Universality and phase diagrams of the Baxter-Wu Model in a Crystal Field: spin-1 and spin-3/2

D. A. Dias\textsuperscript{1,2}, J. C. Xavier\textsuperscript{3} and J. A. Plascak\textsuperscript{1,4,5}

\textsuperscript{1}Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, C.P. 702, 30123-970 Belo Horizonte, MG - Brazil
\textsuperscript{2}Universidade Federal de Uberlândia, Campus Patos de Minas, Av. Getulio Vargas 230, 38700-103 Patos de Minas, MG - Brazil
\textsuperscript{3}Instituto de Física, Universidade Federal de Uberlândia, C.P. 593, 38400-902 Uberlândia, MG - Brazil
\textsuperscript{4}Universidade Federal da Paraíba, Centro de Ciências Exatas e da Natureza - Campus I, Departamento de Física - CCEN Cidade Universitária 58051-970 - João Pessoa, PB - Brazil
\textsuperscript{5}Center for Simulational Physics, University of Georgia, 30602 Athens, GA - USA

E-mail: dani.adias@yahoo.com.br, jcxavier@ufu.br, pla@hal.physast.uga.edu

Abstract. Conventional finite-size scaling and conformal invariance theory are used in order to study the critical behavior of the spin-1 and spin-3/2 Baxter-Wu model. For spin-1 the results are similar to the Blume-Capel model. However, for spin-3/2, the phase diagram is much richer, and presents, besides a pentacritical point, an additional multicritical endpoint. In both cases, the universality class is the same as the spin-1/2 model, even at the multicritical points.

The Baxter-Wu model in a crystal field can be defined by following Hamiltonian

\[ H = -J \sum_{<ijk>} \sigma_i \sigma_j \sigma_k + D \sum_{i=1}^{N} \sigma_i^2, \]

where \(J\) is the exchange interaction, the first sum extends over all elementary triangles of a triangular lattice with \(N\) sites, the classical spin variables \(\sigma_i\) take values \(\sigma_i = -S, -S+1, ..., S-1, S\), with \(S = 1/2, 1, 3/2, ...\), and \(D\) is the crystal field or single ion anisotropy. The above model for \(S = 1/2\) [1] has been exactly solved [2] and the exponents are in the 4-states Potts model universality class [3, 4]. However, for \(S \geq 1\) no exact results are available and even the phase diagram topology is not yet well resolved.

In order to study the critical behavior of the model given by (1) we have employed conventional finite-size scaling and conformal invariance theory through the transfer matrix formalism for infinite strips with finite width \(L\) and periodic boundary conditions in all directions (for more details see [5, 6]). In summary, the second-order transition lines are obtained from

\[ G_L(K, d)L = G_{L+3}(K, d)(L + 3), \quad L = 3, 6, ..., \]

where \(G_L(K, d)\) is the inverse of the correlation length and is given by

\[ G_L(K, d) = \ln \left( \mathfrak{R}(\Lambda_L^d)/\mathfrak{R}(\Lambda_{L+3}^d) \right). \]
In the above equations we define $K = \beta J, d = D/J, \beta = 1/k_B T$, with $k_B$ being the Boltzmann constant, and $\Re[\Lambda^i(K, d)]$ is the real part of the $i$-th largest eigenvalue of the corresponding (non-Hermitian) transfer matrix. Multicritical points are obtained using a heuristic method in such a way that

$$G_L(K, d)L = G_{L+3}(K, d)(L+3) = G_{L+6}(K, d)(L+6), \ L = 3, 6, \ldots$$  \hspace{1cm} (3)

