Monte Carlo study of the interfacial adsorption of the Blume–Capel model

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We investigate the scaling of the interfacial adsorption of the two-dimensional Blume–Capel model using Monte Carlo simulations. In particular, we study the finite-size scaling behavior of the interfacial adsorption of the pure model at both its first– and second–order transition regimes, as well as at the vicinity of the tricritical point. Our analysis benefits from the currently existing quite accurate estimates of the relevant (tri)critical–point locations. In all studied cases, the numerical results verify to a level of high accuracy the expected scenarios derived from analytic free–energy scaling arguments. We also investigate the size dependence of the interfacial adsorption under the presence of quenched bond randomness at the originally first–order transition regime (disorder–induced continuous transition) and the relevant self–averaging properties of the system. For this ex–first–order regime, where strong transient effects are shown to be present, our findings support the scenario of a non–divergent scaling, similar to that found in the original second–order transition regime of the pure model.

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Critical interfacial phenomena have been studied extensively over the last decades, both experimentally and theoretically [1–4]. A well–known example is wetting, where the macroscopically thick phase, *e.g.*, the fluid, is formed between the substrate and the other phase, say, the gas. Liquid and gas are separated by the interface. An interesting complication arises when one considers the possibility of more than two phases. A third phase may be formed at the interface between the two other phases. An experimental realization is the two–component fluid system in equilibrium with its vapor phase [2, 5]. Both of the above scenarios may be mimicked in statistical physics in a simplified fashion, by either the two–state Ising model in wetting – with the state "+1" representing, say, the fluid, and "-1" the gas – or for the case of a third phase via multi–state spin models, simply by fixing distinct boundary states at the opposite sides of the system. In this latter case, the formation of the third phase with an excess of the non–boundary states has been called as interfacial adsorption [6–8].

Throughout the years, various aspects of the interfacial adsorption have been investigated via Monte Carlo methods and density renormalization–group calculations on the basis of specific multi–state spin models, namely Potts and Blume–Capel models [6, 7, 9–17]. Additional scaling and analytic arguments have been presented [7, 10, 13, 18–20], though not all of them have been confirmed numerically, due to the restricted system sizes studied and, in some cases, the uncertainty in the location of (tri)critical points. However, notable results in the field include the determination of critical exponents and scaling properties of the temperature and lattice–size dependencies, as well as the clarification of the fundamental role of the type of the bulk transition, with isotropic scaling holding at continuous and tricritical bulk transitions, and anisotropic scaling at bulk transitions of first–order type. More recently, a formulation of the field theory of phase separation by Delfino and colleagues has provided new insight into the problem [21–28] and, what is more, the role of randomness has been scrutinized on the basis of the disordered Potts model [29–32].

Clearly the Potts model offers the unique advantage that if one considers the system at its self–dual point, then, the phase–transition temperatures between the ordered ferromagnetic phase and the high–temperature disordered phase are known exactly from self–duality for arbitrary values of the internal states q and particular implementations of the randomness distribution [33]. On the other hand, for the Blume–Capel model, one relies upon the existing estimates for the locations of (tri)critical and transition points and this may be a source of systematic error when uncovering the scaling behavior of the interfacial adsorption, as has already been underlined in the literature [10]. However, quite recently important progress has been reported with respect to an accurate reproduction of the phase diagram of the model for a wide range of its critical parameters [34–39], thus motivating the current study. In the present work we investigate the finite–size scaling behavior of the interfacial adsorption of the two–dimensional square–lattice Blume–Capel model, at both the continuous and first–order transition regimes of its phase diagram, as well as at the vicinity of the tricritical point. Furthermore, we study the effect of quenched bond randomness on the interfacial adsorption at the disorder–induced continuous transition. Our discussion below follows the seminal works by Selke and collaborators [9, 10], where the first Monte Carlo results for the pure Blume–Capel model have been presented, corroborated by analytical scaling arguments, which we will also outline for the benefit of

