Baxter-Wu model in transverse magnetic field

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We investigate the low-energy properties as well as quantum and thermal phase transitions of the Baxter-Wu model in a transverse magnetic field. Our study relies on stochastic series expansion quantum Monte Carlo and on series expansions about the low- and high-field limits at zero temperature using the quantum finite-lattice method on the triangular lattice. The phase boundary consists of a second-order critical line in the 4-state Potts model universality class starting from the pure Baxter-Wu limit meeting a first-order line connected to the zero-temperature transition point ($h \approx 2.4, T = 0$). Both lines merge at a tricritical point approximately located at ($h \approx 2.3J, T \approx J$).

I. INTRODUCTION

Spin models play a major role from the early years in statistical mechanics, since they represent ideal systems to study the physics of classical and quantum phase transitions as well as associated critical behaviour$^{1,2}$. The prototypical quantum spin model with two-spin interactions is the Ising model in a transverse field (TFIM). It is (only) exactly solvable in one dimension at zero temperature or, equivalently, on the two-dimensional square lattice for a vanishing field. More generally, the $d$-dimensional TFIM at zero temperature can be mapped to the $(d+1)$-dimensional Ising model at zero field, both displaying a second-order phase transition in the $(d+1)$ Ising universality class which plays an important role for many other classical and quantum many-body systems$^3$, e. g. in the duality to the $Z_2$ gauge theory$^4$ which has been discussed recently in the context of the topologically ordered toric code$^5$ in the presence of a magnetic field$^6-11$.

The Ising model with three-spin interactions is an interesting system with multiple spin interactions which was introduced by Baxter and Wu on the triangular lattice in 1973 to describe ferrimagnetism and critical phase transitions$^{12-14}$. Interestingly, this Baxter-Wu (BW) model is exactly solvable. It displays a second-order thermal phase transition in the 4-state Potts model universality class (without logarithmic corrections). The latter has been confirmed by series expansions$^{15}$ and quantum Monte Carlo simulations$^{16-18}$. Recently, also the Baxter-Wu model in a transverse magnetic field (BWTF) has been studied by series expansions at zero temperature$^{20}$. Here clear signatures are found for a first-order quantum phase transition separating the ordered phase from the polarized phase present at large magnetic fields. As for the toric code in a field, one can also show a duality mapping between the so-called topological color code (TCC)$^{19}$ on the dual honeycomb lattice, a quantum-spin model relevant for topological quantum computation, in a magnetic field and the BWTF$^{20}$.

In contrast, the physics of the BWTF at finite temperatures is to the best of our knowledge unknown. The latter is interesting, since thermal and quantum fluctuations are present simultaneously and one may expect tricritical behaviour between the first-order phase transition at zero temperature and the second-order phase transition at zero field. Consequently, a detailed study of the finite-temperature phase diagram of the BWTF is the major focus of this paper. To this end we perform large-scale stochastic series expansion (SSE) quantum Monte Carlo (QMC) simulations. Furthermore, we discuss the low-energy spectral properties as well as the zero-temperature phase transition of the BWTF by comparing high-order series expansions about the low- and high-field limit using perturbative continuous unitary transformations (pCUTs)$^{21,22}$ with the numerical data obtained by QMC. Here the pCUT allows to set up a quasi-particle picture for the elementary excitations of the BWTF$^{20,23}$.

The outline of the paper is as follows: In Sec. II, we introduce the Baxter-Wu model on the triangular lattice. The BWTF model is obtained by adding a transverse magnetic field in $x$-direction, and we make the connection to the TCC in a parallel field on the dual honeycomb lattice. Thereafter, Sec. III contains a detailed discussion on the methods used in this work. In Sec. III A, we review the basic concepts of the pCUT method and we prepare the reader for Sec. III B where we briefly review the quantum finite-lattice method combined with pCUTs to study the low-energy physics of the system on finite triangular clusters up to high orders in perturbation. The series expansion results are further given in Sec. III C, while Sec. III D present the specificities of the QMC algorithm. Our results for the BWTF both at zero and finite temperature are presented in the main section of this paper (Sec. IV), while the conclusion Sec. V summarizes our main findings.
using a duality transformation, one can introduce pseudospin-\( \frac{1}{2} \) operators \( \tau^z \) living on the dual honeycomb lattice of the triangular faces. The energetic properties of the Baxter-Wu model are then just given by an effective magnetic field

\[
H_{\text{BW}}^{\text{dual}} = -J \sum_{i \in \Lambda} \tau^z_i .
\]  

Here the sum runs over the vertices of the dual honeycomb lattice \( \tilde{\Lambda} \) which corresponds to the centers of triangles in the dual Baxter-Wu model. Let us stress that this duality is only valid for the spectrum, but any information on degeneracies is clearly lost. Indeed, the effective magnetic field has a unique polarized ground state with pseudo-spins pointing in field direction and elementary excitations are dressed spin flips.

