ELSEVIER

Physica A 254 (1998) 477–516

PHYSICA A

# Graphical representations and cluster algorithms II [1]

L. Chayes [a,*], J. Machta [b]

[a] *Department of Mathematics, University of California, Los Angeles, CA 90095-1555, USA*

[b] *Department of Physics and Astronomy, University of Massachusetts, Amherst, MA 01003-3720, USA*

Received 3 November 1997

**Abstract**

We continue the study, initiated in Part I, of graphical representations and cluster algorithms for various models in (or related to) statistical mechanics. For certain models, e.g. the Blume–Emery–Griffths model and various generalizations, we develop Fortuin Kasteleyn-type representations which lead immediately to Swendsen Wang-type algorithms. For other models, e.g. the random cluster model, that are *defined* by a graphical representation, we develop cluster algorithms without reference to an underlying spin system. In all cases, phase transitions are related to percolation (or incipient percolation) in the graphical representation which, via the IC algorithm, allows for the rapid simulation of these systems at the transition point. Pertinent examples include the (continuum) Widom–Rowlinson model, the restricted 1-step solid-on-solid model and the *XY* model. © 1998 Published by Elsevier Science B.V. All rights reserved

*Keywords*: Cluster algorithms; Random cluster models

## 1. Introduction

This paper is a continuation of Ref. [1] and concerns the construction of graphical representations and their corresponding cluster algorithms for various statistical mechanics systems. Although this work is self-contained, some familiarity with this reference will certainly prove helpful to the reader. However, it will be assumed that the reader is well-versed in the standards of the trade i.e. the Fortuin–Kasteleyn random cluster problems [2], the Swendsen–Wang algorithm [3] and the interpretation of these algorithms due to Edwards and Sokal [4].

* Corresponding author. Fax: 310 3920219; e-mail: lchayes@math.ucla.edu.

[1] Work supported in part by the NSF under the grant DMR-96-32898 (J.M.).


*PII* S0378-4371(97)00637-7

As in [1], the present goals are threefold:

(1) The development of *faithful* graphical representations for various statistical mechanics systems.

(2) A demonstration that the representation is *successful*.

(3) The development of *cluster algorithms* associated with these representations.

Let us elaborate on items (1) and (2). A graphical representation for a statistical mechanics system is an expansion in graphical elements (bonds, sites, etc.) such that each graphical configuration is endowed with a non-negative weight. This allows for a probabilistic interpretation of the expansion that is divorced from the original statistical mechanics problem. (Furthermore, the question of convergence of the expansion does not arise.) By a faithful representation, it is meant that the expectation of any (local) observable in the statistical mechanics system can be expressed as the expectation of a local function in the graphical representation. A successful representation is less precisely defined. In general, it may be taken to mean that the representation provides a clear signal – usually percolation – of a phase transition in the statistical mechanics system. Further, one can envision a "percolation uniqueness" classification: The equivalence of Gibbsian uniqueness to a percolation condition – usually the absence of percolation – in the graphical representation.

Depending on the system, items (1), (2) or (3) may be trivial – or already known. E.g. for spin-systems, (3) often follows immediately from (1). We assert (but have by no means proved rigorously) that under the auspices of items (1)–(3), the direct and rapid simulation of the transition region of a system is possible by using the invaded cluster (IC) algorithm as in Refs. [5,6].

Until recently, only one explicit example of a successful representation existed,[2] namely the random cluster representation of the Potts model. Since, according to Ref. [10], these items are essential in the design of effective cluster algorithms, much effort has been invested in the expansion of this repertoire. The results to date (to the best knowledge of the authors) are summarized in Table 1. Although it cannot be claimed that any significant degree of generality has been achieved, it is fair to say that we are no longer in the realm of "isolated examples".

The organization of the remainder of this paper is as follows:

In Section 2, we study the (non-integer) random cluster model. In this case, items (1) and (2) follow by definition but, heretofore, the development of cluster algorithms has proved elusive.

In Section 3, we study lattice gases: The Blume–Emory–Griffths models and various generalizations which, for certain parameter values, include the (lattice) Widom–Rowlinson models. Graphical representations are developed which reduce to the "grey representation" [12,13] in the Widom–Rowlinson limit. In some cases (notably for the various two-component models), complete theorems characterizing the phase structure

[2] We caution the reader that this is subject to interpretation. Several examples of expansions for the partition function (e.g. Refs. [7,8] for the Widom–Rowlinson model) or graphical components of cluster algorithms (e.g. Ref. [9] for the *XY* model) have been described that later turn out to be faithful or even successful.

Table 1
Current status

| System | Graphical representation | Percolation $\Leftrightarrow$ (standard) phase transitions | Characterization of Gibbsian uniqueness | Cluster algoithm |
|---|---|---|---|---|
| Potts ferromagnet | [2] | [11] | ■ [11] | [3] |
| Widom–Rowlinson 2-comp., Hard cores (lattice or cont.) | [12,13] ([7,8]) | [12,13] | ■ [12] | [14,15] |
| Widom–Rowlinson q-comp., and/or soft cores (latt. or cont.) | Above, [15,16] | Plausible | False in general (■ $q=2$, soft core [14]) | [14] (Sft. crs., $q>2$) [15] ($q>2$) |
| Ashkin–Teller & (rs)-cubic | [1] (Or. & Ref.) [17,18] (Orthodox only) | [1] | [1] | [19] (Orth.) [1] (Orth. & Ref.) [17] (Orth.) |
| BEG-model and $q$-component generalizations | [14] | Plausible (Borderline and various regions; [14]) | False in general (■ $q=2$, non-SA [14]) | [14] |
| FK-random cluster (and continuous $q$ versions of all the above) | By definition | By definition | NA | [14] ($q\geqslant 1$) |
| Restricted $k$-step solid-on-solid | [14] | No results | No results | [14] |
| $XY$-type models (O(2), $\mathbb{Z}_{4n,\ldots}$) | [9] (implicit) [20,21] [14] (faithful) | [22]/[14] | ⊠ | [9] |
| O(3) | [9] (implicit) [20] | [23] | ⊠ | [9] |

■ ≡ complete characterization.
⊠ ≡ somewhat incomplete characterization.
Plausible ≡ incomplete derivations; result certainly true.
[14] is the present work.

are established. In other cases, such results are precluded by the presence of intermediate phases found in Ref. [24]. Finally, there are cases where only incomplete results are established: For various types of ordering, percolation in some boundary condition is necessary and percolation in a particular boundary condition is sufficient. (Although it has not yet been ruled out, we deem it unlikely that the two do not coincide.) Various cluster algorithms for all these models are designed. Some are straightforward and others are based on the ideas in Section 2. Continuum versions of some of these models, e.g. the Widom–Rowlinson models can be constructed by a straightforward

limiting procedure and here the algorithms are directly carried over. Thus, it is now possible to do a cluster-based simulations of a continuum liquid-vapor transition; see Ref. [25].

In Section 4, we investigate two-dimensional random surface models and the $XY$-model. In the former case, via equivalent (constrained) 2d spin systems, we develop graphical representations and cluster methods. We have no firm mathematical results that relate the phases of the random surface model to percolation in the associated representation; this issue is an ongoing concern. For the $XY$-model, we adapt Wolff's "Ising embedding algorithm" [9] to multi-cluster methods and investigate the underlying representation. It is demonstrated that the "onset of ordering" in the spin system is equivalent to the "onset of percolation" in the Wolff representation in the sense that the magnetic susceptibility diverges precisely when the average cluster size diverges.

Most of the derivations in this note will concern arbitrary finite graphs with no boundary. This allows us to cover most cases of interest, namely finite subsets of $\mathbb{Z}^d$ with free, periodic and various other significant boundary conditions. It may perhaps be easier for the reader to assume that the "bond-couplings" are uniform but this is by no means a requirement. In particular, the representations/algorithms apply to various non-uniform systems, e.g. systems with quenched randomness and/or with direction dependent coupling strengths; the required conditions on the couplings will be spelled out in each case.

## 2. Random cluster models

### 2.1. Potts models

The random cluster models, introduced in Ref. [2], are a family of graphical measures that, in the simplest cases, depend on two parameters $q$ and $p$. Let us consider a finite graph $\mathscr{G}$ with bonds $\mathbb{B}_{\mathscr{G}}$ and sites $\mathbb{S}_{\mathscr{G}}$. A bond configuration $\omega$ is a subset of $\mathbb{B}_{\mathscr{G}}$, i.e. a function $\omega_{\langle i,j\rangle}$ with value 1 if the bond $\langle i,j\rangle$ is "occupied" and 0 if this bond is "vacant". The set of all such configurations will be denoted by $\Omega_{\mathbb{B}_{\mathscr{G}}}$. In general, there are numbers $p_{i,j}$ associated with each bond (usually assumed to be the same for each bond). The random cluster measure assigns to each $\omega$ the probability proportional to the weight

$$W_{q,p}^{FK,\mathscr{G}}(\omega) = \prod_{\langle i,j\rangle\in\omega} p_{i,j} \prod_{\langle i,j\rangle\notin\omega} (1-p_{i,j}) q^{c(\omega)} \equiv B_p(\omega) q^{c(\omega)}, \tag{2.1}$$

where $p$ denotes the collection $(p_{i,j} \mid \langle i,j\rangle \in \mathbb{B}_{\mathscr{G}})$, $B_p(\omega)$ is shorthand for the "Bernoulli prefactor" and the quantity $c(\omega)$ is the number of connected components – including isolated sites – of the configuration $\omega$.

For integer $q$, the Swendsen–Wang algorithm uses, in an essential way, the connection between these problems and the spin systems they represent. For non-integer $q$, the *existence* of an underlying spin system is far from obvious and the design of cluster

algorithms in these cases has represented something of a challenge. For $q \geqslant 1$, we have the following:

*2.1.1. Random cluster algorithm*

*Step* 0. Let $\omega \subset \mathbb{B}_{\mathscr{G}}$ denote a configuration.

*Step* 1. For each of the components $C_j$, $j = 1, \ldots, c(\omega)$, independently deem the entire components to be "active" with probability $1/q$ and "inactive" otherwise.

*Step* 2. Remove all occupied bonds connecting active sites.

*Step* 3. Each bond joining a pair of active sites $i$ and $j$ is independently deemed to be occupied with probability $p_{i,j}$ or vacant with probability $1 - p_{i,j}$. The newly occupied bonds together with the bonds connecting inactive sites constitute the updated configuration; the active/inactive status is erased.

This cycle constitutes a single *Monte Carlo* step.

*Remark.* For integer $q$, the preceding is nearly identical to the usual SW algorithm. Indeed, for a Potts model, the above algorithm amounts to the following: Starting from a bond configuration, first generate a spin configuration in the usual fashion (by assigning one of $q$ spin states to each connected component). Then just one of these $q$ states is singled out and only the bonds touching this spin type are updated. The bond update, on this reduced graph takes place in the usual fashion (i.e. as in Step 3 above).

For the general $q$ algorithms, a direct proof of detailed balance, running through an entire cycle of the algorithm, is possible but tedious. Instead (here and in what is to follow) we will use the strategy of [4] and show that the algorithm satisfies detailed balance with respect to an appropriate Edwards–Sokal measure – in this case on configurations of active sites and occupied bonds. The bond marginal of this measure is the random cluster measure; for non-integer $q$, the active site marginal has no evident interpretation.

The algorithm may be divided into two stages: Step 1 creates active site configurations given a configuration of occupied bonds. This will be denoted as the "site move". Steps 2 and 3 create a new bond configuration given the inactive bonds and the active sites; let us call this the "bond move". The validity of the algorithm follows from the observation that the site move and the bond move each independently satisfy detailed balance with respect to the Edwards–Sokal measure. However, neither move by itself is ergodic because one or the other marginal remains frozen. Nevertheless, it is easy to see that by carrying out both moves any allowed configuration of occupied bonds and active sites may be transformed into any other allowed configuration in a single cycle. (Ergodicity is almost always straightforward and in the future will only be mentioned on occasion.)

*Proof of detailed balance.* Consider a configuration of active sites $\eta$ and occupied bonds $\omega$ with $\omega \subset \mathbb{B}_{\mathscr{G}}$ and $\eta \subset \mathbb{S}_{\mathscr{G}}$. (Such configurations are present after Step 1 of the Random cluster algorithm.) Let $f(\eta, \omega)$ denote the number of *inactive*

clusters, i.e. the quantity $f(\eta,\omega)$ is the number of components on the graph that consists of all the inactive bonds and sites. Let us write the Edwards–Sokal weights:

$$Y^{\mathcal{G}}_{q,p}(\eta,\omega) = B_p(\omega)[q-1]^{f(\eta,\omega)}\Delta(\eta,\omega)$$
$$= W^{FK,\mathcal{G}}_{q,p}(\omega)\left[\frac{1}{q}\right]^{c(\omega)-f(\eta,\omega)}\left[\frac{q-1}{q}\right]^{f(\eta,\omega)}\Delta(\eta,\omega)\,, \tag{2.2}$$

where $\Delta(\eta,\omega)$ is zero if any occupied bond connects an active site with an inactive (i.e. not active) site and is one otherwise. The bond marginal of the measure corresponding to these weights is easily calculated: According to the constraint, each component of $\omega$ must be completely active or inactive. The coefficient of $[W^{FK,\mathcal{G}}_{q,p}]\times[\Delta]$ is just the distribution for the process that independently labels each component active, with probability $1/q$ or inactive, with probability $1-1/q$. This sums to one.

A proof that the above algorithm samples the measure corresponding to the weights $Y^{\mathcal{G}}_{q,p}(\eta,\omega)$ follows easily: Step 1 is seen to be an independent sampling of an $\eta$ from the fixed $\omega$ conditional distribution. Note that in Steps 2 and 3, the destruction of old bonds and the placement of new bonds between active sites does not effect the number of *inactive* clusters. Suppose then that $\omega\to\omega'$ under Steps 2 and 3. Let us write $\omega=(\omega_a,\omega_i)$ and similarly for $\omega'$ where $\omega_a$ are the active bonds and $\omega_i$ the inactive bonds. Let $\mathcal{G}(\eta)\subset\mathcal{G}$ denote the graph with sites $\eta$ and those bonds of $\mathcal{G}$ with both endpoints in $\eta$. Then the transition probability is simply the Bernoulli factor relative to $\mathcal{G}(\eta)$ which we denote by $B^{\mathcal{G}(\eta)}_p(\omega'_a)$. However $Y^{\mathcal{G}}_{q,p}(\eta,\omega')=B^{\mathcal{G}(\eta)}_p(\omega'_a)B^{\mathcal{G}\setminus\mathcal{G}(\eta)}_p(\omega'_i)(q-1)^{f(\eta,\omega')}$. Since $\omega_i=\omega'_i$ we have $f(\eta,\omega)=f(\eta,\omega')$; the ratio of the transition rates between these two configurations is manifestly the ratio of the probabilities of these configurations. Detailed balance is established. □

*Remark.* Simulations using this algorithm (in conjunction with the invaded cluster method) are currently under way. Results in two and three dimensions are consistent with or improve upon the best known values for the critical $q$ beyond which the transition is first-order. Details will appear in Ref. [26]. We also remark that a device not dissimilar to the "bond-active site" configurations was used in Ref. [27] for the analysis of random cluster models on the complete graph.

