1 and spin-3/2 Baxter-Wu model in a crystal field

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The phase diagram and the critical behavior of the spin-1 and the spin-3/2 two-dimensional Baxter-Wu model in a crystal field are studied by conventional finite-size scaling and conformal invariance theory. The phase diagram of this model, for the spin-1 case, is qualitatively the same as those of the diluted 4-states Potts model and the spin-1 Blume-Capel model. However, for the present case, instead of a tricritical point one has a pentacritical point for a finite value of the crystal field, in disagreement with previous work based on finite-size calculations. On the other hand, for the spin-3/2 case, the phase diagram is much richer and can present, besides a pentacritical point, an additional multicritical end point. Our results also support that the universality class of the critical behavior of the spin-1 and spin-3/2 Baxter-Wu model in a crystal field is the same as the pure Baxter-Wu model, even at the multicritical points.

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I. INTRODUCTION

The Ising model defined on a triangular lattice with three-spin interactions is a quite interesting system because it does not present, like other more well known magnetic models, the up-down spin-reversal symmetry [1]. The Hamiltonian of the so-called Baxter-Wu (BW) model can be defined by

$$H_{BW} = -J \sum_{\langle ijk \rangle} \sigma_i \sigma_j \sigma_k,$$

where $J$ is the exchange interaction, the sum extends over all elementary triangles of the triangular lattice with $N$ sites, and $\sigma_i = \pm 1$ are Ising spin-1/2 variables located at the corresponding lattice sites (here, instead of having $\sigma_i = \pm 1/2$ we consider a renormalized exchange interaction $J$ so that the spin states are just given by $\sigma_i = \pm 1$). The model given by Eq. (1) is self-dual [1,2], having the same critical temperature $T_c$ as that of the spin-1/2 Ising model on a square lattice, namely, $k_B T_c / J = 2 / \ln(\sqrt{2} + 1) = 2.269185 \ldots$, where $k_B$ is the Boltzmann constant. The critical behavior of the Baxter-Wu model is governed by a conformal field theory with central charge $c = 1$ [3,4], and the exact solution shows that its leading exponents [3–5] $\alpha = 2/3$, $\nu = 2/3$, and $\eta = 1/4$ are the same as those of the 4-states Potts model [6]. Although the leading critical exponents are the same, these two models have different corrections to the finite-size scaling exponents. While the 4-states Potts model presents logarithmic corrections with the size of the system, the Baxter-Wu model has power law corrections with correction-to-scaling exponent $w = 4$ [3,4]. It is exactly due to this rather large value of $w$ that we can expect to obtain, in the thermodynamic limit, quite good estimates of physical quantities of the Baxter-Wu model by using finite-size scaling theory, even when exploring just the smaller system sizes and taking into account the effects of corrections to scaling. It should be said that further extensions of the spin-1/2 model given by Eq. (1) above have also been recently made by considering transverse [7] and longitudinal [8] magnetic fields, Monte Carlo studies of the critical amplitude ratios [9] and short-time dynamics [10], among several others.

Another interesting extension of the above model is to consider spins greater than half and to include an extra crystal field coupled to $\sigma_i^2$, in such a way that the new Hamiltonian reads

$$H = -J \sum_{\langle ijk \rangle} \sigma_i \sigma_j \sigma_k + D \sum_{i=1}^{N} \sigma_i^2,$$

where the classical spin variables $\sigma_i$ take now values $\sigma_i = -S, -S + 1, \ldots, S - 1, S$, with $S \geq 1$, and $D$ is the crystal field or single ion anisotropy. Unfortunately, no exact solution is known for $S \geq 1$. However, one can note that when $D \to -\infty$, only configurations with $\sigma_i = \pm S$ are allowed, and we recover the pure two-state Baxter-Wu model with a renormalized critical temperature given by $k_B T_c / J = S^3 / 2 \ln(\sqrt{2} + 1) = S^3 \times 2.269185 \ldots$. On the other hand, when $D \to \infty$, the system is either in the $\sigma_i = 0$ state, for integer values of $S$, or we have another two-state pure Baxter-Wu model with $\sigma_i = \pm 1/2$, for half-integer values of $S$. In the latter case there is an additional second-order phase transition at the exact renormalized critical temperature given by $k_B T_c / J = (4/3)^2 / 2 \ln(\sqrt{2} + 1) = 0.283648 \ldots$

Thus, the Hamiltonian given by Eq. (2) resembles that of the Blume-Capel (BC) model, where the latter has been extensively studied in the literature and can be defined by [11]

$$H_{BC} = -J \sum_{\langle i, j \rangle} \sigma_i \sigma_j + D \sum_{i=1}^{N} \sigma_i^2,$$

where the first sum is over nearest-neighbor spins. Analogous limits $D \to \pm \infty$, as done above for the Baxter-Wu model, are achieved for the model given by Eq. (3), with the two-state...
spin Ising system being the corresponding limits. In addition, it has been well known that for dimensions greater than one (the one-dimensional model has no phase transition at finite temperatures for any value of $S$) the Blume-Capel model exhibits a phase diagram with ordered ferromagnetic and disordered paramagnetic phases separated by a transition line. This transition line changes from a second-order character (Ising universality class) to a first-order character at a tricritical point for integer values of $S$, while it remains always second order for half-integer values of $S$. In the latter case, first-order transition lines appear at low temperatures and terminate at double critical end points. More details about the phase diagram of the general spin-$S$ can be found in Refs. [12–15]. It should be stressed that for the Blume-Capel model with spin-3/2 some renormalization-group procedures predict a tetracritical point instead of a double critical end point [16,17]. We expect, however, double critical end points are the true picture of the model, because extensive Monte Carlo simulations [13,14] and previous finite-size scaling calculations [18] have located such end points quite precisely, contrary to the renormalization-group procedures that have used some limiting small-size cells together with some additional approximations.