Our major objective is to add quantum fluctuations to the classical Baxter-Wu model on the triangular lattice by introducing a transverse magnetic field. We therefore consider the following Hamiltonian:

\[
H_{\text{BWTF}} = -J \sum_{(ijk)} \sigma^x_i \sigma^x_j \sigma^x_k - h \sum_{i \in \Lambda} \sigma^z_i ,
\]

where the first (second) sum runs over the faces (sites) of the triangular lattice. In the following we focus on \( h > 0 \).

A single \( \sigma^z_i \) flips the eigenvalues of the six face operators sharing the site \( i \) on the triangular lattice as illustrated in Fig. 1. In the dual pseudo-spin representation, the action of the transverse magnetic field is equivalent to flipping the six pseudo-spins of the corresponding hexagon. The BWTF after the duality mapping then reads

\[
H_{\text{BWTF}}^{\text{dual}} = -J \sum_{i \in \Lambda} \tau^z_i - h \sum_{p \in \Lambda} \chi_p ,
\]

where \( p \) denotes a hexagon of the dual lattice \( \tilde{\Lambda} \) and \( \chi_p = \tau^x_1 \tau^x_3 \tau^x_4 \tau^x_5 \tau^x_6 \) are plaquette operators where the numbers \( (1...6) \) correspond to the six sites of hexagon \( p \) (see also Fig. 1).

The just derived dual Hamiltonian is closely related to the TCC in a single parallel field on the honeycomb lattice. The TCC is a topological stabilizer code consisting of two types of plaquette operators which all commute pairwise with each other such that eigenvalues \( \pm 1 \) of all these operators are conserved quantities. One of the two types of plaquette operators is identical to \( \chi_p \) introduced above. The other type of plaquette operator commutes with a magnetic field in \( z \)-direction. As a consequence, the low-energy physics of the TCC in a single parallel field is contained in the sector where all of the remaining conserved plaquette operators are \( +1 \). Therefore, the BWTF is, up to a constant, isospectral to this sector of the TCC in a single parallel field.
III. METHODS

A. Perturbative continuous unitary transformation

Consider Hamiltonians of the form $H = H_0 + xV$ where $H_0$ is the unperturbed part, $V$ the perturbation, and $x$ an expansion parameter, the pCUT method is applicable to those models that satisfy the following conditions\textsuperscript{21}:

- The unperturbed part $H_0$ has an equidistant spectrum bounded from below. It can then be written as $H_0 = E_0 + Q$ where $E_0$ is the unperturbed ground-state energy and $Q$ counts the number of bare excitations.

- The perturbation can be expressed as $V = \sum_{m=-N_{\text{max}}}^{N_{\text{max}}} T_n$ where $T_n$ increments (decrements, if $n < 0$) the number of excitations (quasi-particles) by $n$ such that $[H_0, T_n] = nT_n$.

The pCUT method maps, order by order in $x$, the initial Hamiltonian $H$ to an effective one $H_{\text{eff}}$ which conserves the number of quasi-particles\textsuperscript{21,22}

\[ H_{\text{eff}} = E_0 + Q + \sum_{k=1}^{\infty} x^k \sum_{m=0}^{N_{\text{max}}} C(m_1 \ldots m_k)T_{m_1} \ldots T_{m_k}, \]

such that $Q$ commutes with the effective Hamiltonian $[H_{\text{eff}}, Q] = 0$. The first sum runs over the order of perturbation, $k$, while the second one runs over all possible permutations of $\{m_1, m_2, \ldots, m_k\}$ with $m_i \in \{-N_{\text{max}}, \ldots, N_{\text{max}}\}$ which satisfy the condition $m = \sum_i m_i = 0$. The coefficients $C(m_1 \ldots m_k)$ can be computed model independently as exact rational numbers up to high orders in perturbation\textsuperscript{21}.

Physically, operator sequences $T_{m_1} \ldots T_{m_k}$ in order $k$ represent quantum fluctuations of approximately a length scale $k$. These quantum fluctuations can be calculated in the thermodynamic limit by exploiting the linked-cluster theorem\textsuperscript{21,22,24}. The latter implies that only processes which take place on (finite) connected clusters contribute to matrix elements of $H_{\text{eff}}$. Consequently, the pCUT method provides exact results up to the computed perturbative order directly in the thermodynamic limit.

1. High-field limit ($h \gg J$)

In this subsection, we apply the pCUT method to the BWTF about the high-field limit. We therefore rewrite Eq. 3

\[ \frac{H_{\text{BWTF}}}{2h} = -\frac{1}{2} \sum_i \sigma_i^x - \frac{J}{2h} \sum_{<i,j,k>} \sigma_i^z \sigma_j^z \sigma_k^z, \]

such that the magnetic field represents the unperturbed part and the Baxter-Wu model is the perturbation. The ground state of the pure field term is a polarized phase in the $x$-direction and the system has an equidistant spectrum. Therefore, both necessary conditions for pCUTs are fulfilled. Elementary excitations are local spin flips on the sites of the triangular lattice. They can be conveniently described in terms of hard-core bosons represented by creation and annihilation operators $b_i$ and $b_i^\dagger$.