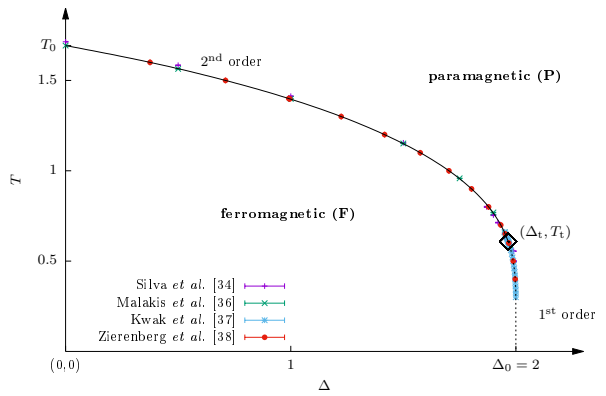

FIG. 1: Phase diagram of the square–lattice zero–field Blume–Capel model in the $\Delta - T$ plane. The phase boundary separates the ferromagnetic (F) phase from the paramagnetic (P) phase. The solid line indicates continuous phase transitions and the dotted line marks first–order phase transitions. The two lines merge at the tricritical point $(\Delta_{\rm t}, T_{\rm t})$, as highlighted by the black diamond. The data shown are selected estimates from previous numerical studies. As usual, we have set $J = 1$ and $k_{\rm B} = 1$ to fix the temperature scale.

the reader in cases where a direct comparison with the numerical data is possible. In a nutshell, the main objectives of the current work are as follows: For the pure case, previous numerical findings [9, 10] based on less extensive simulations, are scrutinized, confirmed, and refined to a high–level of numerical accuracy, especially for the areas around the tricritical point and the first-order transition line in the $\Delta - T$ plane (as will be explicitly elaborated in the discussion of Figs. 2 and 3 below). Completely new results are presented for the random case, an aspect that has not been previously considered in the relevant literature, where an intriguing crossover behavior, with a finite interfacial adsorption, at the randomness–induced continuous transition is observed and explained.

We consider the Blume–Capel model [40, 41] defined by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j + \Delta \sum_i S_i^2. \qquad (1)$$

The spin variable S_i takes on the values -1, 0, or $+1$, $\langle ij \rangle$ indicates summation over nearest neighbors, and $J > 0$ is the ferromagnetic exchange interaction. The parameter Δ denotes the crystal–field coupling and controls the density of vacancies ($S_i = 0$). For $\Delta \to -\infty$ vacancies are suppressed and the model becomes equivalent to the Ising model. The phase diagram of the Blume–Capel model in the crystal–field – temperature plane consists of a boundary that separates the ferromagnetic from the paramagnetic phase, see Fig. 1. The ferromagnetic phase is characterized by an ordered alignment of ± 1 spins. The paramagnetic phase, on the other hand, can be either a completely disordered arrangement at high temperature or a ± 1–spin gas in a 0–spin dominated environment for low temperatures and high crystal fields. At high temperatures and low crystal fields, the ferromagnetic–paramagnetic transition is a continuous phase transition in the Ising universality class, whereas at low temperatures and high crystal fields the transition is of first–order character [40, 41]. The model is thus a classical and paradigmatic example of a system with a tricritical point $(\Delta_{\rm t}, T_{\rm t})$ [42], where the two segments of the phase boundary meet. At zero temperature, it is clear that ferromagnetic order must prevail if its energy $zJ/2$ per spin (where z is the coordination number, $z = 4$ in the present case) exceeds that of the penalty Δ for having all spins in the ± 1 state. Hence the point $(\Delta_0 = zJ/2, T = 0)$ is on the phase boundary [41]. For zero crystal–field Δ, the transition temperature T_0 is not exactly known, but well studied for a number of lattice geometries. A most recent reproduction of the phase diagram of the model can be found in Ref. [38], and is also given here in Fig. 1, where a summary of results is presented from various works in the literature. A recent accurate estimation of the location of the tricritical point has been given in Ref. [37]: $(\Delta_{\rm t}, T_{\rm t}) = (1.9660(1), 0.6080(1))$.