If $q\geqslant 2$, the algorithm can be modified by introducing several species of active particles. Let $m$ denote a positive integer, $m\leqslant q$. Starting from a bond configuration $\omega$, each component of $\omega$ is independently assigned to be in one of $m$ "active" states each with probability $1/q$ or, failing all of these chances, left inactive with probability $(1-m/q)$. The bonds on active clusters are erased and new bonds independently placed, with density $p$, subject to the constraint that they only connect active sites that are of the same species. The graphical problem and the Edwards–Sokal weights for this process are defined as follows: Let $\boldsymbol{\eta}=(\eta_1,\ldots,\eta_m)$ be an $m$-species occupation configuration with $\eta_i\cap\eta_j=\emptyset$ for $i\neq j$. Let $\Delta(\boldsymbol{\eta},\omega)$ be the relevant constraint function:

$\Delta(\boldsymbol{\eta},\omega)=1$ if the bonds of $\omega$ only connect inactive sites or active sites of the same species and zero otherwise. Let $f(\boldsymbol{\eta},\omega)$ denote the number of inactive components. The weights are

$$Y^{\mathcal{G}}_{q,p;m}(\boldsymbol{\eta},\omega)=B_p(\omega)[q-m]^{f(\boldsymbol{\eta},\omega)}\Delta(\boldsymbol{\eta},\omega)$$

$$=W^{FK,\mathcal{G}}_{q,p}(\omega)\left[\frac{1}{q}\right]^{c(\omega)-f(\boldsymbol{\eta},\omega)}\left[\frac{q-m}{q}\right]^{f(\boldsymbol{\eta},\omega)}\Delta(\boldsymbol{\eta},\omega)\,. \tag{2.3}$$

A proof of detailed balance for this algorithm follows the same steps as the case $m=1$. If $m>1$, it is plausible that this modification will speed up the algorithm since it is not dissimilar to performing $m$ steps of the $m=1$ algorithm in a single step.

It is clear that these algorithms can be extended to cover more general FK random cluster models, e.g. extended models featuring higher order geometric objects: triangles, plaquettes, etc. These extended models have been discussed in Ref. [28] and in various other places in the literature, e.g. Ref. [29] and more recently Ref. [30]. The general problem is defined as follows: Let $\mathcal{F}$ denote a *generalized graph* consisting of sites, bonds (certain pairs of sites), triangles (certain triplets of sites), etc. We will denote by $\mathbb{S}_{\mathcal{F}}$ the site set and by $\mathbb{E}_{\mathcal{F}}$ the collection of all the higher objects. (In what follows, it of course is assumed that $|\mathbb{S}_{\mathcal{F}}|$ is finite.) If $\omega\subset\mathbb{E}_{\mathcal{F}}$, the notion of "connected in $\omega$" is defined in the obvious fashion. Explicitly, an object tying together $k$ sites may be formally regarded as $k(k-1)/2$ separate bonds between all pairs of sites and the configuration $\omega$ as the union of all these bonds. Connectivity is then defined as in the standard fashion for bond graphs. For each $A\in\mathbb{E}_{\mathcal{F}}$, there is a $p_A\in(0,1)$. Let $\mathbf{p}$ denote the family of these $p$'s: $\mathbf{p}=(p_A\,|\,A\in\mathbb{E}_{\mathcal{F}})$ and let $B_{\mathbf{p}}(\omega)$ denote the Bernoulli factor

$$B_{\mathbf{p}}(\omega)=\prod_{A\in\omega}p_A\prod_{B\notin\omega}(1-p_B)\,. \tag{2.4}$$

For any positive real $q$, the random cluster weights are given by

$$W^{FK,\mathcal{F}}_{q,\mathbf{p}}(\omega)=B_{\mathbf{p}}(\omega)q^{c(\omega)}\,. \tag{2.5}$$

If $q$ is an integer greater than one, it is easily shown that this is the graphical representation of a $q$-state Potts system on $\mathbb{S}_{\mathcal{F}}$: Let $\sigma_i\in\{1,\ldots,q\}$ denote Potts spin variables for $i\in\mathbb{S}_{\mathcal{F}}$ and consider the Hamiltonian $\mathcal{H}=-\sum_{A\in\mathbb{E}_{\mathcal{F}}}J_A\delta\sigma_A$ where $\delta\sigma_A=1$ if all the spins in $A$ are in the same state and is zero otherwise. Then if $\beta$ is the inverse temperature and $J_A$ and $p_A$ are related by $p_A=1-e^{-\beta J_A}$, a straightforward recapitulation of the usual derivation of the FK representation yields the weights in Eq. (2.5).

The algorithm for these systems is the obvious generalization of the above algorithm: Step 1 is the same using the appropriate notion of connectivity and replacing the word *bonds* with *connecting objects*. Steps 2 are similar but here with the harsher restriction that the new elements are constrained to provide connections *exclusively* between active sites. (E.g. for a triangle to be placed, all three sites must be active.) A proof of detailed balance for this algorithm follows the same lines as the basic case.

In the remainder of this paper, for both Potts and other models, similar generalizations are often possible. It will be clear from context which generalizations are possible (and which ones are not). Hereafter these will not be mentioned explicitly and generalizations of the algorithms and other results will be left an ongoing exercise for the reader.

### 2.2. Cubic models

Another class of spin system that gives rise to successful FK-type graphical representations is the Ashkin–Teller (AT) model and the generalization known as the cubic model. These models are discussed at length in Ref. [1] so here we will be succinct. Let $\mathcal{G}$ denote a graph. For the AT model, at each $i \in \mathbb{S}_{\mathcal{G}}$ there are four spin states: $\sigma_i \in \{-1, 0, +1, 2\}$. On the bonds $\langle i, j\rangle \in \mathbb{B}_{\mathcal{G}}$ the interaction energies satisfy $\mathscr{E}_{i,j}(\sigma_i, \sigma_j) = \mathscr{E}_{i,j}(\sigma_i + \alpha, \sigma_j + \alpha)$-addition mod 4. Two cases have been distinguished in Ref. [1]:

$$\text{Reformed ferromagnet: } \mathscr{E}_{i,j}(0,0) < \mathscr{E}_{i,j}(0,2) \leqslant \mathscr{E}_{i,j}(0,\pm 1) \quad \text{for all } i,j\,,$$

$$\text{Orthodox ferromagnet: } \mathscr{E}_{i,j}(0,0) < \mathscr{E}_{i,j}(0,\pm 1) \leqslant \mathscr{E}_{i,j}(0,2) \quad \text{for all } i,j\,.$$

The coinciding case is, of course, the four-state Potts model. In both regimes, there are successful representations analogous to the random cluster representation of the Potts model.

In the orthodox case, one considers two copies of $\mathcal{G}$ (i.e. two coupled spin systems) denoted by $\mathcal{G}_\tau$ and $\mathcal{G}_\kappa$. A bond configuration, $\omega$, has three types of bonds: Bonds in $\mathcal{G}_\kappa$, denoted by $\kappa$-bonds, bonds in $\mathcal{G}_\tau$, denoted by $\tau$-bonds and a third type that has the same effect as the simultaneous occurrence of a $\tau$-bond and a $\kappa$-bond which are denoted by $\tau\kappa$-bonds. Thus, the configuration is represented as a triple: $\omega = (\omega_\tau, \omega_\kappa, \omega_{\tau\kappa})$. Connectivity in $\mathcal{G}_\tau$ is defined via the bonds in $\omega_\tau$ or $\omega_{\tau\kappa}$ (i.e. in $\omega_\tau \vee \omega_{\tau\kappa}$) and similarly in $\mathcal{G}_\kappa$. The number of connected components, by these definitions, are denoted by $c_\tau(\omega)$ and $c_\kappa(\omega)$ respectively. The AT random cluster weights for the orthodox ($\mathfrak{o}$) region are given by

$$W^{AT;\mathfrak{o},\mathcal{G}}_{(2,2),P} = B_P(\omega) 2^{c_\tau(\omega)} 2^{c_\kappa(\omega)}\,, \tag{2.6}$$

where $P = (p_\tau, p_\kappa, p_{\tau\kappa})$ is determined from the temperature and the energy differences (cf. Ref. [1], Eqs. (III.18)–(III.20)) and $B_P(\omega) = B_{p_\tau}(\omega_\tau) B_{p_\kappa}(\omega_\kappa) B_{p_{\tau\kappa}}(\omega_{\tau\kappa})$ is the product of Bernoulli factors each of which is as described in Eq. (2.1). The generalization of this representation to the cubic models (in their orthodox regime, for the appropriate temperature and energy differences) is achieved by replacing the two corresponding to the $\tau$-layer by an $s$ and the two corresponding to the $\sigma$-layer by an $r$. A graphical model is now be defined for any positive real values of $r$ and $s$; the weights will be denoted by $W^{AT;\mathfrak{o},\mathcal{G}}_{Q,P}$ with $Q \equiv (s, r)$. Such representations have also been described in Refs. [17,18].

An algorithm for the cases $s \geqslant 1$, $r \geqslant 1$ can be designed along the same lines as the one for the random cluster model:

*2.2.1. Cubic model algorithm: Orthodox region*

*Step* 0. Let $\omega = (\omega_\tau, \omega_\kappa, \omega_{\tau\kappa})$ as described.

*Step* 1. Each connected component in the $\tau$-layer is independently deemed to be active with probability $1/s$ or inactive with probability $1 - 1/s$. Similarly, for the $\kappa$-layer with $s$ replaced by $r$.

*Step* 2. All $\kappa$ bonds connecting pairs of active sites are removed and all $\tau$ bonds connecting pairs of active sites are removed. The $\tau\kappa$-bonds are removed only if all four participating sites are active.

*Step* 3. The various bonds are placed in their appropriate slots subject to the constraint that all the participating sites are active. In particular, the viable candidates for the double bonds must have all of the four relevant sites in the active state. The active/inactive status is then erased and a Monte Carlo step has been completed.

*Proof of detailed balance.* The proof scheme is nearly identical to the one used in the ordinary random cluster algorithm. Let $\eta = (\eta_\tau, \eta_\kappa)$ denote configurations of active sites in the $\tau$-layer and $\kappa$-layer, respectively. Let $\Delta(\eta, \omega)$ denote the relevant constraint function which vanishes if any bond connects an active to an inactive site and is one otherwise. (Note that $\Delta$ does *not* vanish if, e.g. a $\tau\kappa$-bond connects two active sites in the $\tau$-layer and two inactive sites in the $\kappa$-layer.) The algorithm evidently satisfies detailed balance for the Edwards–Sokal measure with weights

$$K^{\mathfrak{v};\mathscr{G}}_{Q,P}(\eta, \omega) = B_P(\omega)[s-1]^{f_\tau(\eta_\tau, \omega_\tau, \omega_{\tau\kappa})}[r-1]^{f_\kappa(\eta_\kappa, \omega_\kappa, \omega_{\tau\kappa})}, \tag{2.7}$$

where $f_\tau$ is the number of inactive components in the $\tau$-layer calculated according to the site configuration $\eta_\tau$ and the bond configuration $\omega_\tau \vee \omega_{\tau\kappa}$ and similarly for $f_\kappa$. The right-hand side of Eq. (2.7) may be expressed as in the second part of Eq. (2.2), i.e. $W^{AT;\mathfrak{v},\mathscr{G}}_{Q,P}$ times the constraint function times a factor with the interpretation of two Bernoulli sampling probabilities for independent assignments of active/inactive status to the components in the $\tau$ and $\kappa$ layers. This demonstrates that the bond marginal of the measure defined by the weights in Eq. (2.7) is correct and that detailed balance holds for the site moves. Taking into consideration which bond moves have been allowed and which are forbidden it is seen that the quantities $f_\tau$ and $f_\kappa$ remain constant. Thus, the proof of detailed balance for the bond moves is established as in the usual random cluster case. □

In the reformed region, the graphical representation is confined to a single graph but there are two colors of bonds, black and white. The black bonds may be envisioned as sitting on top of the some of the white ones. Bonds that are one or the other are called "grey". Thus we have $\omega \subset \mathbb{B}_\mathscr{G}$, the grey bonds, $\vartheta \subset \omega$, the black bonds and $\omega \backslash \vartheta$ are the whites. Let $\chi_{\vartheta \subset \omega}$ denote the function that is one if this constraint is satisfied

and zero otherwise. Then the graphical measure for the AT model in reformed region is defined by the weights

$$W^{AT;\mathrm{r},\mathscr{G}}_{(2,2),P}(\omega,\vartheta)=\left[\prod_{\langle i,j\rangle\in\omega}U_{i,j}\prod_{\langle i,j\rangle\in\vartheta}V_{i,j}\right]2^{c(\omega)}2^{c(\vartheta)}\chi_{\vartheta\subset\omega} \tag{2.8}$$

with $P$ representing the parameters $(U_{i,j})$ and $(V_{i,j})$ which in turn are determined from the parameters in the spin system (cf. Ref. [1], the equations in the statement of Proposition III.1). For the cubic generalization of this model, $2^{c(\omega)}$ is replaced by $r^{c(\omega)}$ and $2^{c(\vartheta)}$ is replaced by $s^{c(\vartheta)}$. Defining $Q=(r,s)$, the corresponding weights are denoted by $W^{AT;\mathrm{r},\mathscr{G}}_{Q,P}$. For convenience, let us define $u_{i,j}$ and $y_{i,j}$ by $U_{i,j}=u_{i,j}/(1-u_{i,j})$ and $U_{i,j}V_{i,j}=y_{i,j}/(1-y_{i,j})$. If $r\geqslant 1$ and $s\geqslant 1$, we have:

*2.2.2. Cubic model algorithm: Reformed region*

*Step* 0. Let $(\omega,\vartheta)$ denote a black and white configuration as described.

*Step* 1. Each grey component (component of $\omega$) is independently deemed to be inactive with probability $(1-1/r)$ or *partially activated* with probability $1/r$. The partially activated sites may be envisioned as grey sites. The restriction of $\vartheta$ to the clusters of partially active sites defines black connected components. Each such connected component is assigned the fully active status with probability $1/s$ or it remains partially active with probability $1-1/s$.

*Step* 2. Remove all bonds connecting active sites. Leave intact all bonds (and their colors) connecting the inactive sites.

*Step* 3. Independently, each neighboring pair $i,j$ of fully active (black) sites is joined by a black bond with probability $y_{i,j}$ or left unjoined with probability $1-y_{i,j}$. Next, all unjoined neighboring pairs of active sites $i$ and $j$ (including the black pairs that failed to get a black bond) are joined by a white bond with probability $u_{i,j}$ or left unjoined with probability $1-u_{i,j}$. The active status of all sites is now erased and a full Monte Carlo step has been completed.