One finds

\[ \frac{H}{2h} = -\frac{N}{2} + \sum_i n_i + \frac{J}{2h} \sum_{<i,j,k>} (b_i^\dagger b_j^\dagger b_k^\dagger + b_i b_j b_k + b_i^\dagger b_j b_k^\dagger + b_i^\dagger b_k b_j + h.c.) \]

\[ = E_0 + Q + \frac{J}{2h} (T_3 + T_1 + T_{-1} + T_{-3}), \]

where $N$ is the number of triangular lattice sites and $n_i = b_i^\dagger b_i$ is the local density on site $i$.

The three-spin interactions of the Baxter-Wu model do therefore change the number of QPs by $n = \{\pm 1, \pm 3\}$. The pCUT then maps Hamiltonian (7) to an effective Hamiltonian $H_{\text{eff}}^{\text{BWTF}}$ which conserves the number of QPs. This allows the investigation of the low-energy properties of the BWTF in the high-field limit along the lines discussed in Ref. 20. The series expansion results for the ground-state energy per site $\varepsilon_0^{\text{BWTF}}$ as well as the 1-QP gap $\Delta_1^{\text{BWTF}}$ will be presented in Sec. III C.

2. Low-field limit ($J \gg h$)

Here we aim at a linked cluster expansion for the low-field limit of the BWTF. To this end we can benefit from the duality mapping discussed in Sec. II and we can apply the pCUT method to the dual Hamiltonian (4) on the dual honeycomb lattice\textsuperscript{20}. Since the first term of Eq. (4) is an effective field term, the unperturbed part is exactly the same as the one in the high-field limit and we can again apply the pCUT method using spin-flip excitations of the dual model as the appropriate QPs. The plaquette operators $\chi_p$ represents the perturbation which are six-spin interactions on hexagons. The latter operators change the number of QPs by $n = \{0, \pm 2, \pm 4, \pm 6\}$. Consequently, the dual Hamiltonian (4) can be recast into the following form

\[ \frac{H_{\text{dual}}^{\text{BWTF}}}{2J} = E_0 + Q + \frac{h}{2J} \sum_{n=0,\pm 2,\pm 4,\pm 6} T_n, \]

where $E_0 = -N$. The explicit expressions of $T_n$ operators have been already given in Ref. 20.

The pCUT then maps Eq. (8) to an effective Hamiltonian $H_{\text{eff}}^{\text{BWTF}}$ in the low-field limit. The energetics of the BWTF in the low-field limit is then accessed by calculating the ground-state energy per site and the low-energy gap of the QP excitations.

However, one should note that although a single spin flip on one site of the dual honeycomb lattice is the lowest excited state, the 1-QP sub-block is not the most
relevant sector close to the phase transition\textsuperscript{20}. In the original BWTF, the transverse field $\sigma_i^x$ creates (out of the unperturbed ground state) six QPs on the six neighboring triangles which share site $i$. This condition implies that this 6-QP excitation having all six spins of a hexagon flipped to be the most relevant low-energy excitation. We therefore discuss $\varepsilon_0$ and the corresponding 6-QP gap of the BWTF in the low-field limit in the next section.

B. Quantum finite-lattice method

As we have already outlined in Sec. III\textsc{a}, the pCUT method maps the initial problem to a QP conserving Hamiltonian which is a sum over virtual fluctuations that are represented by sequences of the $T_n$ operators. This property has important consequences when the method is applied to Hamiltonians with local property has important consequences when the method is applied to Hamiltonians with local operators\textsuperscript{21}. By local, we mean $T_n = \sum_i T_{n,i}$ where $i$ are a finite number of neighboring sites.

In Ref. 25, it has been shown that $H_{\text{eff}}$ can alternatively be represented by an infinite sum of nested commutators of these local operators. This property is a direct consequence of the so-called linked-cluster theorem\textsuperscript{21,24,26} which states that only those processes contribute to the matrix elements of the effective Hamiltonian which take place on linked clusters.

According to Gelfand et al.\textsuperscript{26}, the series expansion of any extensive quantity $F$ per site on a lattice $\Lambda$ can be expressed as a sum over linked clusters $c$:

$$F(\Lambda)/N = \sum_c L(\Lambda,c)W(c),$$

where

$$W(c) = F(c) - \sum_{c' \subset c} W(c').$$

Here $N$ is the number of lattice sites, $L(\Lambda,c)$ is the number of embeddings of cluster $c$ per lattice site, and $W(c)$ is the reduced weight of the cluster $c$. In order to obtain $W(c)$, one first calculates the series expansion of $F$ on cluster $c$ and then subtracts the contributions of all subclusters $c' \neq c$ which can be embedded in $c$ ($c' \subset c$). In the present work, $F$ denotes the matrix elements of $H_{\text{eff}}$ which correspond to the ground-state energy or hopping amplitudes of elementary quasi-particles.