In order to study the interfacial adsorption, denoted hereafter as W, and following the work of Selke and collaborators [9, 10] we shall employ special boundary conditions, distinguishing the cases $[1:1]$ and $[1:-1]$ that will favor the formation of an interface within the system. For the case $[1:1]$, the spin variable is set at all boundary sites equal to 1, while for the case $[1:-1]$ the variable is set equal to 1 at one half of the boundary sites and to -1 at the opposite half of the boundary sites. Typical equilibrium configurations have verified that under these special boundary conditions an excess of the non–boundary states, $S_i = 0$, is generated at the interface (see for instance Fig. 1 in Ref. [9]). This phenomenon is described quantitatively by the net adsorption per unit length of the interface, that is defined with the help of the following mathematical expression [9]

$$W = \frac{1}{L} \sum_i \left[\langle \delta_{0,S_i} \rangle_{[1:-1]} - \langle \delta_{0,S_i} \rangle_{[1:1]} \right], \qquad (2)$$

where the angular brackets denote thermal averages and L is the linear dimension of the square lattice. The critical behavior of W is characterized by the critical exponents x and ω via [10]

$$W_L \sim L^x \quad (T = T_{\rm c}), \qquad (3)$$

and

$$W_{t_{\rm c}} \sim t_{\rm c}^{-\omega} \quad (L = \infty), \qquad (4)$$

where $t_{\rm c} = (T_{\rm c} - T)/T_{\rm c}$ is the reduced critical temperature for the standard case of a critical point. Although the above Eqs. (3) and (4) are expressed for the usual case of continuous transitions, they can be similarly generalized for the case of a tricritical point, where $t_{\rm t} = (T_{\rm t} - T)/T_{\rm t}$, or for a first–order phase transition, $t^* = (T^* - T)/T^*$,

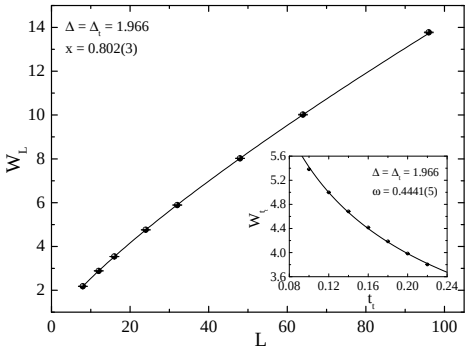

FIG. 2: Finite–size scaling of the interfacial adsorption W_L (main panel) and W_{t_t} (inset) at the tricritical point.

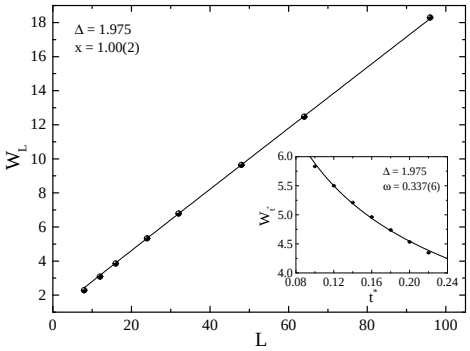

FIG. 3: Finite–size scaling of the interfacial adsorption W_L (main panel) and W_{t^*} (inset) at the first–order transition regime.

where T^* denotes now the corresponding transition temperature.