Returning to the present system, we can see in fact a close analogy between the Baxter-Wu model defined by Eq. (2) and the Blume-Capel Hamiltonian (3). Having the Baxter-Wu model in a crystal field, the same kind of competition between the ordered ($\langle \sigma \rangle \neq 0$) and the disordered ($\langle \sigma \rangle = 0$) phases (which is mediated by the crystal field in this case) as in the Blume-Capel model, one may expect for both models a similar phase diagram, but with different classes of critical behavior. A similar type of competition appears also in the dilute $q$-states Potts model [19]. As has been discussed above, the Baxter-Wu model and the 4-states Potts model have the same critical exponents (see, for example, Ref. [5]). Because the dilution in the Potts model with 4-states has the same effect as the above crystal field in the Baxter-Wu model, one should also expect the critical behavior of both models to be the same. Indeed, some previous calculations of the phase diagram of both models have been reported in the literature. Nienhuis et al. [19], based on a renormalization-group study, concluded that for the dilute 4-states Potts model the phase diagram is similar to that of the spin-1 Blume-Capel model, in the sense that there is a transition line from the ordered states to the disordered state that changes from a second-order character to a first-order character at a multicritical point. In this case, however, the critical behavior is governed by only one fixed point, giving along the second-order line the same exponents as those of the pure 4-states Potts model. On the other hand, Kinzel et al. [20], using finite-size methods, conjectured a different kind of phase diagram. These authors interpreted the changes of the estimated thermal exponents $1/\nu$ along the transition line as a signal that a second-order transition should happen only for $D \to \infty$ (the pure Baxter-Wu model). Nevertheless, more recently [21], renormalization-group, conventional finite-size scaling, and conformal invariance techniques have been applied to the spin-1 Baxter-Wu model and the presence of a multicritical point has in fact been achieved.

So far, up to our knowledge, no results have been reported in the literature about the critical behavior of the spin-3/2 (and higher values of $S$) Baxter-Wu model in a crystal field. The main question that arises is concerning its phase diagram. Besides the second- and first-order lines, does it also exhibit (i) one quadruple critical end point, (ii) one multicritical point, or (iii) one multicritical end point and one pentacritical point? In case (i) the first-order transition line ends up in an isolated critical point, as in the Blume-Capel model, while in case (ii) one would have an octocritical point, where eight phases become equal. However, there is still an additional possibility, because case (iii) corresponds to having a multicritical end point and a pentacritical point that are separated by a first-order transition line. As we see below, the most probable phase diagram could indeed present a topology corresponding to the scenario depicted in case (iii) above, while case (i) is definitely improbable to happen for this model.

This paper is organized as follows. In the next section we present the transfer matrix formalism of the model, together with the relations used in our finite-size studies. The results are discussed in Sec. III, where we have revisited the spin-1 case taking larger finite strips than previously considered and presenting the new results of the spin-3/2 model. We then close the paper in Sec. IV with some concluding remarks.

II. FINITE-SIZE SCALING AND CONFORMAL INVARIANCE

Consider first an infinite strip with finite width $L$ having periodic boundary conditions along the infinite direction. The column-to-column transfer matrix $\hat{T}$ of the Hamiltonian (2) for spin-$S$ on such a triangular lattice strip has then a dimension $(2S + 1)^2 \times (2S + 1)^2$. Its coefficients $T_{n_1,n_2}$ are the Boltzmann weights generated by the spin configurations $n_i = \{\sigma_i^1,\sigma_i^2,\ldots,\sigma_i^L\}$ and $n_{i+1} = \{\sigma_{i+1}^1,\sigma_{i+1}^2,\ldots,\sigma_{i+1}^L\}$ of adjacent columns $i$ and $i + 1$, respectively. If we consider a periodic boundary condition in the vertical direction as well, the transfer matrix elements can be written as

$$T_{n_i,n_{i+1}} = e^K \sum_{\sigma} \langle \sigma | e^{-\beta H} | \sigma_i^1,\ldots,\sigma_i^L \rangle \langle \sigma_i^1,\ldots,\sigma_i^L | \sigma_{i+1}^1,\ldots,\sigma_{i+1}^L \rangle - \delta(\sigma_i^1-\delta(\sigma_i^2)^2, (4)$$

with $K = \beta J, d = D/J$, and $\beta = 1/k_BT$. The finite-size behavior of the eigenvalues of $\hat{T}$, namely, $\Lambda_1(K,d) > \Lambda_2(K,d) > \cdots > \Lambda_{L}(K,d)$, where $n = (2S + 1)^2$ and $\Lambda_{L}(K,d)$ is the $L$th eigenvalue of $\hat{T}$, can be used to determine the critical line and the critical exponents [22–24]. The critical line $t_c$, where $t_c$ is the reduced critical temperature given by $t_c = k_BT_c/J = K_c^{-1}$, is evaluated by extrapolating to the bulk limit ($L \to \infty$), the sequences obtained by solving