The finite-lattice method (FLM) was first introduced by Enting et al.\textsuperscript{27} in the framework of classical statistical mechanics and applied to the Ising model on the square lattice. The main idea of the FLM was to consider rectangular clusters $C_{mn}$, with $m \times n$ sites and their embeddings in the lattice $\Lambda$. Then any extensive quantity such as the free energy is calculated on rectangular clusters and the physical quantity in the thermodynamic limit is obtained by proper summation and subtraction rules. The main benefit of this method is that the total number of clusters is dramatically decreased compared to a full graph expansion. Furthermore, the embedding number can be determined analytically for some lattices such as the square lattice\textsuperscript{27}. The FLM was first brought to the realm of quantum many-body problems by Dusuel et al. in Ref. 25 where it has been applied to the transverse field Ising model and the XXZ model on the square lattice.

We have applied Enting’s finite-lattice method for the triangular lattice\textsuperscript{28,29} to the BWTF model and we calculated the ground-state energy and the 1-QP gap of the system in the high-field limit. In contrast to the square lattice, there is no algebraic relation for the embedding factor of subclusters for the triangular lattice. One therefore has to determine these factors numerically. The interested reader can find an efficient algorithm for generating the subclusters and obtaining their embedding number in Ref. 29. After identifying the clusters and their embedding number, we calculate the matrix elements of $H_{\text{eff}}$ by acting on each cluster and thereafter subtracting the contributions of subclusters $c' \subset c$ using Eqs. (9,10).

C. Series expansion results

1. High-field results

Using the quantum finite-lattice method on the triangular lattice, we calculated the ground-state energy $e_{0}^{hf}$ and the 1-QP gap $\Delta_{1}^{hf}$ of the system about the high-field limit for $h = 1$:

$$e_{0}^{hf} = -1 - \frac{1}{3} j^2 - \frac{19}{216} j^4 - \frac{5359}{34020} j^6 - \frac{500690327}{1371686400} j^8 - \frac{74305313819}{7201356000} j^{10},$$

$$\Delta_{1}^{hf} = 2 - 24 j^2 + 64 j^4 - \frac{268712}{81} j^6 + \frac{37389778504}{893025} j^8 - \frac{29786981411535707}{20253807000} j^{10}.$$  

Note that both series obtained by the quantum finite-lattice method correspond exactly to the ones calculated in Ref. 20 for the TCC in a parallel field.

2. Low-field results

Finally, we also give the series expansion results of the ground-state energy $e_{0}^{lf}$ and the 6-QP gap $\Delta_{6}^{lf}$ (relevant mode close to the transition) of the system in the low-field limit for $J = 1$ obtained by pCUTs:

$$e_{0}^{lf} = -2 - \frac{1}{12} h^2 - \frac{1}{864} h^4 - \frac{19}{155520} h^6 - \frac{1133}{238878720} h^8 - \frac{12026279}{270884684800} h^{10},$$

$\Delta_{6}^{lf}$.
\[ \Delta^R = 12 - \frac{22}{3} h^2 + \frac{88}{27} h^4 - \frac{413}{72} h^6 \]  
(14)

The series are obtained by acting with \( H_{\text{eff}} \) on the appropriate hexagonal clusters in different orders of perturbation as explained in Ref. 20.

**D. Quantum Monte Carlo**

1. **Algorithm**

Working in the standard basis where the Ising interaction is diagonal, all non-vanishing off-diagonal elements of the BWTF are negative for \( h > 0 \); it is therefore amenable to QMC simulations with no sign problem. However, it is non-trivial to devise an efficient algorithm due to the specific form of the three-body Ising interaction. The SSE QMC technique with efficient directed loop updates\(^{30}\) is indeed usually formulated for two-body interactions. For specific models however, one can construct non-local loop algorithms in a slightly different fashion as first formulated by Sandvik\(^{31}\) for the TFIM model in the basis where the Ising interaction is diagonal. We refer the reader to Ref. 31 for full details of the algorithm, and just state the key point: for the TFIM, the matrix element of an Ising (SSE) vertex is unchanged when both spins (all SSE vertex legs) are flipped. Unfortunately, this property does no longer hold for the BWTF due to the odd number of sites in the Ising interaction. However, we can use a similar idea: before starting a global loop update in the SSE configuration, one can freeze randomly one of the three sublattices A, B or C\(^{32}\) by not allowing the loop to touch any of the spins in this sublattice. Then, we use exactly the same rules as for the TFIM case\(^ {31}\), and flip all legs of SSE vertices except those on the frozen sublattice, i.e. four legs among six. By doing so, the weight of the configuration is unchanged and the acceptance rate is one. In the limit of vanishing transverse field, this algorithm is identical to the cluster algorithm first proposed by Evertz and Novotny\(^{33}\) for the classical Baxter-Wu model, exactly as the algorithm proposed by Sandvik\(^ {31}\) reduces to the Swendsen-Wang\(^ {34}\) algorithm for the Ising model.

This remark makes us believe that our QMC algorithm for the quantum Baxter-Wu model is slightly less efficient than the TFIM algorithm, as it was already shown\(^ {33}\) for the classical limit \( h \to 0 \) that the dynamical critical exponent (characterizing the algorithm efficiency to decorrelate Monte-Carlo samples) was larger than for the Swendsen-Wang algorithm. We nevertheless manage to simulate close to criticality large samples of size \( N = L \times L \) up to \( L = 96 \) at finite temperature, and up to \( L = 15 \) in the ground-state. We have checked by comparing with exact diagonalizations (ED) on small lattices that our QMC implementation does reproduce all quantities within error bars.