*Proof of detailed balance.* Consider configurations of the full model simulated: black and white bonds as well as black and white site occupation variables. Let $\eta\subset\mathbb{S}_{\mathscr{G}}$ and $\varsigma\prec\eta$ denote the partially active and fully active sites – or grey and black sites. The whites sites are just the sites $\eta\backslash\varsigma$. Let $(\omega,\vartheta)$ denote the bond configurations and $D(\eta,\varsigma,\omega,\vartheta)$ the constraint function that vanishes unless (i) no bonds connect active sites (partially or fully) to inactive sites, (ii) all black bonds connect only pairs of black sites, and (iii) $\omega\succ\vartheta$ and $\eta\succ\varsigma$; when all these are satisfied, $D=1$. The Edwards–Sokal weights are given by

$$K^{\mathrm{r};\mathscr{G}}_{Q,P}(\eta,\varsigma,\omega,\vartheta)=\left[\prod_{\langle i,j\rangle\in\omega}U_{i,j}\prod_{\langle i,j\rangle\in\vartheta}V_{i,j}\right](r-1)^{f(\eta,\omega)}(s-1)^{f(\varsigma,\vartheta)}D(\eta,\varsigma,\omega,\vartheta)\,, \tag{2.9}$$

where $k(\eta,\omega)$ and $k(\varsigma,\vartheta)$ have the same meanings as in the ordinary random cluster algorithm. After pulling out the weight $W_{Q,P}^{AT;\mathfrak{r},\mathscr{G}}(\omega,\vartheta)$ the site moves are exhibited as an independent sample of the conditional distribution and the bond marginal is seen to be correct. As for the bond moves, the cluster factors are all in order for the same reasons as in the previous algorithms, let us check that the bond weight factors are indeed correct. Suppose that $(\eta,\varsigma,\omega,\vartheta)$ and $(\eta,\varsigma,\omega',\vartheta')$ are two configurations on which $D$ does not vanish and whose bond configurations are identical for all bonds joining sites in $\mathbb{S}_{\mathscr{G}}\backslash\eta$. Let $\mathbb{B}_\eta$ denote the set of bonds in $\mathscr{G}$ with both endpoints in $\eta$ and similarly for $\mathbb{B}_\vartheta$. Let $\omega_\eta=\omega\cap\mathbb{B}_\eta$ and similarly $\vartheta_\varsigma$, etc. To compute the transition probability from $(\eta,\varsigma,\omega',\vartheta')$ to $(\eta,\varsigma,\omega,\vartheta)$ it is seen that the desired black move occurs with probability $y^{N(\vartheta_\varsigma)}(1-y)^{|\mathbb{B}_\varsigma|-N(\vartheta_\varsigma)}$. Then, the necessary white move happens with probability $u^{N(\omega_\eta)-N(\vartheta_\varsigma)}(1-u)^{|\mathbb{B}_\eta|-(N(\omega_\eta)-N(\vartheta_\varsigma))}$. Thus, overall, the transition probability is

$$\prod_{\langle i,j\rangle\in\omega_\eta}\left[\frac{u_{i,j}}{1-u_{i,j}}\right]\prod_{\langle i,j\rangle\in\vartheta_\varsigma}\left[\frac{y_{i,j}}{u_{i,j}}\frac{1-u_{i,j}}{1-y_{i,j}}\right]$$

$$\times\prod_{\langle i,j\rangle\in\mathbb{B}_\eta}(1-u_{i,j})\prod_{\langle i,j\rangle\in\mathbb{B}_\varsigma}(1-y_{i,j})\propto\left[\prod_{\langle i,j\rangle\in\omega}U_{i,j}\prod_{\langle i,j\rangle\in\vartheta}V_{i,j}\right] \tag{2.10}$$

with the constant of proportionality the same for the reverse transition probability. Detailed balance is established. □

## 3. Lattice gases

### 3.1. Formalism

We begin with some notation. For lattice gases, the state space at a single site $i$ consists of an occupation variable – $n_i=0$ or 1 – and, given that $n_i=1$, a variable $\sigma_i$. Here we will focus on the discrete case so $\sigma_i\in\{1,\dots,q\}$. The model may be viewed as an annealed-dilute spin-system (which is generally considered to be somewhat unphysical) or a multi-component lattice gas. In the former case, the variable $\sigma_i$ is interpreted as an internal state and in the latter as a label for the species. Finally, there may be a physical motivation for regarding the model as consisting of a mixture of a $q$-state particle ($n_i=1$) and a single state particle ($n_i=0$). For $q=2$ (written $\sigma_i\in\{+1,-1\}$) these are the BEG models [31] and from this perspective, the entire section concerns generalized BEG models. Notwithstanding, all of these models are mathematically equivalent; much of our terminology will be couched in the language of dilute spin systems.

Consider, then, a graph $\mathscr{G}$ with site variables $n_i$ for each $i\in\mathbb{S}_{\mathscr{G}}$ and spin variables $\sigma_i$ for all $i$ such that $n_i=1$. Let $H$ denote a Hamiltonian for the spin system alone

$$H=\sum_{\langle i,j\rangle\in\mathbb{B}_{\mathscr{G}}}\mathscr{E}_{i,j}(\sigma_i,\sigma_j)\,. \tag{3.1}$$

The corresponding lattice gas is defined by the Hamiltonian

$$\mathscr{H} = \sum_{\langle i,j\rangle \in \mathbb{B}_{\mathscr{G}}} n_i n_j \mathscr{E}_{i,j}(\sigma_i, \sigma_j) - \sum_{\langle i,j\rangle \in \mathbb{B}_{\mathscr{G}}} \lambda_{i,j} n_i n_j - \sum_{i \in \mathbb{S}_{\mathscr{G}}} \mu_i n_i \,, \tag{3.2}$$

where it has been assumed that $\mathscr{E}_{i,j}(\sigma_i, \sigma_j)$ is non-positive and vanishes at its maximum. (Thus, e.g. for the uniform Potts case, $\mathscr{E}_{i,j}(\sigma_i, \sigma_j) = -\delta_{\sigma_i, \sigma_j}$.) The partition function is given by

$$\mathscr{Z}_{\mathscr{H},\beta} = \sum_{\substack{n_i = \pm 1 \\ i \in \mathbb{S}_{\mathscr{G}}}} \sum_{\sigma_i : n_i = 1} e^{-\beta \mathscr{H}} \prod_{i : n_i = 1} v_i(\sigma_i) \,, \tag{3.3}$$

where $v_i(\sigma_i)$ are the a priori weights. Regardless of the model, we will adapt the convention that these weights sum to $q$: $\sum_{\sigma_i} v_i(\sigma_i) = q$. This serves to define the Gibbs measure on the space of particle/spin configurations. It is remarked that the "trace" in Eq. (3.3) may also be defined by summing over $q$ states at all sites and shifting the value of $\mu$. However, the more physical interpretation exemplified by the convention in Eq. (3.3) is that "spins" on the vacant sites are not present. In any case, for a fixed set of occupied sites, the distribution of the spin variables on the complementary sites is simple product measure.

Systems described by Eqs. (3.2), (3.3), fall into two classes depending on the sign of $\lambda_{i,j}$. For $\lambda_{i,j} \geqslant 0$, which we call super attractive (SA), many results from the corresponding uniform systems can be directly transcribed. In particular, the line $\lambda_{i,j} = 0$ gives rise to complete characterization theorems when such results hold in the undiluted system. If $\lambda_{i,j} < 0$, our results are far less general so, to be concise, we will focus our attention exclusively on the Potts cases. However, this region (even for the Potts models) is known to exhibit some unusual phases [24] and also contains the point of departure for the construction of various continuum models. Also, somewhat surprisingly, certain comparison inequalities (e.g. with bond-site percolation) can be derived here which, to date, we have been unable to produce in the SA region. We will therefore devote separate subsections to the SA region and to the dilute Potts model in the region $\lambda_{i,j} < 0$. In a third subsection we will describe continuum limits and in a forth subsection, we will present a unified treatment of the cluster algorithms for all of these models.

### 3.2. The SA region

Consider a non-diluted system with Hamiltonian $H$ and let $W^{\mathscr{G}}_{H,\beta}(\omega)$ denote the weights of the so-called grey representation defined for configurations $\omega \in \Omega_{\mathbb{B}_{\mathscr{G}}}$:

$$W^{\mathscr{G}}_{H,\beta}(\omega) = \sum_{\sigma_i : i \in \mathbb{S}_{\mathscr{G}}} \prod_{\langle i,j\rangle \in \omega} R_{i,j}(\sigma_i, \sigma_j) \tag{3.4}$$

with $R_{i,j}(\sigma_i, \sigma_j) = e^{-\beta \mathscr{E}_{i,j}(\sigma_i, \sigma_j)} - 1$ (cf. [1] (Section II)) and $\Omega_{\mathbb{B}_{\mathscr{G}}}$ is the set of all bond configurations on $\mathbb{B}_{\mathscr{G}}$. Our first result shows that if the grey measure has desirable

monotonicity properties, then, in the SA region, these are inherited in the site-diluted version of the problem.

*Lemma* 3.1. Consider a lattice gas of the type described in Eqs. (3.1)–(3.3) with $\lambda_{i,j} \geqslant 0$ and with the convention that $\mathscr{E}_{i,j}(\sigma_i, \sigma_j)$ is non-positive. Suppose that the graphical representation for the grey measure defined by the weights in Eq. (3.4) is strong FKG. Let $\Omega_{\mathbb{S}_\mathscr{G}}$ and $\Omega_{\mathbb{B}_\mathscr{G}}$ denote, respectively, the set of all site configurations and bond configurations on $\mathscr{G}$. Then there is a probability measure defined on configurations $(n, \theta, \omega) \in \Omega_{\mathbb{S}_\mathscr{G}} \times \Omega_{\mathbb{B}_\mathscr{G}} \times \Omega_{\mathbb{B}_\mathscr{G}}$ that is a faithful representation of this system and is strong FKG with respect to the natural partial order.

*Proof.* First let us write

$$e^{\beta \mu_i n_i} = z_i n_i + (1 - n_i)\,, \tag{3.5a}$$

$z_i = e^{\beta \mu_i}$. Next, using the fact that $\lambda_{i,j} \geqslant 0$ and $-\mathscr{E}_{i,j}(\sigma_i, \sigma_j) \geqslant 0$, we may expand

$$e^{\beta \lambda_{i,j} n_i n_j} = (e^{\beta \lambda_{i,j}} - 1) n_i n_j + 1\,, \tag{3.5b}$$

$$e^{\beta \mathscr{E}_{i,j}(\sigma_i, \sigma_j) n_i n_j} = R_{i,j}(\sigma_i, \sigma_j) n_i n_j + 1 \tag{3.5c}$$

with all the above written quantities non-negative. Expanding $e^{-\beta \mathscr{H}}$ in this function, multiplying out the three products and collecting all terms, each such term is seen to be in a one-to-one correspondence with a configuration on $\Omega_{\mathbb{S}_\mathscr{G}} \times \Omega_{\mathbb{B}_\mathscr{G}} \times \Omega_{\mathbb{B}_\mathscr{G}}$. Such a term, which is a non-negative function of the particle/spin configuration will be denoted by $(n, \omega, \theta)$ and its weight is defined as the trace of this function. Explicitly, for the bond $\langle i, j \rangle$, the quantity $\theta_{\langle i,j \rangle}$ is one if $(e^{\beta \lambda_{i,j}} - 1) n_i n_j$ appears in the term, etc. The particle configuration is its own representation. Indeed if the $n_i$ appears in the term, the term vanishes unless $n_i = 1$ and if $1 - n_i$ appears, the term vanishes unless $n_i = 0$. Hence, these variables are not distinguished notationally. The $\omega$-bonds will sometimes be referred to as grey bonds and, for reasons that will become clear when we introduce the cluster algorithms, the $\theta$-bonds will be referred to as anchor bonds (with apologies to Ref. [32]).

It is observed that in this expansion, there will be constraints between the site and bond configurations: For any bond $\langle i, j \rangle$, regardless of the values of $n_i$ and $n_j$, it is always permitted to select the "vacant bond" terms (i.e. the 1's) in the $\omega$ or $\theta$ expansion. However, if an "occupied" term is selected, e.g. $(e^{\beta \lambda} - 1) n_i n_j$, the weight of the entire configuration will vanish unless $n_i = n_j = 1$. Thus, all the bond configurations – both the $\omega$'s and the $\theta$'s – must satisfy the rule that each occupied bond connects two occupied sites. Let $X(n, -)$ denote the indicator of this constraint, e.g.

$$X(n, \omega) = \begin{cases} 1 & \text{if both endpoints of each occupied} \\ & \text{bond in } \omega \text{ are occupied sites in } n\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{3.6}$$

The weights for the graphical configuration are given by

$$Y^{\mathscr{G}}_{\mathscr{H},\beta} = W^{\mathscr{G}(n)}_{H,\beta}(\omega) \prod_{\langle i,j\rangle\in\theta} L_{i,j} \prod_i z_i^{n_i} X(n,\omega)X(n,\theta)\,, \tag{3.7}$$

where $L_{i,j} = e^{\beta\lambda_{i,j}} - 1$ and where we recall that $\mathscr{G}(n)$ is defined as the subgraph of $\mathscr{G}$ consisting of the sites in $n$ and the bonds that connect them. However, it is noted that $W^{\mathscr{G}(n)}_{H,\beta}(\omega)$ differs from $W^{\mathscr{G}}_{H,\beta}(\omega)$ only in the fact that with the present convention, the vacant sites do not contribute their weight in the sum over the spin configurations. Thus, let us rewrite Eq. (3.7) using $W^{\mathscr{G}(n)}_{H,\beta}(\omega) = W^{\mathscr{G}}_{H,\beta}(\omega) q^{-(|\mathbb{S}_{\mathscr{G}}|-N(n))}$ where $N(n) = \sum_i n_i$ is the total number of particles in the configuration. Then

$$Y^{\mathscr{G}}_{\mathscr{H},\beta} \propto W^{\mathscr{G}}_{H,\beta}(\omega) \prod_{\langle i,j\rangle\in\theta} L_{i,j} \prod_i [qz_i]^{n_i} X(n,\omega)X(n,\theta)\,. \tag{3.8}$$

A proof of the strong FKG follows almost immediately from the hypotheses. First, by definition, the min or max of a configuration is found by taking the min of max of each separate component: $(n^1,\omega^1,\theta^1)\vee(n^2,\omega^2,\theta^2) = (n^1\vee n^2, \omega^1\vee\omega^2, \theta^1\vee\theta^2)$ and similarly for the min. Second, it is seen that if $(n^1,\omega^1,\theta^1)$ and $(n^2,\omega^2,\theta^2)$ satisfy all of the $X$ constraints, $X(n^1,\omega^1) = \cdots = X(n^2,\theta^2) = 1$, then so do the min and max configurations, $X(n^1\vee n^2,\omega^1\vee\omega^2) = \cdots = X(n^1\wedge n^2,\theta^1\wedge\theta^2) = 1$. Thus, let $(n^1,\omega^1,\theta^1)$ and $(n^2,\omega^2,\theta^2)$ denote any two configurations with non-vanishing weights. Then

$$\frac{Y^{\mathscr{G}}_{\mathscr{H},\beta}((n^1,\omega^1,\theta^1)\vee(n^2,\omega^2,\theta^2)) Y^{\mathscr{G}}_{\mathscr{H},\beta}((n^1,\omega^1,\theta^1)\wedge(n^2,\omega^2,\theta^2))}{Y^{\mathscr{G}}_{\mathscr{H},\beta}(n^1,\omega^1,\theta^1) Y^{\mathscr{G}}_{\mathscr{H},\beta}(n^2,\omega^2,\theta^2)}$$

$$= \frac{W^{\mathscr{G}}_{H,\beta}(\omega^1\vee\omega^2) W^{\mathscr{G}}_{H,\beta}(\omega^1\wedge\omega^2)}{W^{\mathscr{G}}_{H,\beta}(\omega^1) W^{\mathscr{G}}_{H,\beta}(\omega^2)} \geqslant 0\,. \qquad \square \tag{3.9}$$

As is often the case, monotonicity can be translated into definitive statements about the unicity of Gibbs states. Here, as in previous cases, these questions can be tied to percolation in the graphical representation.

Let us recall the usual working definition of percolation. For simplicity, we will restrict attention to nearest-neighbor interactions on $\mathbb{Z}^d$ but the following is *not* restricted to graphical representations with the FKG property. Let $\Lambda\subset\mathbb{Z}^d$ be a finite set and $\partial\Lambda = \{i\in\mathbb{Z}^d\backslash\Lambda \mid \text{dist.}(i,\Lambda) = 1\}$. The relevant graph consists of the sites of $\Lambda\cup\partial\Lambda$ and the bonds connecting the neighboring pairs of these sites. Boundary conditions in the spin system are defined in the usual fashion; fixing $n_i$ and, if relevant, fixing $\sigma_i$ at each $i\in\partial\Lambda$. The graphical representations in the presence of boundary conditions lead to weights with measures similar to those defined so far but with constraints (e.g. forbidding any configuration that connects certain portions of the boundary). The details of these modifications are unimportant, it is sufficient to know that in principle, the representation exists. Even in cases where monotonicity properties hold on a general graph (in the absence of boundary conditions) most of the above boundary conditions will *not* lead to FKG measures. However, some do, in particular the free boundary

conditions, $n_i \equiv 0$, $i \in \partial\Lambda$, because this is equivalent to "no boundary conditions" on the graph (whose sites are) $\Lambda$. Percolation is defined as follows: Let $\Lambda_k$ denote a sequence of shapes $\Lambda_{k+1} \supset \Lambda_k$ with $\Lambda_k \nearrow \mathbb{Z}^d$. Let $P_k^{\omega}(\beta)$ denote the probability that the origin is connected to $\partial\Lambda_k$ by occupied $\omega$-bonds using the boundary condition that optimizes this probability. Percolation of the $\omega$-type is said to occur if

$$0 < \lim_{k\to\infty} P_k^{\omega}(\beta) \equiv P_{\infty}^{\omega}(\beta)\,. \tag{3.10}$$

(It is not hard to show the existence of this limit.) For the Potts and cubic model, putting a particle at each boundary site and setting the spins on these sites to the same state corresponds to the maximal FKG state for these systems: The wired and black-wired states respectively. However, back in the spin system, these are just the boundary conditions that one would use to induce the magnetized state (cf. [1] (Theorems III.3 and III.7)). This extra information allows for more complete results in the lattice gas versions of these cases.