$$G_{L}(K',d)L = G_{L+3}(K,d)(L+3), \quad L = 3, 6, \ldots \quad (5)$$

for $K = K' = K_c$, where $G_L(K)$ is the inverse of the correlation length (or the mass gap of the Hamiltonian $H$) and is given by

$$G_L(K,d) = \ln \left( \frac{\Lambda_1}{\Lambda_L} \right). \quad (6)$$

The correlation length exponent $\nu$ is obtained from

$$\nu = \frac{\ln \ell}{\ln(dK'/dK)}.$$
where $\ell = \frac{L+3}{T}$. is the scaling factor and the derivative $dK/\frac{dK}{dt}$ is obtained from Eq. (5) when $K' = K = K_c$ is the fixed point solution for a given value of $\ell$.

The multicritical points are obtained using a heuristic method, which has already been proved to be effective [18,25]. In this case, we have to solve simultaneously Eq. (5) for three different lattice sizes:

$$G_L(K,d)L = G_{L+3}(K,d)(L+3)$$
$$= G_{L+6}(K,d)(L+6), \quad L = 3, 6, \ldots. \quad (7)$$

Note that in Eqs. (5) and (7) we restricted the possible finite strip widths to multiples of 3 in order to preserve the invariance of the Hamiltonian (2) under the reversal of all spins on any two of the three sublattices (each vertex of the triangle of the lattice can be viewed as belonging to three different sublattices in such a way that inverting the spins on any two of these sublattices leaves the Hamiltonian invariant).

As usual, the model is expected to be conformally invariant in the region of continuous phase transition. This invariance allows one to infer the critical properties from the finite-size corrections of the eigenspectrum at the critical temperature [22,23]. The conformal anomaly $c$, which labels the universality class of the critical behavior, can be calculated from the large-$L$ behavior of the ground-state eigenvalue of $\hat{T}$ [23]:

$$\ln \frac{\Lambda^1_L}{L} = \epsilon_\infty + \frac{\pi c v_s}{6L^2} + o(L^{-2}). \quad (8)$$

where $\epsilon_\infty = \ln \frac{\Lambda^1_L}{T}$ is the bulk limit when $L \to \infty$ and $v_s = \sqrt{3}/2$ is the sound velocity. On the other hand, the scaling dimensions $x(n)$ related to the $n$th energy in the sector with zero momentum can be obtained by extrapolating the sequence

$$x_L(n) = \frac{L}{\pi \sqrt{3}} \ln \left( \frac{\Lambda^1_L}{\Lambda^0_L} \right)^{\frac{1}{\nu}}. \quad (9)$$

The corresponding critical exponents can be calculated from the above equation by knowing that $x(2) = \eta/2$ and $x(3) = 2 - 1/\nu$.

Regarding the first-order transition line, a finite-size estimate can be obtained by the same procedure as done in recent works [18,21]. Along the first-order transition line of the Baxter-Wu model with a crystal field, we have the coexistence of $p$ phases. For spin-1, $p = 5$ and we have one ferromagnetically ordered phase, three ordered ferrimagnetically and a disordered one. For spin-3/2, as we see below, $p = 8$. Consequently, for a given lattice size $L$ we calculate the points where the gap corresponding to the $p$th eigenvalue has a minimum. This can be done by looking at the minimum of the following gap function:

$$\Delta_p(K,d) = \Lambda^1_L(K,d) - \Lambda^p_L(K,d). \quad (10)$$

The extrapolation $L \to \infty$ of these points gives us an estimate of the first-order transition line in the thermodynamic limit.

It should be emphasized that the transfer matrix given by Eq. (4) is non-Hermitian. Thus, in the numerical diagonalization of $\hat{T}$ we have used the Lanczos method for non-Hermitian matrices [26]. Despite considering the translational symmetry to block-diagonalize the corresponding transfer matrices, it turns out that the determination of the higher eigenvalues, necessary for computing first-order transitions, becomes a problem, due to the fact the Lanczos base loses the orthogonality, mainly for the larger lattices. In such cases, we had to fully diagonalize the transfer matrix and obtain its entire spectrum, which has a huge computational cost. For this reason, it has been a challenge to estimate the first-order line for large systems.

Finally, it is convenient to mention that, although the sizes of the strip width that we are going to consider are not, at first sight, as large as one might desire, they represent indeed very large systems, because one of the directions of the strip is actually infinite, and the corresponding transfer matrices have practically reached the reasonable computer time and memory limits of our presently available machines (however, they are not truly infinite in the sense that they carry finite-size corrections, since the free energy is just an analytical function of the Hamiltonian parameters).

### III. RESULTS

For the spin-1 model, within our computational power, we can consider strip widths up to $L = 12$, while for spin-3/2 we were limited to $L = 9$. As we could increase the size of the system further when compared to the previous work ($L = 9$) [21] for spin-1, we have revisited this model in order to seek the difference it makes to consider an additional larger strip and to obtain the correlation length exponent given directly from Eq. (6) as well, where the latter quantity was not exploited in the previous study. However, before obtaining the phase diagrams, it is worthwhile to see what happens to the model at zero temperature.