In the QMC simulations, we measure several observables which can be grouped in two types: observables related to the order parameter of the ordered magnetic phase of the BWTF model, and observables related to energy. The sections below give their definitions and expected scaling close to a phase transition.

2. **Observables based on order parameter**

To define properly the order parameter, let us first discuss the symmetries of the model Eq.(3). It is clearly invariant when one performs a \( \pi \) rotation in spin space (i.e. spin inversion) for spins sitting on any two among the three sublattices A, B or C (this fact is explicitly used in the construction of the QMC algorithm, see Sec. IIID 1). As a consequence, any sublattice magnetization

\[ m_{\alpha} = 1/(N/3) \sum_{i \in \alpha} \sigma_i^z \]

(where \( \alpha = \text{A}, \text{B} \) or C\) will have a vanishing expectation value \( \langle m_{\alpha} \rangle = 0 \) on finite systems. This is also true for the expectation value of any cross-correlation \( \langle m_A m_B \rangle = \langle m_B m_C \rangle = \langle m_A m_C \rangle = 0 \).

Using the above symmetry (which is recovered in our simulations within error bars), we can construct an estimator of the square of the order parameter

\[ m^2_s = \frac{m_A^2 + m_B^2 + m_C^2}{3} \]

(15)

which expectation value reaches its maximum value in the four classical ground states. The same quantity was also measured in classical simulations\(^ {35}\). Close to a continuous phase transition at finite temperature, we expect the following scaling form\(^ {36}\):

\[ \langle m^2_s \rangle = L^{-2\beta/\nu} f((T - T_c)/L^{1/\nu}) \]

where \( \beta \) is the order parameter critical exponent, \( \nu \) the correlation length critical exponent, \( T_c \) the critical temperature and \( f \) a universal scaling function. The exponents of the classical BW model are those of the 4-states Potts model in two dimensions (with no logarithmic correction): \( \beta = 1/12, \nu = 2/3 \). For a first-order transition, we expect a jump at the critical point.

A useful way of localizing a continuous phase transition is to consider the associated Binder cumulant

\[ U_L = 1 - \frac{3}{5} \frac{\langle m^4_s \rangle}{\langle m^2_s \rangle^2} \]

(16)

Normalization is such that \( U \to 2/5 = 0.4 \) in the ordered phase, and \( U \to 0 \) in the disordered phase. For a continuous phase transition, the following scaling form is expected:

\[ U_L = g((T - T_c)/L^{1/\nu}) \]
with $g$ a universal scaling function, such that for various sizes $L$, Binder cumulants should cross at the critical point. The exponent $\nu$ can furthermore be extracted from a scaling plot. For first-order phase transitions one does not observe unique crossings and the Binder cumulant reaches very large negative values just above the critical point (in the disordered phase), which should scale as $L^d = L^2$. This has been explained phenomenologically by Vollmayr et al.\textsuperscript{37}. Some continuous phase transitions may also display negative values for Binder cumulants, but the minimum does not scale as $L^d$.

Observables based on the $z$ components of spins are easily measured in QMC as they are diagonal in the chosen $\sigma^z$ basis.

3. Observables based on energy

Singualrities in energy and its derivative can clearly signal phase transitions both at finite and zero temperature. For finite temperature, the specific heat per site:

$$C_v/N = \frac{\langle H^2 \rangle - \langle H \rangle^2}{NT^2}$$

is well-known to display a singularity at a finite-$T$ phase transition. For a continuous transition, we expect the following scaling form:

$$C_v/N = L^{\alpha/\nu} h ((T - T_c) L^{1/\nu})$$

where $\alpha$ is the specific heat critical exponent and $h$ another universal scaling function. For the BW model, we know that $\alpha = 2/3$, in agreement with hyperscaling relation $\alpha = 2 - d\nu$. For a first-order phase transition, we rather expect a (volume-scaling) divergence $C_v/N \sim L^d$.

At zero temperature, the analog of the specific heat is the second-derivative of the ground-state energy,

$$\chi_E = -\frac{1}{N} \frac{\partial^2 E_0}{\partial h^2}$$

with respect to the field strength. For a second-order phase transition, this quantity should scale at the transition as $^{38}$:

$$\chi_E \sim L^{(2/\nu) - (d+z)}$$

where $z$ is the dynamical exponent ($d = 2$ here). For a first-order phase transition on the other hand, we expect a volume divergence: $\chi_E \sim L^d$.