For a configuration $(n, \omega, \theta)$, let $\mathbb{W}$ denote the bonds of $\omega \vee \theta$ and define $P_k^{\mathbb{W}}(\beta)$, and $\mathbb{W}$-type percolation in the same way. (Ostensibly, this could require a different sequence of boundary conditions.) We now establish:

*Theorem* 3.2. (i) Consider a system of the type described by the Hamiltonian in Eq. (3.1) endowed with a group structure: That is, the $\sigma_i$ are elements of a group: $v(\sigma_i) \equiv 1$ and $\mathscr{E}(\sigma_i, \sigma_j) = \varphi(\sigma_i^{-1}\sigma_j)$ with $\varphi(a) = \varphi(a^{-1})$. Then if $P_{\infty}^{\omega}(\beta)$ vanishes, all Gibbs states are invariant under the action of the group. In particular, in the spin language, the spontaneous magnetization is zero. (ii) In the monotone cases, as described in the statement of Lemma 3.1, a sufficient condition for the unicity of Gibbs states is $P_{\infty}^{\mathbb{W}}(\beta) = 0$. For the Potts models and for the cubic models in the reformed region, if $\lambda = 0$, (which implies $\mathbb{W} = \omega$) then $\omega$-type percolation is necessary and sufficient for the existence of multiple limiting Gibbs states.

*Proof* (*Sketch*). We will be content with an outline of the argument since the principle ideas have appeared in Refs. [1,11].

In cases where there is an underlying group symmetry for the spin system, the graphical problem is not effected if the value of all the spins on the boundary are shifted by the same group element. Thus, in those configurations where the support of the observable is disconnected from the boundary, the average of any local observable is invariant under the action of the group. Such disconnections occur with probability tending to one as $\Lambda \nearrow \mathbb{Z}^d$ if there is no $\omega$-percolation. See Ref. [1] (Proposition II.2) for a detailed version of an argument along these lines.

Let us discuss the monotone cases. If free boundary conditions are imposed on $\Lambda_k$ – which means $n_i = 0$ for all $i \in \partial\Lambda_k$ – the limiting measure exists, independent of the sequence $(\Lambda_k)$ by FKG monotonicity. Next, if $k' > k$, the absence of $\mathbb{W}$-percolation implies that the probability of a $\mathbb{W}$-connection between $\Lambda_k$ and $\partial\Lambda_{k'}$ tends to zero as $k' \to \infty$ (holding $k$ fixed) regardless of the boundary conditions on $\Lambda_{k'}$. This implies the existence of a "separating surface" (composed of vacant $\mathbb{W}$-bonds) in $\Lambda_k \setminus \Lambda_{k'}$.

Given such a surface and conditioning on the outermost separating surface the restriction of the measure to the interior is seen, to also provide a free boundary conditions on this surface. Such a conditional measure, restricted to $\Lambda_k$ lies in between – in the sense of FKG – the measure on $\Lambda_k$ with free boundary condition and the restriction to $\Lambda_k$ of the measure in $\Lambda_{k'}$ with free boundary conditions. Evidently then, every limiting measure is the free measure.

Finally, if $\lambda = 0$, then $\omega = \mathbb{W}$ so $\omega$-percolation is necessary for non-uniqueness. For the Potts and cubic models, the optimal finite-volume boundary conditions are as discussed prior to the statement of this theorem. Furthermore for these models under these conditions, percolation implies long-ranged order with a positive broken symmetry order parameter, the magnetization. □

It is noted that for the AT (and cubic) models, the grey representation may be supplanted with the more sophisticated representations discussed in the previous section. In the orthodox region, one uses a double layer representation and the weights are as described in Eq. (3.8) using $W_{Q,P}^{AT;\mathfrak{o},\mathcal{G}}$ as in Eq. (2.6), here subject to the constraint that the bonds of *both* layers connect occupied sites. Similarly, in the reformed region, one can represent the dilute model by going directly to the black and white representation and use $W_{Q,P}^{AT;\mathfrak{r},\mathcal{G}}$ from Eq. (2.8) (here subject to the constraint that all grey bonds connect only occupied sites). A proof of the FKG property for the multi-layer/multicolor measures in the dilute case follows exactly the proof of the FKG property for these measures in the uniform case (Ref. [1] (Propositions III.6 and III.1 respectively)) combined with the arguments of Lemma 3.1. As a consequence we have:

*Theorem* 3.3. For the dilute AT and cubic models with $\lambda \geqslant 0$: (a) In the orthodox region percolation in (at least) one layer is necessary and sufficient for (at least partial) breakdown of symmetry and percolation in both layers is necessary and sufficient for full symmetry breakdown. (b) In the reformed region, percolation of greys without percolation of blacks is necessary and sufficient for partial symmetry breaking and percolation of blacks is the necessary and sufficient condition for the onset of the low temperature phase. In both the reformed and orthodox cases, if $\lambda = 0$, the weaker form of percolation is the sharp criterion for non-uniqueness.

*Proof.* The proof follows closely the arguments of Theorem 3.6 in conjunction with Proposition III.6 (for the orthodox region) and Theorem III.3 (for the reformed region) from Ref. [1]. For brevity, details are omitted. □

*Remark.* In the region $\lambda > 0$, a more definitive statement than that of Theorem 3.2 is not possible. In particular, for some values of the parameters, there will be phase transitions exhibited by the lattice gas variables in which the spin variables only play a peripheral rôle. For example, in the absence of spin interactions, the lattice gas is equivalent to an Ising system and therefore has a coexistence line. The interplay between these two possible phase transitions – and their percolation properties in various graphical representations – presents a challenging topic for study.

### 3.3. The non-SA region

The conclusions of Theorem 3.2 demonstrate that the condition $\lambda \geqslant 0$ is *required* for this type of FKG property in the graphical representation, i.e. if $\lambda < 0$, such a property does not hold in general. Indeed, in Ref. [24], the $\lambda < 0$ were studied.[3] For a variety of site-diluted "large entropy" models, e.g. the $q$-state Potts models, with $q$ large, it was shown that this region possesses a staggered phase characterized by the preferential occupation of the even or the odd sublattice. Under the conditions where such results were established, it is also possible to show that there is no percolation of sites. Hence, the existence of multiple phases without any sort of percolation.

Outside the SA region, it is evident that a different sort of expansion (which appears deceptively similar) is required. At present, the models that are amenable to cluster algorithms are limited in scope; we will focus attention on the dilute ferromagnetic Potts models defined by

$$\mathscr{H} = -\sum_{\langle i,j\rangle} J_{i,j}(\delta_{\sigma_i,\sigma_j} - 1)n_i n_j - \sum_{\langle i,j\rangle} \kappa_{i,j} n_i n_j - \sum_i \mu_i n_i \,. \tag{3.11}$$

Here, $J_{i,j} > 0, \kappa_{i,j} = J_{i,j} + \lambda_{i,j}$ and it is assumed that $\kappa_{i,j} \geqslant 0$. We write

$$e^{-\beta\mathscr{H}} = \left[\prod_{\langle i,j\rangle} [p_{i,j}\delta_{\sigma_i,\sigma_j} + (1 - p_{i,j})]n_i n_j + 1 - n_i n_j\right] \times \left[\prod_{\langle i,j\rangle} K_{i,j} n_i n_j + 1\right]\left[\prod_i z_i n_i + 1 - n_i\right] \,. \tag{3.12a}$$

After expanding the product, it is seen that the terms generated by the second two factors have similar interpretations as their counterparts from the previous representation: occupied/vacant site configurations and occupied/vacant anchor bond configurations. The first factor gives rise to three sorts of terms. First, between neighboring pairs of occupied sites, there are the occupied and vacant random cluster bonds. Second, there is a different sort of vacant bond, the $1 - n_i n_j$ term, that labels pairs of sites that do not have both members occupied. Notwithstanding their similarity, the two sorts of vacant bonds play different roles. In particular, these latter vacant bonds *force* at least one vacant site at the endpoints of the bond and, of further significance, have different weights.

The configurations are described by the triple $(n, \omega, \theta)$. The objects $n$ and $\theta$ are as before while $\omega$ is the random cluster representation on the graph of occupied sites. The other sort of vacant bonds do not require a separate symbol. The weights are

$$V^{\mathscr{G}}_{\mathscr{H},\beta}(n,\omega,\theta) = B_p^{\mathscr{G}(n)}(\omega) q^{k(n,\omega)} \prod_{\langle i,j\rangle \in \theta} K_{i,j} \prod_i z^{n_i} X(n,\omega) X(n,\theta) \,, \tag{3.12b}$$

[3] In Ref. [24] as in this subsection, this condition is expressed as $\kappa < 1$; cf. Eq. (3.11).

where $k(n,\omega)$ is the number of connected components of $\omega$ on the graph $\mathcal{G}(n)$ and $B_p^{\mathcal{G}(n)}(\omega)$ is the Bernoulli factor for the configuration $\omega$ relative to this graph. The $\kappa=0$ $(\Rightarrow\theta=\emptyset)$ version of this representation has been discussed previously, e.g. in Ref. [28].

The difference between this representation and that of Eq. (3.7) for the Potts model can now be made explicit. Here $p_{i,j}=R_{i,j}/(1+R_{i,j})$; let us multiply the weights in Eq. (3.7) by a factor of $\prod_{\langle i,j\rangle\in\mathbb{B}_{\mathcal{G}}}(1-p_{i,j})$ and compare: In the $\lambda\geqslant 0$ case, *all* vacant bonds cost a factor of $(1-p_{i,j})$ whereas when $\lambda<0$, only the vacant bonds between neighboring occupied sites require the factor of $(1-p_{i,j})$.

As a limiting case, we obtain the Widom–Rowlinson model introduced in Ref. [33]. Indeed, on $\mathbb{Z}^d$ with $p_{i,j}\equiv p$ and $K_{i,j}\equiv K$ if $|i-j|=1$ and zero otherwise, the nearest-neighbor Widom–Rowlinson model is just the $K\to 0$, $p\to 1$ limit in the above representation – corresponding to $\kappa\to 0$ and $J\to\infty$. In this limit, there are no anchor bonds and $\omega$ is trivial in the sense that it is identically $\mathbb{B}_{\mathcal{G}(n)}$. The weights for the site configurations $n$ reduce to

$$W_z^{WR,\mathcal{G}}(n)=z^{N(n)}q^{k(n)}\,, \tag{3.13}$$

where $k(n)\equiv k(n,\mathbb{B}_{\mathcal{G}(n)})$ is the number of components of the graph $\mathbb{B}_{\mathcal{G}(n)}$, i.e. the number of "connected clusters" of particles. These are the weights of the grey representation for the Widom–Rowlinson model (see Refs. [12,13] and also Refs. [7,8]). It should be noted that the Widom–Rowlinson (lattice) limit is two limits that may be taken separately. Of particular interest for the next subsection are the cases $\kappa=0$, $p<1$ which lead to "soft core" continuum models that can be analyzed by graphical methods.

As mentioned previously, there is no hope for a general statement that the absence of percolation in the representation defined via Eqs. (3.12a) and (3.12b) characterizes the regime of a unique phase. Furthermore, even the weaker statement that $\omega$-percolation is necessary and sufficient for symmetry breaking contains an unfilled gap: Percolation with respect to *some* boundary conditions is necessary and percolation with respect to the wired boundary conditions is sufficient. The case $q=2$, is exceptional and can be entirely settled; results of this sort were proved for the Widom–Rowlinson limit in Refs. [12,13]:

*Theorem* 3.4. Consider the system defined by the Hamiltonian in Eq. (3.11) with $q=2$ defined, for simplicity on $\mathbb{Z}^d$ with isotropic couplings satisfying $0\leqslant\kappa\leqslant J$ or the $J=\infty$ limits thereof. Then $\omega$-percolation or, for the $J=\infty$ limit, percolation of $n$-sites (as defined by the representation in Eq. (3.13) is the necessary and sufficient condition for the existence of multiple Gibbs states.

*Proof.* If $q=2$, the Hamiltonian in Eq. (3.11) is the usual BEG model with the identification $\sigma_i\in\{+1,-1\}$, $s_i=\sigma_i n_i$. By using the known FKG properties of the latter (see, e.g. Ref. [34]), it may be concluded that the present model has the strong FKG property with respect to the (sitewise) ordering $n_i=1,\sigma_i=+1\succ n_i=0\succ n_i=1,\sigma_i=-1$ provided that $J\geqslant\kappa\geqslant 0$. Thus, by the standard $\pm$-type FKG arguments, positive

spontaneous magnetization characterizes the non-uniqueness regime. The optimal boundary conditions for positive magnetization are, of course, the plus boundary conditions and in the graphical system, these correspond to the wired boundary conditions. Thus, "percolation" in (the limits of) wired states is indeed the characterization of the multiple phase regime.

To establish all the stated claims, it must be demonstrated that whenever there is percolation in some state, there is also percolation in the wired state. To this end, let $\Lambda \subset \mathbb{Z}^d$ denote some finite set with $0 \in \Lambda$ and let $*$ denote some arbitrary boundary condition on $\partial\Lambda$. It may be assumed that $*$ is a "spin-system" boundary condition – an assignment of $n_i = 0$ or 1 to each $i \in \partial\Lambda$ and an assignment of $\sigma_i = \pm 1$ to each such $i$ with $n_i = 1$. (All boundary conditions relevant for the graphical problem may be expressed as superpositions of boundary conditions of this sort.) Let $P^{\omega}_{\Lambda,*}(= P^{\omega}_{\Lambda,*}(\beta,\kappa,z))$ denote the probability that the origin is connected to $\partial\Lambda$ by occupied $\omega$-bonds. For any $*$, we claim that $P^{\omega}_{\Lambda,w} \geqslant \frac{1}{2} P^{\omega}_{\Lambda,*}$ where $w$ denotes the wired boundary condition.

Let $\partial\Lambda^+(*)$ and $\partial\Lambda^-(*)$ denote the $n_i = 1$, $\sigma_i = +1$ and $n_i = 1$, $\sigma_i = -1$ portions of the boundary. In general, if $\Gamma \subset \partial\Lambda$, let $T^{\omega}_{\Lambda,*}(\Gamma)$ denote the probability in the $*$-system that the origin is connected to $\Gamma$. Thus, $P^{\omega}_{\Lambda,*} = T^{\omega}_{\Lambda,*}(\partial\Lambda^+(*)) + T^{\omega}_{\Lambda,*}(\partial\Lambda^-(*))$. The inequality $P^{\omega}_{\Lambda,w} \geqslant \frac{1}{2} P^{\omega}_{\Lambda,*}$ follows if we can establish that $T^{\omega}_{\Lambda,w}(\partial\Lambda^+(*)) \geqslant T^{\omega}_{\Lambda,*}(\partial\Lambda^+(*))$ and $T^{\omega}_{\Lambda,w}(\partial\Lambda^-(*)) \geqslant T^{\omega}_{\Lambda,*}(\partial\Lambda^-(*))$.