#### A. Zero temperature limit

At $T = 0$ and $D < D_0$, where $D_0$ depends on the value of the spin $S$, the model given by Eq. (2) has four different ordered states corresponding to a ferromagnetic phase where all spins are in the $\sigma_i = +S$ state, and three ferrimagnetic phases in which two sublattices have spins in the $\sigma_i = -S$ state and the other sublattice has spins in the $\sigma_i = +S$ state. The free energy per spin for all these four phases is, in this case, given by $g_F = -2JS^3 + D S^2$, which is independent of the spin being integer or half-integer. However, for $D > D_0$ the scenario is quite different. For integer $S$ the stable phase corresponds to all spins in the zero state and we have the corresponding free energy $g_0 = 0$. On the other hand, for half-integer $S$ we have again four different ordered states: one ferromagnetic phase where all spins are in the $\sigma_i = +1/2$ state, and three ferrimagnetic phases in which two sublattices have spins in the $\sigma_i = -1/2$ state and the other sublattice has spins in the $\sigma_i = +1/2$ state. All these ordered states have the same free energy given now by $g_F = -J/4 + D/4$. In Fig. 1, we depict the behavior of the free energies for the cases $S = 1$ and $S = 3/2$. For $S = 1$, as illustrated in Fig. 1(a), we have $D_{10}/J = 2$ and, at this point, five phases are coexisting. On the other hand, for $S = 3/2$, as shown in Fig. 1(b), we have $D_{10}/J = 3.25$ and, at this point, eight phases are coexisting. For nonzero low temperatures we then expect a line of quintuple points and a line of octuple points for spin-1 and spin-3/2, respectively.
As a matter of example, Fig. 2 shows the second-order transition temperature $t_c$ obtained from Eq. (5) for the three different strip widths and the special value $d = -20$. The thermodynamic limit of the critical temperature has been obtained from

$$t_c(L) = t_c^\infty + AL^{-1/\nu}(1 + BL^{-(w-2)}),$$

(11)

with $\nu = 2/3$ and the correction-to-scaling exponent $w = 4$ [3,4]. $A$ and $B$ are nonuniversal constants. As a function of $L^{-1/\nu} = L^{-3/2}$ the above equation can be written as

$$t_c(L) = t_c^\infty + AL^{-3/2}[1 + B(L^{-3/2})^{4/3}],$$

(12)

which is easier to be used in the fittings and gives us an idea of the degree of the corrections to scaling. For this negative value of $d$ we get the bulk value $t_c = 2.26911$, which is indeed close to (and also note that it is smaller than) the expected limit $t_c = 2.26918\ldots$ of the pure model when $d \to -\infty$. This indicates that the present approach is indeed able to obtain quite good estimates of $t_c$ with just the available strip widths. This same procedure is thus used to get the critical temperatures for other values of $d$, and some results are written in Table I. It should be stressed that all digits presented in that table are significant in the sense that the numbers are obtained by solving Eqs. (5) and (7), or by fitting our data to Eq. (12). However, regarding the fitting procedure we expect errors in the estimates of the extrapolated critical temperatures in the thermodynamic limit (when compared with the exact ones, which are not available). A measure of these errors can be inferred by the least-squares fitting $\chi^2$, defined as follows: for a set of $N$ data $d_i$ ($i = 1, \ldots, N$) whose fitted points are $f_i$, $\chi^2$ is given by $\left(\sum_i (f_i - d_i)^2\right)^{1/2}$. In our fits of the second-order transition we have obtained $\chi^2$ of the order $10^{-10}$ in all analyzed points, in such a way that even by considering only three data points the corresponding error goes to higher significant digits than shown in the table.

### Table I. Results for the spin-1 Baxter-Wu model.

<table>
<thead>
<tr>
<th>$d$</th>
<th>$t_\infty^{\text{3-12}}$</th>
<th>$t_\infty^{\text{3-9}}$</th>
<th>$t_\infty^{\text{3-6}}$</th>
<th>$t_\infty^{\text{3-3}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t(3)$</td>
<td>2.2575</td>
<td>2.2743</td>
<td>2.2575</td>
<td>2.26911</td>
</tr>
<tr>
<td>$t(6)$</td>
<td>2.2568</td>
<td>2.2743</td>
<td>2.2575</td>
<td>2.26911</td>
</tr>
<tr>
<td>$t(9)$</td>
<td>2.2575</td>
<td>2.2743</td>
<td>2.2575</td>
<td>2.26911</td>
</tr>
<tr>
<td>$t_c^{\text{3-3}}$</td>
<td>1.8597</td>
<td>1.8597</td>
<td>1.8597</td>
<td>1.8597</td>
</tr>
<tr>
<td>$t_c^{\text{3-6}}$</td>
<td>1.8597</td>
<td>1.8597</td>
<td>1.8597</td>
<td>1.8597</td>
</tr>
</tbody>
</table>

\(^a\)Second-order transition.
\(^b\)Pentacritical point.
\(^c\)First-order transition.
The multicritical point, nevertheless, is given by the condition that the pentacritical point will be located for a crystal field $d = 0.890254$. The first-order line is obtained by minimizing the gap related to the fifth eigenvalue, $p = 5$ in Eq. (10). An example is shown in Fig. 3 for $t = 1$. In this case, it turns out to be better to compute the crystal field for a given value of the temperature, instead of the temperature for each value of the parameter $d$, as has been done along the second-order transition line. However, either the first-order transition temperature $t_1$ for a given $d$, or the crystal field $d_1$ for a given temperature $t$, in the thermodynamic limit, can be obtained by fitting the data to the following equation:

$$x_1(L) = x_1^\infty + A L^{-2} (1 + B/L^2),$$

(13)

where $x_1 = t_1$ or $d_1$, the first exponent $-2$ on the lattice size $L$, as well as the second exponent $2$ on the corresponding correction to the scaling term come from the dimension of the lattice, as expected for first-order transitions [27–30]. Extra care should also be taken in this region because we have noticed that the Lanczos procedure in getting the fifth eigenvalue has degenerated in some instances. For this reason, we have to compute all eigenvalues of the original transfer matrix which took a much longer time, leading us to avoid considering the $L = 12$ lattice in this case. Some values for the first-order transition line, obtained by this fitting procedure, are also presented in Table I.