Another interesting insight on the phase transition is provided by the energy Binder cumulant\textsuperscript{39}:

$$V_L = 1 - \frac{\langle H^4 \rangle}{3\langle H^2 \rangle^2}.$$ 

This quantity is equal to $2/3$ away from the phase transition (both in the disordered and ordered phase)\textsuperscript{39}. For a continuous transition, the same limit $V(T_c) = 2/3$ is obtained in the thermodynamic limit. On the other hand, a finite dip (with $V = V^* \neq 2/3$) is observed in the thermodynamic limit at a first order phase transition point\textsuperscript{39}. For finite systems, the value of the dip is expected\textsuperscript{39} to scale as $V_{min}(L) = V^* + A/L^d$. For a continuous transition, a dip can also be found on finite systems, but it should vanish in the thermodynamic limit where $V(T_c) = 2/3$ is recovered. We are not aware of the precise derivation of a finite-size scaling form of the energy Binder cumulant at a continuous transition, although general arguments\textsuperscript{39,40} suggest the following scaling $V_{min}(L) - 2/3 \sim L^{-d + \alpha/\nu}$.

Even though they correspond to off-diagonal observables, moments of the Hamiltonian are easily computed within the QMC method (by computing the appropriate moment of the expansion order\textsuperscript{30}). The second-derivative of the ground-state energy is also directly accessible as a simple response function within the SSE technique\textsuperscript{30,38}.

IV. NUMERICAL RESULTS FOR PHASE TRANSITIONS

A. Quantum phase transition

In this section, we investigate the zero-temperature phase transition driven by the magnetic field, combining pCUT and QMC results. We have calculated with pCUTs the ground-state energy per site, $e_0$, as well as the 1-QP gap, $\Delta = \omega(K = 0)$, of the system for the small- and high-field limit of the BWTF model (see Sec. III C for the full expressions). Note that exactly the same series have been obtained in Ref. 20 when studying the TCC in a single parallel field. Nevertheless it is in our opinion valuable to give them again here in the appropriate units for the BWTF.

Combining the low- and high-field series expansions, we display $e_0/J$ as a function of $h/J$ in Fig. 2. The crossing point of both expansions signals a first-order phase transition close to $h \approx 2.405 J$ in full agreement with Ref. 20. We refer the interested reader to the latter reference for a detailed discussion on capturing the first-order transition point by analyzing the 1-QP energy gap. Additionally, we also show the QMC expectation value for different system sizes, at a fixed inverse temperature $\beta J = 16$. As we can clearly see from the zoom close to $h \approx 2.4 J$ in the bottom inset, there is a clear discontinuity in the ground-state energy curve which also pleads in favor of a first-order phase transition.

However, we observe that the QMC energy curves for larger sizes $L = 18$ and $L = 24$ deviate from the collapse (data not shown). We attribute this to a lack of equilibration at this temperature of our QMC simulations for these large system sizes. This is confirmed by considering the single sample $L = 18$ for different values of inverse temperature (see top inset of Fig. 2), where the average energy at lower temperature is incorrectly larger than for higher temperature in this field region. Note that in such
cases, a careful statistical analysis does confirm that simulations are not converged so that we do not show error bars. Such hysteretic effects in Monte Carlo simulations are typical of a first-order phase transition.

This is confirmed by the following results for other QMC observables (we now fix the inverse temperature to be $\beta J = 16$, and limit the system size to $L \leq 15$ to ensure correct convergence). In Fig. 3, we plot the magnetization per site along the field $\langle \sigma^x \rangle$ versus transverse field $h$. While this is not an order parameter, this quantity displays a rather nice behaviour with a paramagnetic response at small field, a sharp jump close to $h/J \approx 2.39$, and then approaches saturation. Note that the pCUT fully agrees with the QMC results displaying a jump at slightly larger values $h/J \approx 2.395$ as shown in Fig. 3. The (square of the) order parameter (Fig. 4a) similarly displays a marked jump versus field at the same critical value of the field $h \approx 2.39J$ (see inset). The order parameter Binder cumulant $U_L$ also displays a jump (see Fig. 4a), as well as a large negative (apparently diverging with $L$) value above the transition field. As seen later, this may not indicate a first-order transition though. In order to confirm the discontinuous nature of the transition, we display in Fig. 5 the behavior versus field of the second-derivative of the ground-state energy $\chi_E$, which clearly diverges strongly at the transition. The divergence appears (see inset) to approximatively scale as

$L^2$ (and maybe even with a larger exponent, but this is probably due to the limited range of $L$ available at this low temperature). Note however that the divergence expected in $\chi_E$, and seen in QMC data, comes from the non-analyticity of $e_0(h)$ and thus cannot be captured by the perturbative pCUT approach.

Overall, this set of results clearly point towards a first-order quantum phase transition in the BWTF model Eq. (1). The QMC simulations point to $h_c(T = 0) \approx 2.39J$ while the pCUT results tend to a slightly larger value $h_c(T = 0) \approx 2.4J$. This small difference might arise due to the convergence problem in QMC as explained above or due to the uncertainties in the pCUT originating from the extrapolation of the series.

B. Finite temperature phase diagram

We now turn to finite-temperature properties of the BWTF model. At $h = 0$, the BW model is known to have a second-order transition in the 4-state Potts model universality class (without logarithmic corrections), i.e. with critical exponents $\alpha = \nu = 2/3$, $\beta = 1/12$, at the self-dual point $T_c = 2J/\log(\sqrt{2} + 1) \approx 2.269J$. When switching on a small field $h$, it is not a priori clear whether the transition will remain of second-order type or change to first-order, as will be the case eventually when $h \to h_c$ at zero temperature.