To this end, consider the relevant Edwards–Sokal weights for the problem

$$U^{\Lambda,*}_{\mathscr{H},\beta}(n,\omega,\theta,\sigma) = z^{N(n)} B_p^{\mathscr{G}(n)}(\omega) K^{N(\theta)} X^*(n,\omega) X^*(n,\theta) \Delta^*(\sigma,\omega)\,, \tag{3.14}$$

where the $*$'s denote that the configuration at the boundary has been fixed according to the rule $*$. If $u^{\Lambda,*}_{\mathscr{H},\beta}(-)$ denotes the corresponding measure, and $g^{\Lambda,*}_{\mathscr{H},\beta}(-)$ the Gibbs measure for the spin-system, we may write

$$T^{\omega}_{\Lambda,*}(\Gamma) = \sum_{n\sigma} g^{\Lambda,*}_{\mathscr{H},\beta}(n\sigma) u^{\Lambda,*}_{\mathscr{H},\beta}(\tau^{\omega}(0,\Gamma) \,|\, n\sigma) \tag{3.15}$$

where $\tau^{\omega}(0,\Gamma)$ is the event that the origin is connected to $\Gamma$ by $\omega$-bonds and $n\sigma$ is notation for a particle-spin configuration on $\Lambda$. As noted previously, if $* = w$ in the graphical system, we should see $* = +$ (or $* = -$) in the spin system. In all cases, the relevant connectivity probabilities have been expressed as the *Gibbsian* average of a function. Now, let $*$ denote some specific boundary condition and consider the e.g. the case, $\tau^{\omega}(0,\partial\Lambda^+)$. It is clear that $u^{\Lambda,*}_{\mathscr{H},\beta}(\tau^{\omega}(0,\Gamma) \,|\, n, n\sigma)$ is an increasing function of $(n, n\sigma)$: For fixed spin and particle configuration, this is the Bernoulli probability, at bond density $p$, on the graph consisting of the $+$-sites and the bonds that connect them that there is an occupied connection between 0 and $\partial\Lambda^+$. Raising the particle-spin configuration will only increase this probability. But then, by using the FKG property of the Gibbs measure, we have the desired inequality $T^{\omega}_{\Lambda,w}(\partial\Lambda^+(*)) \geqslant T^{\omega}_{\Lambda,*}(\partial\Lambda^+(*))$. A similar argument establishes the inequality with the $\partial\Lambda^-(*)$'s. From this, it follows easily that the limiting percolation density in the wired state is at least half of the optimal density, and the characterization is complete. □

It is possible to establish a number of modest results for these systems when $\kappa = 0$.

*Proposition* 3.5a. Consider the isotropic nearest-neighbor dilute Potts Hamiltonian on $\mathbb{Z}^d$ with $\kappa = 0$. Let $p = 1 - e^{-\beta J}$ and $a(z,q) = zq/[1+zq]$. Next, consider the bond-site percolation problem on $\mathbb{Z}^d$ with bond parameter $\mathfrak{p}$ and site parameter $\mathfrak{a}$, $0 \leqslant \mathfrak{p}, \mathfrak{a} \leqslant 1$. Let $\Pi \subset [0,1]^2$ denote the percolative region of this model. Then if $(p,a) \in \mathrm{Int}(\Pi^c)$, the interaction $\beta\mathscr{H}$ is completely analytic.

*Proof.* Consider the graphical weights as written in Eqs. (3.12a) and (3.12b) – with $K = 0$ so there are no $\theta$-bonds. The constraint function, $X(n,\omega)$ has the undesirable feature of being increasing in $n$ but decreasing in $\omega$. However, at the special point $\kappa = 0$, this may be overcome by the following device: Let $\omega^{\#}$ denote an arbitrary bond configuration and for a site configuraion $n$, define

$$\omega(\omega^{\#}, n) = \{\langle i,j\rangle \in \omega^{\#} \mid n_i = n_j = 1\}\,. \tag{3.16}$$

Consider the weights

$$V^{\#,\mathscr{G}}_{\mathscr{H},\beta}(n,\omega^{\#}) = B^{\mathscr{G}}_p(\omega^{\#}) z^{N(n)} q^{k(n,\omega(\omega^{\#},n))}\,. \tag{3.17}$$

It is clear that restricting attention to observables that depend only on $n$ and $\omega(\omega^{\#},n)$, the resulting measure is identical to the one defined by the weights in Eqs. (3.12a) and (3.12b). Let us rewrite these weights:

$$V^{\#,\mathscr{G}}_{\mathscr{H},\beta}(n,\omega^{\#}) \propto B^{\mathscr{G}}_p(\omega^{\#}) B_a(n) q^{k(n,\omega)-N(n)}\,. \tag{3.18}$$

We claim that $k(n,\omega(\omega^{\#},n)) - N(n)$ is a decreasing function of $(n,\omega^{\#})$ – which implies FKG dominance of the independent bond-site measure over these graphical representations for the spin-systems. First observe that if $\omega$ increases, then $k(n,\omega)$ will decrease or stay the same; adding bonds to an existing $\omega^{\#}$ will only serve to increase $\omega$. If we add a site, then $k$ can only increase by at most one (here, it can actually decrease if $\omega^{\#} \neq \omega$) so $k - N$ cannot increase.

Now let us discuss the graphical representation defined by the weights in Eq. (3.18) on some finite $\Lambda \subset \mathbb{Z}^d$ with fixed boundary condition on $\partial\Lambda$. Let $A \subset \Lambda$ and consider a (minimal) surface $S$ composed of bonds and sites that separate $A$ from $\partial\Lambda$. Consider the measure conditioned on the event that all of these bonds and sites are vacant. It is not hard to see that this measure, e.g. restricted to $A$ is identical to the measure (restricted to $A$) constructed with free boundary conditions on the exterior of $S$. Similar statements, modified appropriately hold for surfaces that separate $A$ from a portion of $\partial\Lambda$.

When $(p,a) \in \mathrm{Int}(\Pi^c)$, these surfaces are abundant in the independent model due to the exponential decay of the bond-site connectivity function. Using the comparison/decomposition methods in Ref. [35], the proof of Theorem 4 in this reference is easily modified to establish complete analyticity under the stated conditions. □

Using the device of the $\omega^{\#}$ configurations, dominations in the opposite direction may be obtained. Let us write

$$V^{\#,\mathscr{G}}_{\mathscr{H},\beta}(n,\omega^{\#}) \propto B^{\mathscr{G}}_{p}(\omega^{\#}) \frac{1}{q^{N(\omega^{\#})}} \left[\frac{z}{q^{(2d-1)}}\right]^{N(n)} q^{k(n,\omega)+N(\omega^{\#})+(2d-1)N(n)} . \tag{3.19}$$

Now $k(n,\omega) = N(n) - N(\omega) + \ell(\omega)$ where $\ell(\omega)$ is the number of independent loops in the configuration. We claim that $2dN(n) + N(\omega^{\#}) - N(\omega) + \ell(\omega)$ is increasing: Extra bonds can only increase $\ell(\omega)$ and $N(\omega^{\#}) - N(\omega)$. If we add a site, $N(\omega^{\#})$ does not change, by definition, but $N(\omega)$ could go up by as much as $2d$ – without the formation of additional loops. But this has been compensated by the $2dN(n)$ and we may conclude that the above is indeed increasing. We thus have

*Proposition* 3.5b. Let

$$\tilde{p} = \frac{p}{p + q(1-p)}$$

and

$$\tilde{a} = \frac{z}{z + q^{(2d-1)}} .$$

Then if $(\tilde{p},\tilde{a}) \in Int(\Pi)$, the spin system is in the high-density/magnetized phase.

*Proof.* Rewriting the weights

$$V^{\#,\mathscr{G}}_{\mathscr{H},\beta}(n,\omega^{\#}) \propto B_{\tilde{p}}(\omega) B_{\tilde{a}}(n) q^{2dN(n)+N(\omega^{\#})-N(\omega)+\ell(\omega)} , \tag{3.20}$$

the corresponding measure dominates the independent measure at parameters $(\tilde{p},\tilde{a})$. Now if, in finite volume with wired boundary conditions, the probability that any site is connected to the boundary by a bond/site path is uniformly positive, there is symmetry breaking in the infinite volume limit. Such uniform positivity is evident if $(\tilde{p},\tilde{a})$ is in the percolative region for the independent bond/site model. □

*Remark.* Graphical representations for the AT model along the lines of Eqs. (3.12a) and (3.12b) are of course possible, and presumably the analog of Proposition 3.5 can be established in these cases. However, nothing along the lines of Theorem 3.4 has been shown in any (non-trivial) case. More pertinent to the central theme of this work is the fact that, at present, we cannot even write down cluster algorithms for these cases. These matters are currently under intensive study. However, for the interim, there is a continuum version of the (orthodox region) AT model introduced in Ref. [36] that does admit a cluster algorithm. Since this model is certainly not the straightforward limit of the AT model, we will discuss this model solely in the context of continuum systems.

### 3.4. Continuum limits

If $\kappa = 0$, continuum limits of the dilute Potts systems along with their graphical representations are readily obtained.[4] This provides a vehicle for the proof of various results about these continuum gases but also (and of primary importance here) allows for the construction of cluster algorithms directly in the continuum. Around the time that the results of this subsection were derived, another group (H.O. Georgii and O. Häggström) studied the same set of problems and arrived at essentially the same graphical representations. The principal differences are: (i) The degree of generality – Georgii and Häggström have treated all of the sysems discussed here with the addition of a species independent "background interaction" which we have not considered. (ii) A cleaner proof of the existence of a region of multiple phases (the analog of Theorem 3.5b in the continuum). In light of (i) and (ii) – not to mention that the work [16] was written up well in advance of the present work – we will keep details to the minimum requirements for self-containment and defer altogether to Ref. [16] for the proof of Theorem 3.6. However, certain results in this section, e.g. Theorem 3.7 are in the complement of Ref. [16].

Let us start with the Hamiltonian in Eq. (3.11) on $\mathbb{Z}^d$ with $\kappa_{i,j} \equiv 0$ and the ferromagnetic term given by $-\sum_{\langle i,j\rangle} J_{i,j}[\delta_{\sigma_i,\sigma_j} - 1]$, with $J_{i,j} \geqslant 0$ and the value $J_{i,j} = \infty$ formally permitted and understood as a restriction on the particle configurations. Now suppose that $J_{i,j}$ is of the form

$$J_{i,j} = J(|i-j|/\varepsilon)\,, \tag{3.21}$$

where $|i-j|$ denotes Euclidean distance and for simplicity it is assumed that $e^{-J(r)}$ is piecewise continuous identically one for $r \geqslant 2a > 0$. The number $a$ is called the interaction radius. Let $y > 0$ denote a real number and let us scale the fugacity $z$ according to $z = y\varepsilon^d$. Now, let $\mathscr{A} \subset \mathbb{R}^d$ a finite regular region. Let $\mathscr{G}(\varepsilon; \mathscr{A}, a)$ denote the following graph: the site set of $\mathscr{G}(\varepsilon; \mathscr{A}, a)$ is given by $(\varepsilon\mathbb{Z})^d \cap \mathscr{A}$ where $(\varepsilon\mathbb{Z}^d)$ denotes the $d$-dimensional hypercubic lattice with lattice spacing $\varepsilon$ and the bonds of $\mathscr{G}(\varepsilon; \mathscr{A}, a)$ are all pairs of such sites that are separated by Euclidean distance less than $2a$. For case of exposition, let us temporarily consider the case of free boundary conditions on $\mathscr{G}(\varepsilon; \mathscr{A}, a)$. It is straightforward to show (e.g. as in Ref. [37]) that with this scaling, the $\varepsilon \to 0$ limit is a classical $q$-component gas with mutual fugacity $y$ and a pair interaction, $V_{A,B}(\boldsymbol{r})$ that depends on the species $(A,B); A,B = 1,\ldots,a$ that is given by

$$V_{A,B}(\boldsymbol{r}) = \begin{cases} J(|\boldsymbol{r}|), & \text{if } A \neq B\,, \\ 0, & \text{otherwise}\,. \end{cases} \tag{3.22}$$

[4] The same holds e.g. for the AT model but for reasons mentioned in the above remark, these will not be discussed. Similarly, $\kappa < 0$ limits are possible but will not be described in the present work. Note that if $\kappa > 0$ then the continuum limit is unstable.

These models admit a class of continuum graphical representation that may be derived directly in the continuum or via the lattice approximations. (To the author's knowledge, such models were first discussed in Ref. [7].) We start with the multispecies versions: Let $\underline{n}$ denote $q$ collections of points in $\mathscr{A}$ and let $\mathscr{G}_{\underline{n},a}$ denote the graph imbedded in $\mathscr{A}$ with sites at the points $\underline{n}$ and bonds connecting all sites separated by a distance less that $2a$. Let $\omega \subset \mathbb{B}_{\mathscr{G}_{\underline{n},a}}$, let $p(r) = 1 - e^{-\beta J(r)}$ and let $B_{p(r)}(\omega)$ denote the Bernoulli factor for the configuration $\omega$ with independent bond probabilities determined according to the length of the bond by the function $p(r)$. Finally, let $\Delta(\underline{n}, \omega)$ denote the function that is zero if any occupied bond of $\omega$ connects points of different species and is one otherwise.

Given that there are $n_1$ particles of type 1,... and $n_q$ particles of type $q$, the density (with respect to Lebesgue measure on $\mathscr{A}^{|n_1+\cdots+n_q|}$) for having the graph $\mathscr{G}_{\underline{n},a}$ and the bond configuration $\omega \subset \mathbb{B}_{\mathscr{G}_{\underline{n},a}}$ is $B_{p(r)}^{\mathscr{G}_{\underline{n},a}}(\omega)\Delta(\underline{n}, \omega)$. The constant of proportionality, $Z_{V,\beta;\underline{n}}(\mathscr{A})^{-1}$ is, of course, the inverse of the canonical partition function at inverse temperature $\beta$ and interaction Hamiltonian determined by the pair potentials in Eq. (3.22). The probability of observing a configuration of this constituency is given by $y^{n_1+\cdots+n_q}[Z_{V,\beta;\underline{n}}(\mathscr{A})/\Xi_{A,\beta,y}(\mathscr{A})]$ where $\Xi_{V,\beta,y}(\mathscr{A})$ is the grand canonical partition function for the region $\mathscr{A}$. Summing over all possible colorings of $|n|$ particles located at the points $n = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{|n|})$, we obtain the grey densities for the graph $\mathscr{G}_{n,a}$ and the bond configuration $\omega \subset \mathbb{B}_{\mathscr{G}_{n,a}}$ that are given by $B_{p(r)}(\omega)q^{k(n,\omega)}$ where $k$ is the number of components (clusters) of $\mathscr{G}_{n,a}$ is the configuration $\omega$.

A few elementary calculations show that the above describes graphical representations of the previously discussed continuum models and it is not hard to see that this is exactly the continuum limit of the ($\kappa = 0$) graphical representations that were analyzed in the previous subsection. Indeed, this follows almost immediately from elementary considerations of continuity, much the same as the arguments used in Ref. [37].

So far, we have only discussed the case of free boundary conditions. Other boundary conditions for the continuum gas may be constructed in a straighforward fashion: finite (fixed) particle configurations may be (approximately) placed outside $\mathscr{G}(\varepsilon; \mathscr{A}, a)$ and the limiting finite volume Gibbs measures constructed accordingly. In the context of these models, various infinite densities (outside $\mathscr{A}$) can also be handled in a straighforward fashion. Of principal concern in this work will be the *wired* boundary conditions. In the $\varepsilon \to 0$ limiting procedure, one of the species is selected and a particle of this type is placed at every site in $(\varepsilon\mathbb{Z})^d \setminus \mathscr{G}(\varepsilon; \mathscr{A}, a)$ that is within a distance $2a$ of the boundary. In the continuum limit, this forces every particle (in $\mathscr{A}$) that is within a distance $2a$ of the boundary to be of the same species as the outside particles. In the graphical representation, these boundary conditions dictate that we count components according to the rule that all particles within a distance $2a$ of the boundary are considered to be in the same cluster.

It is highly plausible that percolation (the formation of infinite clusters of sites connected by occupied bonds) in the graphical representation provides the signal for the species density symmetry breaking phase transitions in these models. (Although we

caution that in $d=3$, if $q \gg 1$, there may be crystalline phases with no broken symmetry among the various species.) However, as is the case in the lattice models, the characterization of symmetry breaking via percolation falls somewhat short of a complete theorem: Percolation in the wired state is sufficient and percolation in some state is necessary. Furthermore, even to prove the existence of multiple phases dominated by a single species requires some effort:

*Theorem* 3.6. Consider the soft-core WR models as described above with $e^{-J(r)} > 0$ for $r < 2a$. Then, for $\beta$ and $z$ sufficiently large, there is percolation in any state that is the limit of wired states which further implies the existence of multiple Gibbs states.

*Proof.* See Ref. [16] (Theorem 1.1).

For $q=2$, the $+ \succ \emptyset \succ -$ FKG property is inherited in the (two-component) continuum version by continuity – as was the case in the Widom–Rowlinson limit [12,13]. A proof of the analog of Theorem 3.3 follows in this case from nearly identical arguments.