It is interesting to look at Fig. 4, where we present all results we have obtained by considering all the strips for this model, including second-order transitions, first-order transitions, pentacritical points, as well as the thermodynamic limit extrapolation. One can clearly note that in this scale, and apart from the first-order results from the lattice size $L = 3$, all the data are quite close to each other, except for the location of the pentacritical point. Closer views of the second-order transitions and of the first-order transitions are depicted in Figs. 5(a) and 5(b), respectively. Only on such a finer scale is it possible to distinguish the different results and the corresponding thermodynamic limit. In addition, one can see that the broken lines of the first-order transitions start at $T = 0$ and $d = 2$ and finish at the pentacritical point. As a matter of simplicity, in Fig. 6 we give the complete phase diagram just in the thermodynamic limit for the spin-1 Baxter-Wu model. Although the location of the pentacritical point has considerably changed by taking one larger strip, the final result for the transition lines have not changed so much, so we really expect that the full phase diagram given in Fig. 6 is indeed what we should expect for this model.

At this point it should be interesting to make some comments about the order of the transition lines we get in Fig. 6. In fact, for the finite sizes of the transfer matrices, all eigenvalues depend quite smoothly on the parameters $t$ and $d$, and nothing looks singular. That is why one gets the so-called analytical continuation of the transition lines, regardless of being first or second order (this also happens in Monte Carlo simulations). Figure 7 shows the region of the first-order transition line where the second-order character is still present for $d \sim 1.3$. However, we clearly see that the thermodynamic limit of the first-order transition line is below the corresponding limit of the second-order line, giving us an indication that the first-order transition takes place before the second-order one. For $d < d_m$ the situation is the inverse. Thus, we can infer the order of the transition in this simple way. The multicritical point, nevertheless, is given by the condition expressed in Eq. (7) and not by the crossing of the first- and second-order lines (although they are close together).
In order to determine the universality class of critical behavior, we calculate the central charge $c$ along the critical line. The finite-size estimates of the central charge can be estimated by

$$c_{L,L+3} = \frac{12}{\sqrt{3\pi}} \left( \frac{\ln A_{L+3}^1}{L+3} - \frac{\ln A_{L}^1}{L} \right) \left( \frac{1}{(L+3)^3} - \frac{1}{L^3} \right)^{-1},$$

(14)

while the extrapolated values, $c_\infty$, can be obtained from the $L$-large behavior of $c_{L,L+3}$, given by

$$c_{L,L+3} = c_\infty - a[L^{-w} + (L + 3)^{-w}]L^{-2} + (L + 3)^{-2}]^{-1},$$

(15)

where $a$ is a constant and $w = 4$ is the dominant dimension associated to the operator governing the finite-size corrections [3].

In Table II, we present some finite-size estimates of the central charge as well as the extrapolated values along the second-order transition line. As we can see, our results support that the critical behavior of the critical line is described by a conformal field theory with $c = 1$. Although we do not have a precise location of the pentacritical point, we have calculated the central charge $c$ for hundreds of values $d$ along the second-order transition line and close to our finite estimate of the pentacritical point and we found no abrupt change in the values of $c$, $\nu$, and $\eta$. This indicates that even in the pentacritical point $c = 1$. It is convenient to mention that this scenario is quite different from the spin-1 Blume-Capel model, where the central charge changes abruptly from $c = 1/2$ at the critical line to $c = 7/10$ at the tricritical point (see Ref. [18]). But, it is

<table>
<thead>
<tr>
<th>$d$</th>
<th>$-10$</th>
<th>$-1$</th>
<th>0.890254</th>
</tr>
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<tbody>
<tr>
<td>$c_{3,6}$</td>
<td>0.9381</td>
<td>0.9408</td>
<td>0.9530</td>
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<tr>
<td>$c_{6,9}$</td>
<td>0.9864</td>
<td>0.9868</td>
<td>0.9875</td>
</tr>
<tr>
<td>$c_{9,12}$</td>
<td>0.9945</td>
<td>0.9946</td>
<td>0.9933</td>
</tr>
<tr>
<td>$c_\infty$</td>
<td>1.0017</td>
<td>1.0016</td>
<td>0.9984</td>
</tr>
</tbody>
</table>
TABLE III. Finite-size estimates of the critical exponents $\nu$ and $\eta$ for different values of $L$ for some points along the second-order transition line for the spin-1 Baxter-Wu model. $\nu_{L,L+3}$ is obtained from Eq. (6) and $\nu_L$ and $\eta_L$ are obtained from Eq. (9).