Our QMC simulations discussed below indicate that the finite-temperature transition remains continuous in the same universality class as for the classical BW model in a large region of transverse field, up to at least $h = 2.25J$. Additionally, we have indications that the
The full \((h=2J, h=2.35J)\) phase diagram is indicated by the dotted vertical line.

An independent check of the nature of the phase transitions is obtained by considering the energy Binder cumulant \(V_L\). In all three cases, we observe a dip close to \(T_c(h)\) (see Fig. 9). However, the data at \(h=0, 2J\) have a different finite-size behavior as can be observed in Fig. 8b: the minimum value \(V_{min}\) converges to 2/3 with \(1/L\) (as expected from the scaling ansatz presented in Sec. III.D3 with \(\alpha/\nu = 1\)), while \(V_{min} - 2/3\) appears to reach a non-zero value with a different power-law \(L^{-2}\) for \(h=2.35J\). The existence and scaling of the dip in \(V\) was also reported in \(h=0\) classical studies [40,41]. This is again a sign of a first-order phase transition for this latter field value, which is confirmed by the fact that a (phenomenological) collapse of the full \(V_L\) curves can be obtained for \(h=0, 2J\), but not for \(h=2.35J\) (see Fig. 10).

Fig. 11 represents the (squared) order parameter \(m^2\) as a function of temperature, for the three selected field values and for different \(L\). A rather sharp drop is observed at the values of \(T_c\) estimated from the above energetics considerations. While the curves for different system sizes can be reasonably well collapsed with the BW exponents \((\beta/\nu = 1/8)\) for the field values \(h=0, 2J\) (see Fig. 12), this is not the case for \(h=2.35J\). The results for the
FIG. 7: (Color online) Collapse analysis using the same data as in Fig. 6. Using the known results for BW model and the obtained $T_c$’s, we plot $C_v/L^{\alpha/\nu}$ vs $(T - T_c(h))L^{1/\nu}$ with $\alpha = \nu = 2/3$.

FIG. 8: (Color online) (a) Specific heat maximum vs length $L$ for various $h$. (b) Dip size of $V_L$ vs $1/L$ for various $h/J$.

magnetization Binder cumulant $U_L$ confirm this analysis, albeit with a further anomaly in the high-temperature phase. Indeed on the largest clusters, a nice crossing for different $L$ is observed (with value close to 0.27) in Fig. 13 for $T_c(h = 0) \simeq 2.269J$ and $T_c(h = 2J) \simeq 1.523J$, but not for the largest field value where curves do not cross at a single point. We note also the existence of negative values for larger $T$ (for all fields): we find (data not shown) that this minimum does diverge in the thermodynamic limit for $h = 2.35J$ but not for $h = 0, 2J$, therefore implying a first-order character for the largest field and a continuous nature for the two other field values. This is confirmed by the excellent data collapse for $U_L$ presented in Fig. 14 obtained using the exact value $\nu = 2/3$.

Note that we have also performed a systematic data collapse (without any prior knowledge) for all the above quantities. For instance, data analysis of the Binder cumulant $U_L$ for the three cases $h = 0, h = 2J$ and $h = 2.35J$ respectively leads to estimates of $\nu = 0.6701 \pm 0.003$, $\nu = 0.6664 \pm 0.004$ and $\nu = 0.5205 \pm 0.01$. Such results are fully compatible with our claim that the first

FIG. 9: (Color online) Energy Binder cumulant $V_L$ vs $T$ for various sizes and transverse fields. A dip in this quantity signals a phase transition (see text).

FIG. 10: (Color online) Tentative data collapse of the $V_L$ dip times $L$ vs $(T - T_c) L^{1/\nu}$ using the critical exponents of the BW model. A rather good collapse can be obtained for $h = 0$ and $2J$, but not for $h = 2.35J$.

FIG. 11: (Color online) Order parameter squared $\langle m^2 \rangle$ as a function for temperature $T/J$ for different system sizes, for different field values.
two cases are second-order phase transitions in the same universality class as the BW model, while the third one is first-order with an effective $\nu = 1/d = 1/2$.

In order to provide a more physical picture in the change of nature of the phase transition when varying $h/J$, we provide now some analysis of the full energy and order parameter histograms. In Fig. 15, the order parameter histograms for various $h$ (taken at the transition, i.e. fixing $T/J$ at the maximum slope of $m_T^2(T)$) display some characteristic bimodal structure. This bimodal form is reinforced when increasing $h$, although there is no qualitative change, and is responsible for the negative $U_L$ values that were discussed previously.