*Theorem* 3.7. Consider the above described systems for $q=2$. Then percolation occurs iff it occurs in the (unique) limiting wired state and thus is the necessary and sufficient condition for multiple Gibbs states.

*Proof.* The absence of percolation in *any* state implies uniqueness while percolation in the wired state implies symmetry breaking. All that remains is to show that percolation in some state implies that there is percolation in the wired state. Consider some boundary condition on a regular $\mathscr{A} \subset \mathbb{R}^d$ and let $\partial\mathscr{A}^+$ and $\partial\mathscr{A}^-$ denote the portions of the boundary that permit a connection of the $+$ and $-$ type, respectively. Assume, for simplicity, that the probability of a connection between the origin and $\partial\mathscr{A}^+$ is not smaller than the corresponding probability for a connection to $\partial\mathscr{A}^-$. By considering these probabilities given the (approximate) locations of all particles in $\mathscr{A}$, the relevant Edwards–Sokal coupling allows us to conclude that this is an increasing function of the configuration: Indeed, the rules of the conditional measure are to independently place bonds between particles of the same type. The presence of additional $+$ particles allows for additional mechanisms for connections to $\partial\mathscr{A}^+$. Evidently, the overall probability of a connection to the boundary does not exceed twice the probability in the wired state. □

### 3.4.1. Graphical algorithms

We now proceed with graphical algorithms defined for all the problems and their representations described in this section. These algorithms are not dissimilar to the ones in the previous section. Thus, in these systems, it also turns out that there is no obstruction to the use of non-interger values of $q$ provided that $q \geqslant 1$. Most of our attention will focus on the lattice versions. The continuum problems are, in

essence, an afterthought: Here, as with the graphical representations themselves, the limit of the algorithm is the algorithm of the limit. To simplify all descriptions, we have ignored listing the provisos required for various boundary conditions; what follows is strictly true for free boundary conditions (i.e. on a general graph, no boundary conditions). Other boundary conditions may be incorporated in a routine fashion – usually by freezing appropriate graphical elements (and, possibly, their connected components for the duration of the Monte Carlo step).

The simplest case is the WR model described by Eq. (3.13). Let us start here and work our way upwards.

*3.4.2. Hard core lattice WR ($p = 1,\ \kappa = 0$) algorithm*

*Step* 0. Let $n \subset \mathbb{S}_{\mathscr{G}}$ denote a site configuration. The configuration $n$ is divided into connected clusters $K_1, \ldots, K_{k(n)}$.

*Step* 1. Each cluster is removed with probability $1/q$ or left intact with probability $1 - 1/q$. The removal decisions are independent from cluster to cluster.

*Step* 2. The vacant sites are of two types: Those that border on one or more of the surviving clusters and those that are "out in the open". Those sites that neighbor a cluster remain vacant. The vacant sites in the open are independently left vacant with probability $1 - s$ or awarded a new particle with probability $s$ where $s = z/(1 + z)$.

This cycle constitutes a single *Monte Carlo* step.

*Proof of detailed balance.* Detailed balance will be verified by the construction of an intermediate model – which for integer $q$ essentially is the WR model – and demonstrating that this is an Edwards–Sokal coupling. Consider then a model with two species of particles, brown and white. There is no interaction among whites but the system is constrained so as to forbid browns and whites to occupy the same or neighboring sites. For each connected brown cluster, there is a weight factor of $q - 1$ and a particle (brown or white) located at the site $i$ provides a fugacity factor of $z$ (assumed, for simplicity to be independent of $i$). Thus, if $(n_B, n_W)$ is a particle configuration, the weight is given by

$$U(n_B, n_W) = z^{n_B(i)+n_W(i)}(q-1)^{k(n_B)}\chi(n_B, n_W)\,, \tag{3.23}$$

where $\chi(n_B, n_W)$ vanishes if any brown particle shares a site or neighbors with a white particle and is one otherwise and $k(n_B)$ is the number of brown clusters.

It is immediately seen that if we sum over all brown-white particle configurations that have particles at the positions $n \subset \mathbb{S}_{\mathscr{G}}$, we get the grey representation weights of Eq. (3.13). Step 1 is a random selection of $(n_B, n_W)$ given $n$ and step 2 is a random selection of $n_W$ given $n_B$. Detailed balance is established. □

*Remark.* For integer $q$, the brown particles consist of $q - 1$ particle species and the algorithm may be reformulated as one that keeps track of all the $q$ species at all times. In step 1, one of the $q$ species is selected and the lattice is depleted of that particle type. In step 2, the lattice is repopulated with the species that was depleted in step 1

by independently occupying, with probability $s$, each vacant site that does not neighbor a site already occupied by another species. Finally, in a third step, a new species is randomly assigned to each cluster and the cycle is complete.

The case with $p < 1$ and $\kappa = 0$ is nearly identical with a redefinition of "clusters" and an extra step for the bonds.

*3.4.3. Soft core lattice WR ($p < 1$, $\kappa = 0$) algorithm*

*Step* 0. Let $n \subset \mathbb{S}_{\mathscr{G}}$ denote a site configuration and $\omega \subset \mathbb{B}_{\mathscr{G}}$ a bond configuration satisfying $X(n, \omega) = 1$. The configuration $n$ is divided into clusters $K_1, \ldots, K_{k(n,\omega)}$ where connectedness is here defined via the occupied bonds.

*Step* 1. Each cluster – bonds and particles – is removed with probability $1/q$ or left (completely) intact with probability $1 - 1/q$.

*Step* 2. Independently, for each vacant site $i$, a particle is placed at the site with probability $s(i)$ or $i$ is left vacant with probability $1 - s(i)$. The quantity $s(i)$ is given by

$$\frac{s(i)}{1 + s(i)} = z \prod_{j \in n_B} e^{-\beta J_{i,j}},$$

where $n_B$ is the configuration of the sites that were *not* removed.

*Step* 3. Of the bonds connecting the newly arrived particles at sites $i$ and $j$, independently, with probability $p_{i,j}$ such a bond is declared to be occupied or with probability $1 - p_{i,j}$ it is vacant.

Steps 1–3 constitute single a Monte Carlo step.

*Remark.* It is of course observed that if $p_{i,j}$ is identically one, the above collapses into the algorithm for the usual lattice Widom–Rowlinson model with the notion of neighborhood determined by the graph.

*Proof of detailed balance.* A proof of detailed balance along the lines of the previous proof follows immediately once we have set up the intermediate model. Here we again consider brown and white particle configurations $(n_B, n_W)$. Let $n = n_B \cup n_W$ and let $\omega$ be a bond configuration on $\mathscr{G}(n)$. These bond configurations will be subject to the further constraint that no occupied bond connects a white to a brown site. For convenience, let us therefore wite $\omega = \omega_W \cup \omega_B$ with $\omega_W \cap \omega_B = \emptyset$. The full weights are similar to those in Eqs. (3.12a) and (3.12b) – with $K = 0$:

$$\tilde{V}^{\mathscr{G}}_{q,p,z}(n_B, n_W, \omega_B, \omega_W) = B_p^{\mathscr{G}(n)}(\omega) z^{|n|} (q-1)^{k(n_B,\omega)} X(n_B, \omega_B) X(n_W, \omega_W). \quad (3.24)$$

Summing over all $(n_B, n_W)$ that are consistent with a given $\omega$ and satisfy that $n_B \cup n_W$ is equal to some fixed $n$, we get the weights of Eqs. (3.12a) and (3.12b) with $K = 0$. The various steps of the algorithm are seen as selections from appropriate conditional distributions of the measure defined by the $\tilde{V}^{\mathscr{G}}_{q,p,s}$. □

### 3.5. Continuum limits

The above-described algorithms themselves converge to a continuum algorithm that manifestly satisfies detailed balance for the limiting continuum system. Thus, in these cases, there is nothing that can be added beyond an informal description of the limiting algorithm. Let us first consider the usual $q$-component WR (hard core) models:

Here particles are regarded as spheres of radius $a$ with connectivity defined in the sense of overlapping spheres. A specification of points constitutes a *grey* configuration which is then divided into distinct connected clusters. In the first step of the algorithm, with probability $1/q$, each cluster is removed from the system or, with probability $1-1/q$, left in place. The *free volume* is defined to be the set of points a distance greater than $2a$ from any of the remaining particles – so that if a new particle of radius $a$ is placed in the free volume, it does not intersect any of the particles in the cluster that survives the first step. In the second step, particles are placed in this free volume according to a Poisson process at intensity $y$ and we are back to a full configuration. If $q$ is an integer, a $q$-component configuration may be obtained from a grey configuration by independently assigning, with equal probability $1/q$, any of the $q$ labels to the individual clusters. This hard core algorithm was discovered independently by Ref. [15] and has been used effectively in simulations [25].

The algorithm for the soft-core continuum models is similar. Here there are grey particles and bonds (of length $\leqslant 2a$) connecting certain pairs of particles with connectivity defined via these bonds. Starting with a configuration of particles and connecting bonds, clusters are independently retained, with probability $1-1/q$ or discarded with probability $1/q$. Denote by $n_B$ the set of locations of the remaining particles. Particles are replenished in the free volume by a Poisson process with position dependent intensity $\tilde{y}(x)$ given by $\tilde{y}(x)=y\exp\{-\beta\sum_{x'\in n_B}J(|x-x'|)\}$. Finally, bonds are occupied between pairs of the new particles with a probability $p(r)$ where $r$ is the distance separating the pair; no bonds are permitted between the old and the new particles. It is clear that this algorithm reduces to the hard core algorithm when $p(r)=1$ for $r\leqslant 2a$ and zero otherwise. For integer $q$, a multi-component configuration is obtained from a grey configuration in the same way as described above.

In closing, let us remark that other continuum models of the WR-type admit cluster algorithms of this sort. For example, in the model introduced in Ref. [38], there are four species, R, Y, G and B at mutual fugacity $y$ and two interaction radii, $a$ and $A$ with $A > a$. The interactions between R and Y and the interactions between B and G are hard core exclusion with the smaller radius. All other pairings of distinct species interact with hard core repulsion at a distance $2A$ and there is no interaction between particles of the same species. The two radii define two notions of connected, $a$-connected and $A$-connected. The algorithm for this model is a straightforward extension of the previous ones.

We now return to the lattice for the analysis of the more complicated models. As should be clear, the introduction of anchor bonds will require some additional dynamics:

*3.5.1. Dilute Potts model algorithm (non-SA region) I*

*Step* 0. Consider a configuration $(n,\omega,\theta)$ consisting of occupied sites $(n)$, occupied bonds $(\omega)$ satisfying $X(n,\omega)=1$ and anchor bonds $(\theta)$ satisfying $X(n,\theta)=1$. The $\omega$-bonds divide $\mathscr{G}(n)$ into connected clusters of which there are $k(n,\omega)$.

*Step* 1. Each $\omega$-cluster is, independently, with probability $1-1/q$ left alone or, with probability $1/q$, selected for removal. All $\omega$-bonds of these clusters are removed as well as all sites within a given selected cluster except for those that are attached to an anchor bond. These preserved sites will be denoted as *anchored* sites and they remain in place for the duration of the Monte Carlo step.

*Step* 2. This is identical to Step 2 from the soft core (lattice) WR algorithm but it is understood that the anchored sites do *not* contribute to $n_B$.

*Step* 3. This is identical to Step 3 from the soft core WR algorithm with the exception that here new $\omega$-bonds *are* permitted between the new sites placed in Step 2 and the anchored sites preserved from Step 1.

*Step* 4. All $\theta$-bonds are removed. New $\theta$-bonds are independently placed between any pair of occupied sites with probability $r_{i,j}=K_{i,j}/(1+K_{i,j})$ or, such a pair is left without an anchor bond with probability $1-r_{i,j}$.

Steps 1–4 constitute a complete Monte Carlo step.

*Proof of detailed balance.* It is again only necessary to present the joint model and verify (1) that the marginal is the (full) grey measure defined by the weights in Eq. (3.12) and (2) that each step of the algorithm is a random selection from an appropriate conditional distribution. Here, the relevant joint distribution is the generalization of Eq. (3.24):

$$\tilde{V}^{\mathscr{G}}_{q,\,p,s}(n_B,n_W,\omega_B,\omega_W,\theta)=B_p^{\mathscr{G}(n)}(\omega)z^{|n|}B_r^{\mathscr{G}(n)}(\theta)(q-1)^{k(n_B,\omega)}$$

$$\times X(n_B,\omega_B)X(n_W,\omega_W)X(n,\theta)\,. \tag{3.25}$$

In brief: Given $(n,\omega,\theta)$, the weights in Eq. (3.13) are obtained by summing over all $(n_B,n_W)$ and $(\omega_B,\omega_W)$ consistent with $n$ and $\omega$. Step 1 starts with a selection of $(n_B,n_W)$ and $(\omega_B,\omega_W)$ given $n$ and $\omega$. Step 2 and the rest of Step 1 results in the selection of a new $n_W$ given $n_B$ and $\theta$. Observe that in these steps, the white particles attached to the $\theta$-bonds must remain in place because the presence of an anchor bond – without a brown particle at one or both ends – necessarily implies the presence of a white particle at these sites. Clearly, Step 3 produces an $\omega_W$ configuration with the correct statistics given $n_W$ and Step 4 a $\theta$-bond configuration given $n$. □

An alternative representation and algorithm is possible in which the vacancies are elevated to a dynamical status but acts as the soft core algorithm/representation with

regards to the occupied sites. Indeed, let us write

$$\sum_{\langle i,j\rangle} \kappa_{i,j} n_i n_j = \sum_{\langle i,j\rangle} \kappa_{i,j}[(1-n_i)(1-n_j) + n_i + n_j - 1] \tag{3.26a}$$

and define

$$\tilde{\mu}_i = \mu + \sum_{j:\langle i,j\rangle \in \mathbb{B}_{\mathscr{G}}} \kappa_{i,j} \,. \tag{3.26b}$$

We may write $e^{\beta\kappa_{i,j}(1-n_i)(1-n_j)} = (e^{\beta\kappa_{i,j}} - 1)(1-n_i)(1-n_j) + 1 \propto r v_i v_j + 1 - r_{i,j}$ where $v_i = 1 - n_i$ and $r_{i,j} = 1 - e^{-\beta\kappa_{i,j}}$.

Upon expansion, this produces a different set of bond configurations – here denoted by $\vartheta$ which have the property that they must connect pairs of vacant sites. The weight of a (total) configuration is given by

$$U^{\mathscr{G}}_{q,p,\tilde{z},r} = B_p^{\mathscr{G}(n)}(\omega) B_r^{\mathscr{G}(v)}(\vartheta) \prod_i \tilde{z}_i^{n_i} q^{k(n,\omega)} X(n,\omega) X(v,\vartheta) \tag{3.27}$$

where $v \equiv \mathbb{S}_{\mathscr{G}} \backslash n$ is notation for a configuration of vacancies and $\tilde{z}_i = e^{\beta\tilde{\mu}i}$. A cluster algorithm for this representation is a simple extension of the Soft Core Lattice WR Algorithm that includes $\vartheta$-bonds.

*3.5.2. Dilute Potts model algorithm (non–SA region) II*

*Step* 0. Start with a configuration $(n,\omega,\vartheta)$ satisfying $X(n,\omega) = X(n,\vartheta) = 1$. The $\omega$ bonds divide $\mathscr{G}(n)$ into $k(n,\omega)$ components.

*Step* 1. Each $\omega$-cluster is independently removed with probability $1/q$ or left intact with probability $1 - 1/q$. The configuration of remaining occupied sites is denoted by $n_B$.

*Step* 2. Independently, for each vacant site that is *not* attached to a $\vartheta$-bond, a particle is placed with probability $s(i)$ which is given by

$$\frac{s(i)}{1+s(i)} = \tilde{z}_i \prod_{j \in n_B} e^{-\beta J_{i,j}}$$

or otherwise left vacant.

*Step* 3. Independently, for each pair of newly occupied sites, $i$ and $j$, place an $\omega$-bond on $\langle i,j\rangle$ with probability $p_{i,j}$

*Step* 4. Remove all $\vartheta$ bonds. Between every pair of vacant sites, $i$ and $j$, place a $\vartheta$-bond with probability $r_{i,j}$

Steps 1–4 constitute a single Monte Carlo step.