<table>
<thead>
<tr>
<th>$d$</th>
<th>$-20$</th>
<th>$-10$</th>
<th>$-1$</th>
<th>$0$</th>
<th>$0.890254$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu_{3,6}$</td>
<td>0.6828</td>
<td>0.6828</td>
<td>0.6748</td>
<td>0.6631</td>
<td>0.6297</td>
</tr>
<tr>
<td>$\nu_{6,9}$</td>
<td>0.6706</td>
<td>0.6706</td>
<td>0.6632</td>
<td>0.6515</td>
<td>0.6137</td>
</tr>
<tr>
<td>$\nu_{9,12}$</td>
<td>0.66826</td>
<td>0.66825</td>
<td>0.66099</td>
<td>0.64879</td>
<td></td>
</tr>
<tr>
<td>$\nu_3$</td>
<td>0.7172</td>
<td>0.7172</td>
<td>0.7021</td>
<td>0.6814</td>
<td>0.6505</td>
</tr>
<tr>
<td>$\nu_6$</td>
<td>0.6733</td>
<td>0.6732</td>
<td>0.6656</td>
<td>0.6537</td>
<td>0.6282</td>
</tr>
<tr>
<td>$\nu_9$</td>
<td>0.6693</td>
<td>0.6693</td>
<td>0.6621</td>
<td>0.6505</td>
<td>0.6188</td>
</tr>
<tr>
<td>$\nu_{12}$</td>
<td>0.6681</td>
<td>0.6681</td>
<td>0.6610</td>
<td>0.6494</td>
<td>0.6164</td>
</tr>
<tr>
<td>$\eta_3$</td>
<td>0.2346</td>
<td>0.2346</td>
<td>0.2328</td>
<td>0.2295</td>
<td>0.2194</td>
</tr>
<tr>
<td>$\eta_6$</td>
<td>0.2472</td>
<td>0.2472</td>
<td>0.2447</td>
<td>0.2403</td>
<td>0.2264</td>
</tr>
<tr>
<td>$\eta_9$</td>
<td>0.2490</td>
<td>0.2490</td>
<td>0.2463</td>
<td>0.2418</td>
<td>0.2264</td>
</tr>
<tr>
<td>$\eta_{12}$</td>
<td>0.2490</td>
<td>0.2490</td>
<td>0.2463</td>
<td>0.2418</td>
<td>0.2264</td>
</tr>
</tbody>
</table>

C. Spin-3/2 Baxter-Wu model

For the spin-3/2 Baxter-Wu model, the maximum lattice size we considered in our numerical studies was $L = 9$. However, we did learn from the previous section that by increasing the size of the strips no significant change has been noted for the transition line. Due to this fact, we expect to obtain quite good results by taking $D \rightarrow +\infty$ as we did with the central charge, and again we found that these exponents do not change significantly. The results above, indeed, support that the second-order transition line as well as the pentacritical point are described by a conformal field theory with $c = 1$ and whose critical exponents are the same of the pure spin-1/2 Baxter-Wu model.

As mentioned in the introduction, in the limit $D \rightarrow -\infty$ one has $t_c = S^3 \times 2.269185 \ldots = 7.65850 \ldots$, and in the limit $D \rightarrow +\infty$ one has $t_c = 0.28364 \ldots$, which are the exact values of the extremes of the second-order phase transition line separating coexisting ordered phases from the disordered one. Figure 8 shows the reduced critical temperature for the two different lattices and $d = -20$. Since we have only two points, the thermodynamic limit estimate of $t_c$ has been obtained from Eq. (12) with $B = 0$. For this value of crystal field one has $t_c = 7.64169$, which is indeed close to the expected value for $D \rightarrow -\infty$. Thus, despite the fact of having only two data points to estimate $t_c$, we are obtaining an estimate of the bulk value which is already within 0.2% of the exact result. As shown in Table IV, we observe that for $d \leq 3$ the difference between $t_c$ and $t_c(3,6)$ is quite small, which indicates, indeed, that our estimates are quite good. On the other hand, we have noticed that for $d \geq 3$ this difference is relatively large; for this reason we believe that our results are not so accurate in this region of the phase diagram (this is exactly the region where the steepest curvature of the second-order transition line changes to an almost flat curve, which can be seen in the next figures).

The signature that the universality class of critical behavior does not change at the pentacritical point appears also in the critical exponents $\nu$ and $\eta$. We report in Table III the finite-size estimates of the critical exponent $\nu$ obtained from Eqs. (6) and (9), as well as the critical exponent $\eta$ obtained from Eq. (9). Note that $\eta_9 = \eta_{12}$ due to Eqs. (5) and (9) and the fact that we have used $t_c = t_c(3,12)$ in order to get $x^9(1)$ and $x^{12}(1)$. As we can note in this table, our results are consistent with $\nu = 2/3$ and $\eta = 1/4$, which are the same as the pure Baxter-Wu model. We also calculate the critical exponents $\nu$ and $\eta$ around our finite estimate of the pentacritical point, as we did with the central charge, and again we found that these exponents do not change significantly

![FIG. 8. Reduced critical temperature $t_c$ as a function of $L^{-3/2}$ for $d = -20$ for the spin-3/2 Baxter-Wu model. The solid line is the best fit according to Eq. (12) with $B = 0$.]

t_c = 7.64169, which is indeed close to the expected value for $D \rightarrow -\infty$. Thus, despite the fact of having only two data points to estimate $t_c$, we are obtaining an estimate of the bulk value which is already within 0.2% of the exact result. As shown in Table IV, we observe that for $d \leq 3$ the difference between $t_c$ and $t_c(3,6)$ is quite small, which indicates, indeed, that our estimates are quite good. On the other hand, we have noticed that for $d \geq 3$ this difference is relatively large; for this reason we believe that our results are not so accurate in this region of the phase diagram (this is exactly the region where the steepest curvature of the second-order transition line changes to an almost flat curve, which can be seen in the next figures).