Note that Eqs. (2) and (3) are restricted to multiples of 3 to preserve the invariance of the Hamiltonian (1) under the reversal of all spins on any two of the three sub-lattices (each vertex of the triangle of the lattice can be viewed of belonging to three different sublattices in such a way that inverting the spins on any two of these sublattices leaves the Hamiltonian invariant). First-order transition lines are estimated by looking at the minimum of the following gap function

$$\Delta_p(K, d) = \Re[\Lambda^1(K, d)] - \Re[\Lambda^p(K, d)],$$  \hspace{1cm} (4)

where $p$ is the number of coexisting phases along the first-order transition. The conformal anomaly $c$ can be calculated from the large-$L$ behavior of the ground-state eigenvalue

$$\frac{\ln \Re[\Lambda^1]}{L} = \epsilon_{\infty} + \frac{\pi c v_s}{6 L^2} + o(L^{-2}),$$  \hspace{1cm} (5)

where $\epsilon_{\infty} = \frac{\ln \Re[\Lambda^1]}{L}$ 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 $x(n)$ can be obtained by extrapolating the sequence

$$x_L(n) = \frac{L}{\pi \sqrt{3}} \ln \left( \frac{\Re[\Lambda^n]}{\Re[\Lambda^1]} \right).$$  \hspace{1cm} (6)

The corresponding critical exponents of the correlation function and correlation length are, respectively, given by $x(2) = \eta/2$ and $x(3) = 2 - 1/\nu$. The numerical diagonalization of the transfer matrix has been done by using the Lanczos method for non-Hermitian matrices [7] and, when needed, full diagonalization algorithms.

**Spin $S = 1$**

For the spin-1 model, within our computational power, we can consider strip widths up to $L = 12$, and the results are shown in Figs. 1. It is interesting to look at Fig. 1 (a) where we have the whole set of the results obtained by considering all the strips for this model, which includes second-order transitions, first-order transitions, pentacritical points, as well as the thermodynamic limit extrapolation. Concerning the thermodynamic limit, we should emphasize that we have taken into account corrections to finite-size scaling. One can note that the first-order transition lines tend to meet the second-order transition lines at the pentacritical point. From the above results there is a strong indication that the spin-1 Baxter-Wu model shows a second-order transition line separated from a first-order transition line by a pentacritical point. Although this scenario is in disagreement with a picture from a previous paper by Kinzel et al. [8] (where the second-order transition line appears only in the limiting case $d \to -\infty$), the phase diagram has the same topology of the spin-1 Blume-Capel model [9, 10]. In the present case, the best estimate of the pentacritical point for the spin $S = 1$ model is $t^1_p = 1.4020$ and $d^1_p = 0.890254$.

The central charge has also been computed and the results support that the critical behavior of the critical line is described by a conformal field theory with $c = 1$. In addition, our results for the critical exponents are consistent with $\nu = 2/3$ and $\eta = 1/4$, which are the same of the pure Baxter-Wu model, even at the pentacritical point, meaning that the model belongs to the same universality class as the spin $S = 1/2$ model.
Spin $S = 3/2$

Regarding the spin-3/2 model we are limited to the width size $L = 9$, but we expect to obtain good results by taking $L = 3, 6$ and $9$. The results are shown in Figs. 2. As before, in Fig. 2 (a) we have the whole set of results obtained by considering all the strips. At a first look, it seems that we have an octocritical point. However, by closely analysing the data, we can also expect to have another multicritical point at lower temperatures (although we cannot rule out completely the presence of an octocritical point). This extra multicritical point turns out to be a quadruple tetracritical endpoint, and is located at $t_{tce} = 1.05(5)$ and $d_{tce} = 3.01(5)$, while the previous one is a pentacritical point and is located at $t_{3/2}^{p} = 2.0620$ and $d_{3/2}^{p} = 2.9145$.

The global phase diagram, in the thermodynamic limit, is shown in Fig. 2 (b). Independent of each above scenarios, one can say that the spin $S = 3/2$ Baxter-Wu model has a different phase diagram as the Blume-Capel, where the latter one presents only a double critical endpoint below the second-order transition line [11, 12, 13, 14, 15].

We have also computed the critical exponents and the central charge. The latter quantity is shown in Fig. 3. One can clearly see that the central charge, in the thermodynamic limit, is
Figure 3: Central charge as a function of the crystal field. Full dots are some extrapolated results for spin-1 up to the pentacritical point, and the lines correspond to the results for spin-3/2.

also close to 1 (and comparable to those from the spin $S = 1$ model), but drastically changes in the region where a possible first-order transition may occur. In fact, for first-order transitions the central charge $c$ is zero (note that $c$ indeed oscillates around zero close to the multicritical endpoint). The critical exponents $\nu$ and $\eta$ are also compatible with those from the pure model.

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