Both of the above algorithms can be used in the Potts case when $\kappa > J (\lambda > 0)$ however in these cases, a somewhat different algorithm associated with the representation from Eq. (3.7) or (3.8) may be used. We will start with the simplest version – Potts at $\lambda = 0$ – and then treat the general case.

*3.5.3. Dilute Potts model algorithm (integer $q$, $\lambda=0$)*

*Step* 0. Let $(n,\omega)$ denote a site-bond configuration with $X(n,\omega)=1$

*Step* 1. All isolated sites are removed from the lattice. Now, *all* vacant sites of the lattice are independently repopulated with probability $t$ where $t=zq/(1+zq)$.

*Step* 2. Each connected component of sites is independently assigned one of the $q$ spin states. All $\omega$-bonds are removed and new bonds independently placed between spins of the same type with probability $p$.

A single Monte-Carlo step has been completed.

*Remark.* Notice that despite apparent similarities to the non-SA algorithms, there are a number of important distinctions. First, clusters do not get removed, only isolated sites. (In this sense, the rôle of the anchor bond has merged with that of the $\omega$-bond. Nevertheless, for $\lambda>0$, the anchor bond reemerges as an independent entity.) Second, in this algorithm, the sites are removed without regard to their species – the criterion is isolation. Third, in this algorithm new sites may be placed at vacancies on the boundary of the present clusters without any apparent "interaction penalty". Despite these peculiar features, this algorithm satisfies detailed balance with respect to the representation that percolates precisely at the phase boundary of the uniqueness regime.

*Proof of detailed balance.* We will omit any specifics save for the explicit form of the Edwards–Sokal weights for the bond-site-spin configurations. In this case, these read $B_p^{\mathcal{G}(n)}(\omega)(qz)^{|n|}X(n,\omega)\Delta(\sigma,\omega)$ where $\Delta(\sigma,\omega)$ is one if each bond of $\omega$ connects only spins that are of the same type and is zero otherwise. Using these weights, it is easy to verify detailed balance in this case. A more complete proof may be obtained as a special case of the proof for the general SA algorithms. □

The generalization is as follows:

*Proposition* 3.8 (*General dilute systems*; $\lambda\geqslant 0$). Suppose that a graphical problem for bond configurations on graphs $\mathcal{G}$ has the weights $W^{\mathcal{G}}(\omega)$ for bond configurations $\omega\subset\mathbb{B}_{\mathcal{G}}$. Suppose, further, that for all graphs $\mathcal{G}$, if a site and no bonds are added; $\mathcal{G}\to\mathcal{G}'$ with $\mathbb{B}_{\mathcal{G}}=\mathbb{B}_{\mathcal{G}'}$, $\mathbb{S}_{\mathcal{G}'}=\mathbb{S}_{\mathcal{G}}\cup s$ then for all $\omega\subset\mathbb{B}_{\mathcal{G}}, W^{\mathcal{G}'}(\omega)=qW^{\mathcal{G}}(\omega)$. Next suppose that $W^{\mathcal{G}}(\omega)$ is the marginal of some joint measure, with weights $M^{\mathcal{G}}(\omega,\sigma)$, where $\sigma\equiv(\sigma_i\,|\,i\in\mathcal{S}^{\mathbb{S}_{\mathcal{G}}})$ It is supposed that for any $\mathcal{G}$ and $\mathcal{G}'$ as described above, $M^{\mathcal{G}'}(\omega,\sigma,\sigma_s)=v(\sigma_s)M^{\mathcal{G}}(\omega,\sigma)$ where $v(\sigma_s)$ sums to $q$. Finally, suppose that for any finite graph $\mathcal{G}$ there is an ergodic algorithm $T^{\mathcal{G}}:(\omega,\sigma)\to(\omega',\sigma')$ satisfying detailed balance with respect to measure defined by the weights $M^{\mathcal{G}}(\omega,\sigma)$, the first step of which is to randomly select a $\sigma'$ from the conditional distribution given $\omega$. Then, let $\mathcal{G}$ denote a graph and consider the algorithm for configurations $(n,\omega,\theta)$ with $n\subset\mathbb{S}_{\mathcal{G}}$, $\omega\subset\mathbb{B}_{\mathcal{G}}$ and $\omega\subset\mathbb{B}_{\mathcal{G}}$ defined by

*Step* 0: Let $(n,\omega,\theta)\subset\mathbb{S}_{\mathcal{G}}\times\mathbb{B}_{\mathcal{G}}\times\mathbb{B}_{\mathcal{G}}$.

*Step* 1: Remove all sites of $n$ that are not the end points of any bond in or $\omega$ or $\theta$. At each vacant site (including those freshly created) independently, with probability $qz/(1+qz)$ install an occupied site.

*Step* 2: All $\theta$-bonds are removed. New $\theta$-bonds are independently with probability $L/(1+L)$ placed between each pair of occupied sites.

*Step* 3: On the graph consisting of the sites that are endpoints of bonds in $\omega$ (and all bonds of $\mathcal{G}$ that join them) apply the first step of $T$ to obtain spin values for the sites. On the remaining sites $i$ of the current $n$, independently assign spin-values $\sigma_i$ with probability $v(\sigma_i)/q$. Then $\omega$ and all these spin values constitute a bond-spin configuration on $\mathcal{G}(n)$ to which the second step of $T$ is applied in order to obtain the updated $\omega$-bond configuration.

A single Monte-Carlo step is completed.

Then this algorithm satisfies detailed balance with respect to the measure defined by the weights

$$Y^{\mathcal{G}}_{\mathbf{H},L,z} = W^{\mathcal{G}}(\omega) \prod_{\langle i,j\rangle\in\theta} L_{i,j} \prod_i [qz_i]^{n_i} X(n,\omega)\, X(n,\theta)\,.$$

In particular, this is a cluster algorithm for any dilute spin systems with a graphical representation of the type described in Eq. (3.7).

*Proof*. Given the bond configurations $\omega$ and $\theta$, there have to be occupied sites at all endpoints of occupied bonds. The (conditional) distribution of the remaining sites is that of independent Bernoulli variables with density $qz_i/(1+qz_i)$. Step 1 is therefore a random selection of one such configuration. Similarly, given the site configuration $n$, Step 2 is seen to be a random selection of a $\theta$-bond configuration from this conditional distribution. Finally, the desired consequences of Step 3 follow directly from the hypotheses: Starting with the endpoints of $\omega$, the first step of $T$ assigns a spin configuration to these sites. Next, the selection of spin values for the "newly occupied" sites of $n$ are seen to be independent of $\omega$ (and one another) which, due to the hypothesized factorization, $M^{\mathcal{G}'}(\omega,\sigma,\sigma_s) = v(\sigma_s) M^{\mathcal{G}}(\omega,\sigma)$, evidently satisfies detailed balance for the joint measure defined by the $M$-weights on $\mathcal{G}(n)$. The remainder of the $T$ algorithm now generates a new $\omega$-bond configuration for the graph $\mathcal{G}(n)$ in such a way as to satisfy detailed balance for the measure defined by the weights $W^{\mathcal{G}(n)}(\omega)$. Now recall that for any $\omega\subset\mathbb{B}_{\mathcal{G}(n)}$ we have $W^{\mathcal{G}}(\omega) = W^{\mathcal{G}(n)}(\omega) q^{|\mathbb{S}_{\mathcal{G}}|-N(n)}$. It therefore follows that for any $\omega,\tilde{\omega}\subset\mathbb{B}_{\mathcal{G}(n)}$, the ratio $W^{\mathcal{G}(n)}(\omega)/W^{\mathcal{G}(n)}(\tilde{\omega})$ equals $W^{\mathcal{G}}(\omega)/W^{\mathcal{G}}(\tilde{\omega})$. It thus follows that the new $\omega$-configuration is a random selection from the conditional distribution given $n$. Detailed balance of the algorithm is established. □

## 4. 2-D SOS and *XY* models

### 4.1. The restricted SOS model

The connection between certain two-dimensional random surface models and spin systems is well known (see, e.g., Ref. [39]). Usually, the approach is to start with

a familiar spin system and show that the system admits a *height representation*. Of course one consequence is that the resulting surface model may have "peculiar" features – for example the restriction that neighboring height differences are always $\pm 1$ or that the height variable itself is a multi-dimensional object. Here (as in Ref. [40]) we will follow a less traditional approach: We consider familiar random surface models – explicitly the restricted $k$-step SOS models – and demonstrate that these are height representations of various spin systems. Of course, now the latter may be a bit peculiar – e.g. have constraints but nevertheless will be amenable to some analysis: graphical representations and cluster algorithms. Our prototypical example will be the one step restricted solid-on-solid model that is defined as follows:

*Definition.* Let $\Lambda \subset \mathbb{Z}^2$ denote a finite connected set, and, for $i \in \Lambda, h_i \in \mathbb{Z}$ an integer valued height variable. It is assumed that the height on the boundary is identically zero. The Hamiltonian is given by the formal expression

$$H = \sum_{\langle i,j \rangle} |h_i - h_j| T_1(|h_i - h_j|) \tag{4.1}$$

with $T_1(s)$ infinite if $s > 1$ and one otherwise. In particular, $h_i$ is an integer-valued height field on $\Lambda$ with the restriction that the height difference between neighbors does not exceed one.

It is anticipated that such a model differs in no essential way from the usual SOS model (defined as in Eq. (4.1) but without the factor of $T_1$) and in particular to have a roughening transition at some temperature that is the order of unity. (Cf. the discussion in Ref. [41] on p. 29.) In more generality, we may consider models of this form with nearest neighbor interactions given by $F(|h_i - h_j|)T_k(|h_i - h_j|)$ with $T_k$ infinite if its argument exceeds $k$ and one otherwise. Depending on the details of $F$ (and the size of $k$) the preceding sentence may or may not apply.

Focusing attention on the model described by Eq. (4.1), consider the following spin-system with four spin-states per site: $\sigma_i \in \mathbb{Z}_4 \equiv$ which may be better envisioned as colors $\{Y, B, G, R\}$. Let $(\sigma_i - \sigma_j) \in \{0, \pm 1, 2\}$ denote the $\mathbb{Z}_4$ difference between states and $|\sigma_i - \sigma_j|$ $(=0, 1$ or $2)$ the distance between states. We define the Hamiltonian

$$-H = \sum_{\langle i,j \rangle} [\delta_{\sigma_i,\sigma_j} - \chi_{\sigma_i,\sigma_j}] \sum_{\langle\langle i,j,k,\ell \rangle\rangle} \Phi_{\sigma_i,\sigma_j,\sigma_k,\sigma_\ell} \,. \tag{4.2}$$

In the above, $\chi_{\sigma_i,\sigma_j}$ is infinite if $|\sigma_i - \sigma_j|$ is 2 and is zero otherwise; the objects $\langle\langle i, j, k, \ell \rangle\rangle$ are the elementary squares of the lattice and $\Phi_{\sigma_i,\sigma_j,\sigma_k,\sigma_\ell}$ is infinite if all four colors appear on the square and is zero otherwise. On a finite $\Lambda \in \mathbb{Z}^2$, the boundary conditions that are of relevance are those in which all the spins on the boundary are in the same state.

Thus we have a four state Potts (or clock) model with constraints. Clearly, we may define the difference in "heights" vis-à-vis $h_i - h_j = (\sigma_i - \sigma_j)$ and the restriction enforced by $\chi_{\sigma_i,\sigma_j}$ forces this difference to be one. What is not so clear is that it is

possible to define an unambiguous $h_i$ in the first place. In particular, assuming $h \equiv 0$ on the boundary, let $P: \partial\Lambda \to i$ denote a path from the boundary to $i$. We may of course define $h_i(P) = \sum_{\langle i,j\rangle_D \in P} (\sigma_j - \sigma_i)$ where $\langle i, j\rangle_D$ is a directed bond, but then we must address the question of whether $h_i(P)$ is independent of $P$. This is where the second constraint comes in and is the subject of our first proposition.

*Proposition* 4.1. Let $\Lambda \subset \mathbb{Z}^2$ denote a finite connected set, let $\sigma_\Lambda \in \{0, +1, -1, 2\}^\Lambda$ denote a spin configuration on $\Lambda$ and set $\sigma_{\partial\Lambda} \equiv 0$. Suppose that the two constraints discussed are satisfied: $\chi_{\sigma_i,\sigma_j}$ is finite for every $\langle i, j\rangle$ and $\Phi_{\sigma_i,\sigma_j,\sigma_k,\sigma_\ell}$ is finite for every $\langle\langle i, j, k, \ell\rangle\rangle$. Then if $P: x \to i$ is any directed path from the point $x$ on the boundary to the point $i$ in $\Lambda$, the quantity $h_i(P) = \sum_{\langle i,j\rangle_D \in P} (\sigma_j - \sigma_i)$ is independent of $P$.

*Proof.* The proof is elementary and involves nothing more than the Stokes theorem: Let $\langle\langle i, j, k, \ell\rangle\rangle$ denote an elementary square. The quantity $(\sigma_j - \sigma_i) + (\sigma_k - \sigma_j) + (\sigma_\ell - \sigma_k) + (\sigma_i - \sigma_\ell)$ is, of course, zero mod 4; it is sufficient to show that it is actually zero. Since the absolute value of each term is bounded by 1, it is enough to show that it cannot achieve $\pm 4$ without a violation of the four-color rule. This is easily checked: suppose that there are two of the same color on the square and that the $\chi$-constraint is enforced on each bond. If the said two colors occupy adjacent sites on the square, then $|\sigma_a - \sigma_b|$ is only non-zero on three legs of the square and the fact that $|\sigma_a - \sigma_b| \leqslant 1$ does not permit an overall change of four. On the other hand, if the two sites with the distinguished color are diagonally opposed – say at $i$ and $k$ – then any choice of $\sigma_j$ for which $|\sigma_i - \sigma_j| = |\sigma_k - \sigma_j| \leqslant 1$ puts $(\sigma_j - \sigma_i) = (\sigma_k - \sigma_j) = 0$ Similarly, in this case, the last two legs add up to zero. □

From the above example, it is clear that virtually any restricted SOS-model can be described in this fashion; if the height restrictions are $|h_i - h_j| \leqslant k$ all that is needed is a spin model with $q \geqslant 2k + 1$ states. The only requirement, which is both necessary and sufficient, is that the constraints force the height change around each elementary plaquette to be zero; the more spin states, the fewer constraints. In particular, if $q > 4k$ (for the square lattice) the only needed constraint is that $|\sigma_i - \sigma_j| < k$ on each bond. The simplest example, namely $q = 5$ for the one-step restricted SOS model was discussed a while ago in Ref. [40]. However, as we shall see, the spin representations with the *extra* constraints are particularly useful for the construction of cluster algorithms.

A graphical representation for these spin-systems is readily developed; for simplicity, let us confine attention to the four-state spin-model corresponding to the one-step restricted SOS model. Let $\Lambda \subset \mathbb{Z}^2$ be a connected finite set and consider the system with $\sigma_i$ constant on $\partial\Lambda$. Let $\omega \subset \mathbb{B}_\Lambda$ denote an occupied bond configuration and let $\mathbb{Q}_\Lambda(\omega)$ denote the number of ways that the components of $\omega$ can be assigned one of four colors in such a way that the $\chi$ and $\Phi$ constraints are satisfied at each site. (Note that $\mathbb{Q}(\omega) > 0$ since we can always color every site red.) It is evident that if we write the weights

$$W^{SOS}_{\Lambda;p}(\omega) = B_p(\omega)\mathbb{Q}_\Lambda(\omega)\,, \tag{4.3}$$

then the resulting graphical measure, denoted by $\mu^{SOS}_{\Lambda;p}(-)$ faithfully describes the spin system and the associated SOS-model.

The representation is somewhat difficult to work with and its properties have not yet been fully explored. Although we are tempted to believe that the roughening and percolation transitions coincide, we have only partial evidence to this effect. In particular, if there *is* percolation then the surface cannot be "rough" in the sense that $h_0 = 0$ with uniformly positive probability. Further, if we consider the toy "Wedding Cake" model in which (loosely speaking) the surface is only allowed to go up, the corresponding underlying spin-system is precisely the Ising model [42]. Here, the analog of our representation turns out to be exactly the FK representation and thus percolation and "roughening" indeed coincide.