In the present case, we were also able to solve Eq. (7) for $L = 3$, which is indicative of the existence of a multicritical point (for this spin-3/2 model, as we see below, either an octocritical or a pentacritical point). The finite-size estimate of this point is $d_m = 2.0620$ and $t_m = 2.9145$.

Now, we can consider two possible scenarios for the low-temperature topology of the phase diagram. First, similar to the Blume-Capel model, we assume that the first-order line can be determined by considering Eq. (10) with $p = 8$. As before, for the first-order transition, we also have to diagonalize the full matrix (note that, in the present case, we need up to the eighth eigenvalue of $\hat{T}$). In Fig. 9, we present the transition lines found for $L = 3$ and $L = 6$, as well as the extrapolated values to the thermodynamic limit. As we can notice in this figure, the first-order transition lines start at $T = 0$ and $d = 3.25$ and seem to cross the second-order critical line at almost the multicritical point obtained from Eq. (7), i.e., $d_m = 2.0620$.

TABLE IV. Reduced critical temperature $t_c(L,L+3)$ for various values of crystal field $d$ for the spin-3/2 model. The extrapolated values, $t_c^*$, are depicted in the last row.

<table>
<thead>
<tr>
<th>$d$</th>
<th>$-10$</th>
<th>$-1$</th>
<th>$1$</th>
<th>$2.9$</th>
<th>$3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_c(3,6)$</td>
<td>7.2554</td>
<td>5.2325</td>
<td>4.0007</td>
<td>1.3308</td>
<td>1.0560</td>
</tr>
<tr>
<td>$t_c(6,9)$</td>
<td>7.2842</td>
<td>5.2449</td>
<td>4.0044</td>
<td>1.3295</td>
<td>1.0559</td>
</tr>
<tr>
<td>$t_c^*$</td>
<td>7.3331</td>
<td>5.2661</td>
<td>4.0107</td>
<td>1.3288</td>
<td>1.0558</td>
</tr>
</tbody>
</table>
and \( t_m = 2.9145 \). For this scenario, we could interpret this multicritical point as an octocritical point.

If we look, however, at a finer scale on the region \( 2 < d < 3 \), which is depicted in Fig. 10, we further notice that the first-order transition line also crosses the second-order transition line at \( d_{\text{mep}} = 3.01(5) \) and \( t_{\text{mep}} = 1.05(5) \), at least for the system sizes considered herein. In fact, when we take the thermodynamic limit with just the two considered finite strips, we find that the second-order transition line is always below the corresponding first-order transition line (with \( p = 8 \)), although the difference between them is very small, as can be seen in Fig. 10 and, more quantitatively, in Table V. Table V shows the thermodynamic limit of the first-order transition temperatures for some values of the crystal field in this range, in comparison with the second-order transition temperatures (note that the difference is at most 3%).

**TABLE V.** Thermodynamic limit of the first-order transition temperatures \( t^\infty(p) \), as a function of the crystal field \( d \), for the spin-3/2 Baxter-Wu model for the values \( p = 5 \) and \( p = 8 \). For comparison, the last row gives the corresponding extrapolated values of the second-order \( t^\infty \) transition temperature.

<table>
<thead>
<tr>
<th>( d )</th>
<th>2</th>
<th>2.2</th>
<th>2.4</th>
<th>2.6</th>
<th>2.8</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t^\infty(p = 5) )</td>
<td>2.9919</td>
<td>2.7307</td>
<td>2.4207</td>
<td>2.0429</td>
<td>1.5888</td>
<td>1.0586</td>
</tr>
<tr>
<td>( t^\infty(p = 8) )</td>
<td>2.9888</td>
<td>2.7248</td>
<td>2.4155</td>
<td>2.0423</td>
<td>1.5912</td>
<td>1.0883</td>
</tr>
<tr>
<td>( t^\infty )</td>
<td>2.9846</td>
<td>2.7144</td>
<td>2.3992</td>
<td>2.0215</td>
<td>1.5764</td>
<td>1.0558</td>
</tr>
</tbody>
</table>

So, from what we have seen above, we cannot discard the possibility of the existence of another multicritical point, since Eq. (7) is only phenomenological. For this reason, we can also consider a second possible scenario, which is discussed in the following.

Let us assume that there indeed exists another multicritical point at \( d_{\text{mep}} = 3.01(5) \) and \( t_{\text{mep}} = 1.05(5) \), as suggested by the previous results (this point should be named a multicritical end point). Thus, close to this multicritical end point we may expect that the disordered phase is dominated by spins \( \sigma_i = \pm 1/2 \), while the ordered phases are mainly dominated by \( \sigma_i = \pm 3/2 \), and on the phase transition line the density of \( \sigma_i = \pm 3/2 \) spins should present a jump. In this scenario, this transition line must be first order. However, this first-order line corresponds now to a quintuple line, where five phases coexist (the disorder one, and four phases associated with spins coming from the states \( \pm 3/2 \)). For this reason, we have also determined the first-order transition line between these two multicritical points assuming \( p = 5 \) in Eq. (10). Some estimates are presented in Table V as well. We can notice that the results are still very similar to those found with \( p = 8 \) in Eq. (10) and are systematically above the second-order line.