Concerning the energy distribution at the transition, we know from the analysis of its Binder cumulant $V_L$ that it is non gaussian. In fact, if we plot separately energy histograms obtained with configurations having $m_T^2$ smaller or greater than 0.25 (i.e. we separate contributions from both peaks in the $m_T^2$ histograms), then we observe in Fig. 16 that data can be well represented by two gaussians centered at slightly different positions $E_\pm$. As explained in Ref. 39, at the transition the two gaussians have the same weight leading to a dip in $V_L$ of size $2(E_1^2 + E_2^2)/3(E_1^2 + E_2^2)^2$. Therefore a first (respectively second) order transition will occur if $E_\pm$ are distinct in the thermodynamic limit (respectively if they merge). We have already performed this analysis in Fig. 8(b) indicating that phase transitions for $h = 0$ or $h = 2J$ are second-order, while $h = 2.35J$ corresponds to first order. Looking at data on a single size $L = 36$ does not give any indication since the peaks are more separated for small $h$ where the transition is second-order, than for $h = 2.35J$ (see Fig. 16). Clearly, this confirms that a careful finite-size study is necessary to ascertain the order of the phase transition.

C. Phase diagram and discussion

In summary on this numerical study, we have been able to identify clear signatures of second-order thermal phase transitions for various transverse field amplitudes ranging from $h = 0$ up to $h/J \sim 2.25$, all occurring in the same universality class (4-state Potts model, with
Simulations, the situation is particularly challenging for critical exponents of tricritical points from finite-lattice critical exponents. While it is always difficult to extract this multi-critical point (for instance computing precise $L^{\nu}$ with the current lattice sizes), knowledge of the correlation length (effective) critical exponent $\nu$ that the correlation length $\nu$ and then finally $\nu = 0.52$ at $h = 2.35J$ corresponding to first-order behaviour.

V. CONCLUSION

We have studied quantum and thermal phase transitions of the Baxter-Wu model in a transverse magnetic field using large-scale quantum Monte Carlo simulations and series expansions. This has allowed us to characterize the full phase diagram vs $(h/J, T/J)$ (see Fig. 17). On the one hand, our results confirm that the BWTF undergoes a first-order quantum phase transition at $(h \approx 2.4, T = 0)$ that extends to finite temperature regime. On the other hand, the classical second-order phase transition at $(h = 0, T \approx 2.226)$, known to be in the 4-state Potts model universality class, also persists at finite magnetic field, up to rather large values of $h \approx 2.25J$, with the same critical exponents. Therefore, we naturally predict the existence of a tricritical point located where these two phase boundaries merge, i.e. approximately at $(h \approx 2.3J, T \approx J)$, but its determination (including critical exponents) remains challenging. Indeed, even the second-order phase transition line exhibits typical signatures of first-order transitions such as negative Binder cumulant $U_L$ or double peaked energy histograms, which vanish in the thermodynamic limit but hinder the analysis.

Given the central role played by tricritical points in

![FIG. 15:](image_url) Order parameter histograms on $L = 36$ cluster for (a) $h = 0$, $T/J = 2.274$; (b) $h/J = 2$, $T/J = 1.53$; (c) $h/J = 2.35$, $T/J = 0.86$. In each case, we have split data depending whether $m^2_s$ is smaller or greater than 0.25.

![FIG. 16:](image_url) Energy histograms on $L = 36$ cluster for (a) $h = 0$, $T/J = 2.274$; (b) $h/J = 2$, $T/J = 1.53$; (c) $h/J = 2.35$, $T/J = 0.86$. In each case, we have split data depending whether $m^2_s$ is smaller or greater than 0.25.

![FIG. 17:](image_url) Phase diagram of the BWTF vs $(h, T)$. Full (respectively dashed) lines are used for second (respectively first) order phase transitions. Both lines meet at a putative tricritical point close to $h^* \approx 2.3J$ and $T^* \approx J$. No logarithmic corrections) as the classical BW model at $h = 0$. At the same time, the quantum critical point at $T = 0$ (obtained for $h_s(T = 0) \approx 2.4J$) is clearly of first-order nature. We therefore expect that this first-order character subsists at finite temperature, at least close to $h_s(T = 0)$. We have found indications that this is indeed the case in our QMC simulations at $h = 2.35J$. All results are summarized in the phase diagram Fig. 17.

We would thus expect a tricritical point at $(h^*, T^*)$ where the first and second order transition lines meet (dots in Fig. 17). Our best estimates are $h^* \in [2.25J, 2.35J]$ and $T^* \in [0.85J, 1.15J]$. We are not aware of a theoretical prediction for the universality class of a tricritical point separating a Baxter-Wu universality class continuous transition line from a first-order line. With the current lattice sizes $L$ at hand in our QMC simulations, we have not been able to further characterize this multi-critical point (for instance computing precise critical exponents). While it is always difficult to extract critical exponents of tricritical points from finite-lattice simulations, the situation is particularly challenging for
interactions a general uniform magnetic field or ferromagnetic Ising well as its zero-temperature robustness in the presence of magnetic field, is to the best of our knowledge not known.

As stated above, the TCC in a parallel magnetic field on the honeycomb lattice is isospectral to the BWTF. The finite temperature error threshold of the TCC in the framework of the random 3-body Ising model as well as its zero-temperature robustness in the presence of a general uniform magnetic field or ferromagnetic Ising interactions has already been studied. However, the finite temperature physics of the TCC in a parallel magnetic field, is to the best of our knowledge not known.

It is certainly also an interesting project to extend the investigation of the finite-temperature properties to the TCC in a parallel magnetic field.

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