In the present work we have studied the interfacial properties of the system at three values of the crystal–field coupling Δ, including both the first– and second–order lines of the transition but also the tricritical point of the phase diagram shown in Fig. 1. We have considered the values $\Delta = 1$ (second–order regime), $\Delta = \Delta_{\rm t} = 1.966$ (tricritical point), and $\Delta = 1.975$ (first–order regime). The corresponding transition temperatures for the cases $\Delta = 1$ and $\Delta = 1.975$ have been estimated to be $T_{\rm c} = 1.398$ and $T^* = 0.574$, respectively [36], whereas for the case of the tricritical point we have used the most recent estimate $T_{\rm t} = 0.608$ [37]. Additionally, for the case $\Delta = 1.975$ of the originally first–order transition regime, we have also considered the disordered version of the Hamiltonian (1) by selecting ferromagnetic couplings $J \to J_{ij}$ between nearest–neighbor sites i and j, to be either J_1, with probability p, or J_2 with probability $1 - p$. In the case $J_1 > J_2$, one has either strong or weak bonds. Then, the ratio $r = J_2/J_1$ defines the disorder strength, where $(J_1 + J_2)/2 = 1$. Clearly, the value $r = 1$ corresponds to the pure model. For the needs of the present work we fixed the ratio $r = 0.6$, for which the critical temperature of the disorder–induced continuous transition has been estimated to be $T_{\rm c} = 0.626$ [36].

Our numerical protocol consists of canonical Monte Carlo simulations, employing a combination of a Wolff single–cluster update [43] of the ± 1 spins and a single–spin flip Metropolis update that enables the necessary updates of the vacancies $S_i = 0$ [44–46]. We adapted the relative frequencies of using the two updates to optimize the performance and discarded the initial part of each time series to ensure equilibration. Using this approach, we simulated for both versions of the model and for all values of Δ system sizes in the range $L = 8 - 96$, which, as will be shown below, is enough for a safe estimation of the asymptotic behavior, in accordance with the expected scaling arguments. For the pure model we performed several independent runs to increase statistical accuracy, whereas for the disordered system an extensive averaging over the disorder [...] has been undertaken, varying from 5×10^3 realizations for the smaller system sizes down to 1×10^3 for the larger sizes studied. For the disordered case, error bars were computed from the sample–to–sample fluctuations which in all cases were found to be larger than the statistical errors of the single disorder realizations.

For the various cases of phase transitions in the Blume–Capel model along the $\Delta - T$ plane, some very useful analytic and scaling arguments for the interfacial adsorption have been presented in the early work of Selke, Huse, and Kroll [10]. In what follows, we shall only provide the main results of this discussion that are also relevant for comparison with our numerical data; for more details we refer the reader to Ref. [10]. The main point in this description is the reformulation of the interfacial adsorption W with the help of the interface tension σ. According to Ref. [10], using that $\langle \delta_{0,S_i} \rangle = 1 - \langle S_i^2 \rangle$, the interface adsorption may be written in the form $W = (1/L) \sum_i \left[\langle S_i^2 \rangle_{[1:1]} - \langle S_i^2 \rangle_{[1:-1]} \right]$. Denoting the total free energy for $[1:1]$ boundary conditions by $F_{[1:1]}$ (similarly $F_{[1:-1]}$ for $[1:-1]$), W can then be expressed in terms of the interface tension, $\sigma = (1/L)(F_{[1:1]} - F_{[1:-1]})$, as $W = \beta^{-1} \partial \sigma / \partial \Delta$, where $\beta = 1/(k_{\rm B} T)$.

The presentation of our finite–size scaling analysis starts with the most interesting cases referring to the vicinity of the tricritical point and the first–order transition regime. As already mentioned above, the location of the tricritical point of the Blume–Capel model is known today with very good accuracy [37], thus removing one source of error inherent in previous simulation works [9, 10]. According to the scaling arguments of Ref. [10] the exponents appearing in Eqs. (3) and (4) take on the values $x = 4/5$ and $\omega = 4/9$, respectively, for the case of the tricritical point. In Fig. 2 we present our numerical data and the relevant scaling analysis for

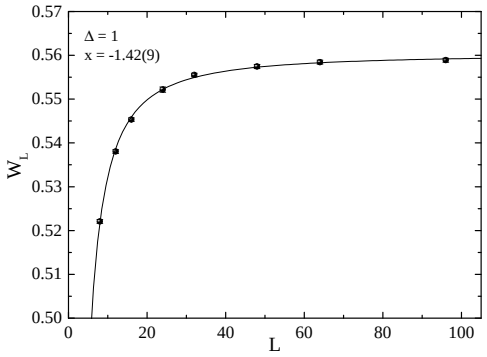

FIG. 4: Finite–size scaling of the interfacial adsorption W_L at the second–order transition regime.