It is clear that with just the present lattices one cannot completely resolve this region of the phase diagram and certainly further studies should be done in order to confirm which of the two presented scenarios corresponds to the true phase diagram. However, some additional information can be obtained by looking at the central charge and critical exponents.

In Table VI we have the finite-size estimates of the central charge \( c \), and the critical exponents \( \nu \) and \( \eta \). These estimates were obtained by the same procedures used in the \( S = 1 \) case. As we can note in this table, the values of \( c, \nu, \) and \( \eta \) are consistent with \( c = 1, \nu = 2/3, \) and \( \eta = 1/4 \) for \( d \leq -1 \), which are the same as the spin-1/2 Baxter-Wu model. We observe that for \( d > -1 \) those values decrease when \( d \) increases. The decrease is even more pronounced in the region between the two multicritical points, as can be seen in Fig. 11 for the central charge. Note that if we calculate \( c \) along a first-order line, its value, in the thermodynamic limit, should be zero.

It seems then more plausible to associate this region to a first-order transition and to assume that the second scenario should be the correct one, since the finite-size estimates of the central charge \( c \), depicted Fig. 11, between the two multicritical points, decrease with the crystal field and, in addition, suggest being zero in the thermodynamic limit, as expected for a first-order transition line (despite that the results oscillate in the difficult region close to \( d = 3 \)). As a further observation, the precise location of such a multicritical end point should be a
real challenge and not an easy one, because, as pointed out by Fisher and Upton [31], the corresponding first-order line itself has a singularity in this case. On the other hand, we believe that the class of the critical behavior along the second-order portions of the critical line of the spin-3/2 Baxter-Wu model is the same as the corresponding spin-1/2 model.

The global phase diagram so obtained is presented in Fig. 12. Note that this phase diagram is different from the is the same as the corresponding spin-1/2 Baxter-Wu model. The global phase diagram so obtained is presented in Fig. 12. Note that this phase diagram is different from the spin-1 model shows a second-order transition line separated from the dimension of the lattice, as shown in Fig. 13(d), increase the width of the strips by 3 in order to accommodate all three different sublattices) to actually support its character. So, different approaches would be very welcome to treat such behavior. In fact, in Fig. 13 we have some preliminary Monte Carlo results for the specific value \( d = 1.4 \) [32]. The probability distribution shown in Figs. 13(a)–13(c) are obtained by using the mixing field technique (for a recent review see Ref. [33]) in the same way as was previously done for the Blume-Capel model in Ref. [34]. According to this method, the double peak distribution, at the same height, is a way of determining the location of the first-order transition for a given lattice size. The finite-size scaling (FSS) behavior of the temperatures \( T_L \) as a function of \( L^{-2} \), the exponent 2 coming from the dimension of the lattice, as shown in Fig. 13(d), also indicates the first-order character of the transition with its thermodynamical limit \( T = 1.1723(3) \). This value is quite close to the present procedure where one gets \( T = 1.1690 \).

For the spin-3/2 Baxter-Wu model the scenario is completely different from what we naively expected, and rather new; as far we know no results have been reported in the literature for the case \( S = 3/2 \). While the corresponding Blume-Capel model presents a double critical end point, our results support that the spin-3/2 Baxter-Wu model has a pentacritical point, with the first-order transition line, at low temperatures, terminating at an additional multicritical end point (from the present data, however, we cannot rule out completely the presence of an octocritical point). Our results show that for \( d \leqslant -1 \) the universality class of critical behavior.

### IV. CONCLUDING REMARKS

We have calculated the phase diagram and critical properties of the spin-1 and spin-3/2 Baxter-Wu model in the presence of a crystal field by using renormalization group, finite-size scaling, and conformal invariance.
Finally, some short comments on the present higher-order critical points would be worthwhile to mention. First, as stated in Griffith’s 1974 paper [35], Kohnstamm [36] was quite pessimistic about experimentally observing such points (higher than the tricritical ones), due to the large number of involved thermodynamic variables, especially when thinking about the Gibbs phase rule, and mainly for fluid systems where the lack of symmetry is well known. In the present case we can see that a rather simple theoretical system, such as the Baxter-Wu model, is able to present such a richness of a variety of higher multicritical phenomena, by just properly tuning the number of the spin states. Second, regarding the nomenclature of the present multicritical points, we tried, as far as we could throughout the text, to avoid using a kind of flowery language in their definitions. For instance, according to the literature, the continuous transition lines for the spin-1 and spin-3/2 models should be named tetracritical lines, and the multicritical end point for spin-3/2 is in fact a quadruple tetracritical end point located, in this case, where the octuple line becomes a quintuple line.

ACKNOWLEDGMENTS

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[32] M. L. M. Costa (unpublished). The Monte Carlo results have been obtained on finite lattices with periodic boundary conditions and using the Metropolis algorithm allied with the single histogram technique. The first $3 \times 10^5$ Monte Carlo steps (MCSs) have been discarded and the histograms have been computed taking $5 \times 10^5$ MCSs.