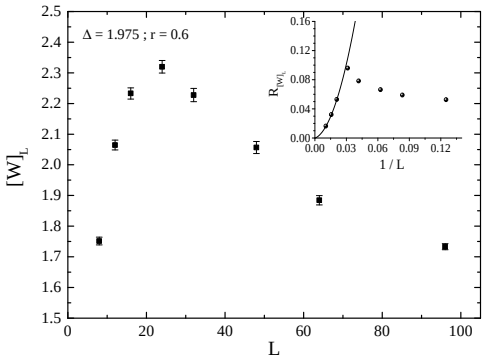

FIG. 5: Finite–size scaling of the disorder–averaged interfacial adsorption $[W]_L$ of the random–bond Blume–Capel model at the disorder–induced continuous transition. The inset illustrates the relevant self–averaging properties in terms of the relative–variance ratio $R_{[W]_L}$ as a function of the inverse system size.

the interfacial adsorption W_L (main panel) and W_{t_t} (inset) at $\Delta = \Delta_t = 1.966$. Fits of the form (3) and (4) shown by the solid lines in the main panel and the corresponding inset respectively, provide us with the estimates $x = 0.802(3)$ and $\omega = 0.4441(5)$, both fully consistent with the expected values $x = 4/5$ and $\omega = 4/9$. We should point out here that the numerical estimation of the exponent x for the tricritical point has been reported as a quite difficult task in the literature, due to the imprecise knowledge of the tricritical coordinates (see Fig. 7 in Ref. [9] where $\Delta_t \approx 1.92(2)$) and the presence of strong finite–size effects for small system sizes (see Fig. 3 in Ref. [10] where for the actual value of $\Delta_t = 1.966$ an effective exponent of the order of ~ 0.65 is obtained). Both of these adversities have been satisfied in the present work, leading to a clear verification of the scaling arguments presented in Ref. [10].

As it is well known, at the critical (and tricritical) points, the singularities in the interfacial adsorption are induced by bulk critical fluctuations. On the other hand, at first–order phase transitions there are no bulk critical fluctuations and the divergence of W arises from an interface delocalization transition [48]. In the latter case and for lattices of square shapes a linear divergence of the form $W_L \sim L$ is expected, *i.e.*, $x = 1$ [10]. Additionally, the critical exponent ω appearing in Eq. (4) is expected to take the value $1/3$, as was originally found in the case of interface unbinding [49], and further generalized for first–order phases transitions in two–dimensions [9, 10, 48, 50]. For the case of the Blume–Capel model, the prediction $\omega = 1/3$ has been numerically confirmed [9, 10], though the numerical data for W_L did not allow for an accurate estimation of the exponent x. In particular, in Ref. [9] a value $x = 0.7 \pm 0.05$ has been found that was subsequently explained as an apparent exponent due to strong metastability effects [10]. To fill in the gap with the scaling analysis of W_L at the first–order transition regime of the Blume–Capel model, we present in Fig. 3 our numerical data for the interfacial adsorption obtained at $\Delta = 1.975$. The fitting results using the Eqs. (3) and (4) as in Fig. 3, give $x = 1.00(2)$ and $\omega = 0.337(6)$, in excellent agreement with the theoretical expectations $x = 1$ and $\omega = 1/3$.

For the spin–1/2 Ising model it is known that $\sigma \sim t_c$ for $t_c \to 0^+$ at the critical point. Given that the Blume–Capel model for $\Delta < \Delta_t$ belongs to the same universality class, we also expect a similar statement to hold, where now t_c may be the distance from the critical curve. Since Δ is a non–ordering field [47], as was also concluded in [10], $W \sim \partial\sigma/\partial t_c \sim$ const. We present in Fig. 4 the finite–size scaling behavior of the interfacial adsorption W_L for $\Delta = 1$. Indeed, a simple power–law fit of the form $W_L = W_\infty + bL^x$ gives a negative exponent $x = -1.42(9)$ and a finite value of W_∞, thus a non–divergent behavior, in agreement with the above arguments. Similar results have been presented in Ref. [9] for a few values of Δ in the second–order transition regime but for smaller system sizes and are overall in contrast to the Potts case, where a clear diverging behavior has been observed in many relevant works [6, 7, 31, 32]. This may be due to the different geometric nature of the interfacial adsorption among the two models, which in the present Blume–Capel model occurs in a layer–like fashion as expected on the basis of single spin–flip energy considerations, see Fig. 1 in Ref. [9], whereas in Potts models a droplet–like adsorption of non–boundary states takes place due to the energetic equivalence of all states [6].

The last part of our work is dedicated to the study of the interfacial adsorption under the presence of quenched bond randomness at the originally first–order phase transition regime of the phase diagram and particularly at the crystal–field value $\Delta = 1.975$. Simulations have been performed for a single value of the disorder strength, namely $r = 0.6$, at the estimated in Ref. [36] critical temperature $T_c = 0.626$. The numerical data for the

disorder–averaged $[W]_L$ are shown in the main panel of Fig. 5, where a very strong saturation is observed [51] and should be compared to the diverging behavior of the corresponding pure system (see Fig. 2). This result is in agreement with the theoretical expectations discussed above for a non–divergent behavior of W in the case of continuous transitions for the present model. Finally, in the inset of Fig. 5 we present the self–averaging properties of the system using the relative–variance ratio $R_{[W]_L} = V_{[W]_L}/[W]_L^2$, where $V_{[W]_L} = [W^2]_L - [W]_L^2$. The limiting value of this ratio is characteristic of the self–averaging properties of the system [52, 53]. The solid line in the inset illustrates a simple polynomial fit over the larger system sizes, indicating the restoration of self–averaging at the thermodynamic limit, given that $R_{[W]_L} \to 0$ as $L \to \infty$. Similar results have been presented for the the case of various random–bond Potts models in two–dimensions [32]. Finally, it is worth noting that the finite–size scaling behavior of both $[W]_L$ and $R_{[W]_L}$ is affected by strong transient effects with a crossover length–scale $L^* \approx 32$, where a turnaround in the behavior sets off. This is consistent with previous observations on the scaling behavior of the correlation length and other thermodynamic observables of the system for the same range of parameters [39]. Indeed, in Ref. [39] it has been explicitly shown that $L \approx 32$ is the apparent size where the first–order characteristic signatures of the transition disappear. Of course, we expect that the value of L^* depends on the disorder strength r as well as on the strength of the first–order transition and it would be interesting to investigate the shift of this crossover length–scale as a function of Δ and r. However this is a task that goes beyond the scope of the present work.

To conclude, we have investigated the scaling aspects of the interfacial adsorption of the two–dimensional Blume–Capel model using a combined Monte Carlo scheme. We presented a detailed analysis of the finite–size scaling behavior of the interfacial adsorption of the pure model at both its first– and second–order transition regimes, as well as at the area of the tricritical point, taking advantage of the current high–accuracy estimates of (tri)critical–point locations. A dedicated part of our work regarding the scaling of the interfacial adsorption under the presence of quenched bond randomness at the originally first–order transition regime (disorder–induced continuous transition) revealed the scenario of a non–divergent scaling, similar to that found in the original second–order transition regime of the pure model. Overall, our results and analysis nicely verified the predicted from analytic arguments scaling scenarios of Ref. [10], overcoming the numerical difficulties highlighted in that seminal work.

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