Finally, it is noted that $\mathbb{Q}(\omega)$ is a decreasing function (because a "greater" bond configuration implies that there are more constraints). Hence, the measures $\mu^{SOS}_{\Lambda;p}(-)$ are dominated by the density $p$ Bernoulli measures which implies the surface is rigid if $p > 1/2$.

The standard approach to the design of cluster algorithms for surface models which dates back to Refs. [43,44] is based on reflections of the surface itself. Here, the graphical representation of the constrained spin system leads to a different sort of algorithm. The following simulates the restricted one-step SOS model and the above described graphical representation:

#### *4.1.1. SOS algorithm*

*Step* 0. Let $\omega \subset \mathbb{B}_\Lambda$ and $\sigma_\Lambda \in \{R, Y, G, B\}$ denote a legitimate bond-spin configuration. In particular, (i) there is no elementary square that is occupied by more than four distinct colors, (ii) the combinations RB and YG never appear on any neighboring pair of sites, and (iii) each occupied bond of $\omega$ connects only sites that are of the same color.

*Step* 1. Select two "compatible" colors i.e. any pair except RB or YG. This may be done randomly or according to some sensible deterministic rule that regularly selects all allowed pairs. For the sake of definitiveness, let us proceed assuming that R and Y have been chosen. Remove all R-sites that are not neighbors of G-sites or connected to an R neighbor of a G-site by occupied bonds. Similarly, remove all Y-components save for those that border on a B-component. (For the duration of this step, all bonds of $\omega$ are to be left in place.) There are now uncolored $\omega$-components left behind where the "internal" R and Y sites used to be. These may be divided into components according to the usual connectivity rules for sites and bonds.

*Step* 2. Each blank $\omega$-component is colored R or Y with probability one half.

*Step* 3. Remove all bonds of $\omega$. On each satisfied (i.e. same color) neighboring pair of sites, a bond is independently occupied with probability $p$ or the bond is left vacant with probability $1 - p$.

Steps 1–3 constitute a single Monte-Carlo step.

*Remark.* It is noted that there are certain similarities between the preceding and the algorithm used for the three-state Potts antiferromagnetic in Refs. [45,46].

*Proof of detailed balance.* We consider the joint measure with weights

$$Y^{SOS}_{p;\Lambda}(\sigma,\omega)=B_p(\omega)Q(\sigma)\Delta(\sigma,\omega)\,, \tag{4.4}$$

where $Q(\sigma)$ is one only if all the $\chi$ and $\Phi$ constraints are satisfied and is zero otherwise and $\Delta(\sigma,\omega)$ is the usual enforcer of the constraint that occupied bonds connect only satisfied pairs. It is evident that the marginals of the joint measure resulting from these weights reproduce the appropriate bond and spin models defined by Eqs. (4.2) and (4.3).

The third step of the algorithm is the usual selection of a bond configuration from the conditional distribution given the spin configuration. Similarly, but slightly less obviously, steps 1 and 2 are seen to be a random selection from the conditional distribution for the two selected colors given the specification of the other two colors and the bond configuration $\omega$. With the stated boundary conditions, the algorithm is obviously ergodic since, e.g. the all red configuration can be reached from any given configuration in a few steps. □

### 4.2. The XY model

In this final subsection, we treat the standard $XY$ model on a graph $\mathscr{G}$. Here, to fix notation, for $i$ in $\mathbb{S}_{\mathscr{G}}$ let $\boldsymbol{s}_i$ denote the spin variable at $i$ which is a two-dimensional vector of length one. The $XY$-Hamiltonian is given by

$$H^{XY}=-\sum_{\langle i,j\rangle}J_{i,j}\boldsymbol{s}_i\cdot\boldsymbol{s}_j \tag{4.5}$$

with $J_{i,j}>0$. For this system, we will use (and modify) the representation implicit in the Wolff algorithm [9] that was described in Refs. [20,21]. Let $\hat{a}$ denote a unit vector and $\hat{b}$ an orthogonal unit vector – to be definitive, rotated by $-\pi/2$. We define $a_i=|\boldsymbol{s}_i\cdot\hat{a}|$ and similarly for $b_i$. Letting $\tau_i=\mathrm{sgn}(\boldsymbol{s}_i\cdot\hat{a})$ and $\sigma_i=\mathrm{sgn}(\boldsymbol{s}_i\cdot\hat{b})$ we may write the Hamiltonian as a sum of three terms: $H^{XY}=-\sum_{\langle i,j\rangle}J_{i,j}(a_ia_j+b_ib_j)+I_{\underline{a}}(\underline{\tau})+I_{\underline{b}}(\underline{\sigma})$ where $\underline{\sigma}=(\sigma_i\,|\,i\in\mathbb{S}_{\mathscr{G}})$ denotes an Ising configuration on $\mathbb{S}_{\mathscr{G}}$, similarly for $\underline{\tau}$ while $\underline{a}$ and $\underline{b}$ are configurations of $a$'s and $b$'s and $I_{\underline{a}}(\underline{\sigma})$ is the Ising Hamiltonian

$$I_{\underline{b}}(\underline{\sigma})=-2\sum_{\langle i,j\rangle}J_{i,j}b_ib_j(\delta_{\sigma_i\sigma_j}-1)\,. \tag{4.6}$$

Thus, for each realization $\underline{b}$, we have one or two Ising models that can be expanded in an FK representation. This is the basis of Wolff's algorithm.[5]

[5] It should be noted that two non-trivial ingredients were introduced in [9]: First, a cluster method for various continuous systems – including the $XY$-model and second the use of *single* cluster methods. The single cluster methods will not concern us in this work.

*4.2.1. The Wolff algorithm*

*Step* 0. Let $\underline{S} = (\boldsymbol{s}_i \mid i \in \Lambda)$ denote a spin configuration. Select an $\hat{a}$ uniformly from the circle. For each $i$ define $\sigma_i = \mathrm{sgn}(\boldsymbol{s}_i \cdot \hat{b})$.

*Step* 1. Independently, for each neighboring pair of sites $\langle i, j \rangle$, if $\sigma_i = \sigma_j$ occupy a bond between these spins with probability $p_{i,j} = 1 - e^{-2\beta J_{i,j} b_i b_j}$. If $\sigma_i \neq \sigma_j$ the bond is vacant.

*Step* 2. Perform a standard SW Ising spin-flip move: each connected cluster – including isolated sites – is independently assigned a new $\sigma$ value that is constant throughout the cluster. All the bonds are erased, the new $\sigma$'s and the old $b$'s are constitute the updated spin configuration.

A single *Monte-Carlo* step has been completed.

*Proof of detailed balance.* Since a proof of detailed balance for (the single cluster version of) this algorithm already appeared in Ref. [9], we will be concise. Let $\alpha$ denote an angle on the circle corresponding to the direction of $\hat{a}$. Let $A_i = \boldsymbol{s}_i \cdot \hat{a} \equiv a_i \tau_i$ and let $\underline{A}$ denote the configuration $(A_i \mid i \in \mathbb{S}_{\mathscr{G}})$ and similarly for $\underline{\sigma}$, etc. Then the spin configuration $\underline{S}$ is completely determined by the variables $(\alpha, \underline{a}, \underline{\sigma})$. Denoting the bond variables by $\omega$, the algorithm evidently samples some joint measure, $W$, on the configurations $(\alpha, \underline{A}, \underline{\sigma}; \omega)$. We may denote by $W(\underline{\sigma}, \omega \mid \alpha, \underline{A})$ the weights for the (Ising) spin configuration and the bond configuration given $\alpha$ and $\underline{a}$. Here, it is clear that $W(\underline{\sigma}, \omega \mid \alpha, \underline{A})$ is of the form of the standard Edwards–Sokal weights – as in Eq. (2.2) – for the Ising Hamiltonian in Eq. (4.6). Now it is seen that summing over the bond configurations gives the (conditional) Boltzmann distribution for the configuration of $\underline{\sigma}$'s. Since the spin and bond moves select independent samples of bonds and spins from the appropriate conditional distributions (given the fixed values of $\alpha$ and $\underline{a}$) detailed balance is satisfied.

Needless to say, if we stuck with a single value of $\hat{a}$, the entire system would be all but frozen. However, a fresh direction for $\hat{a}$ is selected on the zeroth step – which obviously satisfies detailed balance. It is easy to see that in finite volume, it is possible to get arbitrarily close to any spin configuration in a finite number of steps. □

*Remark.* It is obvious that this algorithm can be "improved" (presumably only by a constant factor) by the introduction of a second set of Ising/FK variables associated with the $a$-components of the spins. The algorithm is essentially the same as above only there are now two bond moves – one for the $\tau$'s and one for the $\sigma$'s – and two spin-flip moves. Note that while the bonds associated with the two types of spins are not mutually exclusive they tend to be non-cooperative in the sense that a large $b_i b_j$, which enhances the probability of a $\sigma$-bond implies a smaller value of $a_i a_j$ which disfavors the $\tau$-bond. Although we do not expect substantial improvement in this algorithm over the usual Wolff algorithm, this extra ingredient may be important in the analogous IC algorithm.

Any cluster algorithm is of limited use for the simulation of a phase transition unless this phase transition is reflected in the underlying graphical representation. Although the numerical evidence (e.g. in Ref. [9]) is convincing, to date there has been limited theoretical understanding of this problem and, with the exception of Ref. [21], essentially no rigorous work on the subject. Below we will show that indeed percolation (or more accurately, the onset of percolation) in the underlying graphical representation indeed coincides with a phase transition in the $XY$ model.

Let us start with some notation. We will assume, for the bulk of this analysis that we are dealing with some finite connected $\Lambda \subset \mathbb{Z}^d$. Infinite volume analogs of all statements in general follow via a limiting procedure. Here, we will consider, for once and all, a fixed values of $\hat{b}$ and $\hat{a}$ say the $X$ and $Y$ directions, respectively. Unless otherwise specified it will be assumed that the boundary conditions on $\Lambda$ are free, periodic or that all of the $b_i$ on the boundary are positive. We denote by $M^W(\underline{b}, \underline{\sigma}; \omega)$ the Wolff density for such a configuration and by $\mathbb{E}_{M^W}(-)$ the expectation with respect to this measure. Let $m^W(\underline{b})$ denote the density for the configuration $\underline{b}$ alone ($m^W(\underline{b}) = \sum_{\underline{\sigma}, \omega} M^W(\underline{b}, \underline{\sigma}; \omega)$) and finally, $\mu_{\underline{b}}^W(\omega)$ the conditional probability of the configuration $\omega$ given $\underline{b}$. Note that at least here the measure $\mu_{\underline{b}}^W(-)$ may be explicitly computed via the random cluster weights with $p_{i,j} = 1 - e^{-2\beta|b_i||b_j|}$ and $q = 2$. Observe, if relevant, that the boundary conditions in these conditional measures will be the wired ones. We establish the following, half of which was already proved in Ref. [21]:

*Lemma* 4.2. Let $\langle s_i^{[X]} s_j^{[X]} \rangle \equiv \mathbb{E}_{M^W}(b_i b_j \sigma_i \sigma_j)$ denote the usual correlation function for the $X$-components of the spins for the $XY$ on model $\mathbb{Z}^d$ in any finite volume system with boundary conditions as described or an infinite volume limit thereof. Let $T_{i,j}$ denote the probability in the Wolff measure that the site $i$ is connected to the site $j$ – including, if relevant, connections via the boundary component. Then, for $|i - j| > 1$

$$C[T_{i,j}]^{3/2} \leqslant \langle s_i^{[X]} s_j^{[X]} \rangle \leqslant T_{i,j}$$

where $C$ is a constant that depends only on the temperature and the dimension.

*Proof.* We follow Ref. [21] for the upper bound. Let us start by writing

$$\langle s_i^{[X]} s_j^{[X]} \rangle = \int_{\underline{b}} dm(\underline{b}) b_i b_j \mathbb{E}_{M^W}(\sigma_i \sigma_j \,|\, \underline{b}) \,. \tag{4.7}$$

Let $\mathscr{T}_{i,j}$ denote the event that $i$ is connected to $j$ by occupied bonds. It is noted that if $\omega \notin \mathscr{T}_{i,j}$, then $\mathbb{E}_{M^W}(\sigma_i \sigma_j \,|\, \underline{b})$ vanishes because in one or both of the components of the sites $i$ and $j$, the $\sigma$ value is $+$ and $-$ with equal probability. Indeed, this holds for the expectation of any $f(b_i b_j)\sigma_i \sigma_j$. On the other hand, if $\omega \in \mathscr{T}_{i,j}$ then $\sigma_i = \sigma_j$ and the contribution is one. We thus have the identity

$$\mathbb{E}_{M^W}(\sigma_i \sigma_j \,|\, \underline{b}) = \mathbb{E}_{M^W}(\mathbb{1}_{\mathscr{T}_{i,j}}(\omega) \,|\, \underline{b}) \,, \tag{4.8}$$

where $\mathbb{1}_{\mathscr{T}_{i,j}}(\omega)$ is the indicator for the event $\mathscr{T}_{i,j}$. However, since $b_i b_j \leqslant 1$, the integrand in Eq. (4.7) is bounded by $\mathbb{E}_{M^w}(\mathbb{1}_{\mathscr{T}_{i,j}}(\omega)\,|\,\underline{b})$ which integrates to $T_{i,j}$.

As for the lower bound, let $\varepsilon > 0$ and define the set $g_\varepsilon = \{\underline{b}\,|\,b_i > \varepsilon \text{ and } b_j > \varepsilon\}$. Then, the integral in Eq. (4.7) may be split into a sum of two pieces one from the $\underline{b}$'s in $g_\varepsilon$ and the other from $b$'s in $g_\varepsilon^c$. By the identity in Eq. (4.8), both terms are positive so we may discard the latter and degrade further the remaining term by the replacement of $b_i b_j$ with $\varepsilon^2$:

$$\langle s_i^{[X]} s_j^{[X]} \rangle \geqslant \varepsilon^2 \int\limits_{\underline{b} \in g_\varepsilon} dm(\underline{b}) \mathbb{E}_{M^w}(\mathbb{1}_{\mathscr{T}_{i,j}}\,|\,\underline{b})\,. \tag{4.9a}$$

Adding to both sides of this equation the integral of $\mathbb{E}_{M^w}(\mathbb{1}_{\mathscr{T}_{i,j}}|\underline{b})$ over $g_\varepsilon^c$, we get

$$\langle s_i^{[X]} s_j^{[X]} \rangle + \varepsilon^2 \int\limits_{\underline{b} \in g_\varepsilon^c} dm(\underline{b}) \mathbb{E}_{M^w}(\mathbb{1}_{\mathscr{T}_{i,j}}\,|\,\underline{b}) \geqslant \varepsilon^2 T_{i,j}\,. \tag{4.9b}$$

We claim that this extra (unwanted) integral is at least of the order $\varepsilon^4$. Indeed, if $\mathscr{T}_{i,j}$ is to occur, then $i$ must be connected to one of it's neighbors as must $j$. However, the occupation for the bonds emanating from $i$ and $j$ are themselves of the order $\varepsilon$: If $i'$ denotes a neighbor of $i$ then $p_{i,i'} = 1 - e^{-2\beta b_i b_{i'}} \leqslant 2\beta\varepsilon$. Furthermore, in a $q \geqslant 1$ random cluster system, the probability of any given bond being occupied is bounded above by the associated $p$ parameter. Thus for any $\underline{b}$ in $g_\varepsilon^c$, we have $\mathbb{E}_{M^w}(\mathbb{1}_{\mathscr{T}_{i,j}}\,|\,\underline{b}) \leqslant [2d\beta\varepsilon]^2$ (where here we have used the fact that $|i-j| > 1$).

Finally, the measure of the set $g_\varepsilon^c$ is itself of the order $\varepsilon^2$. Indeed, consider this event with the configurations neighboring $i$ and $j$ that optimize the probability of this event. (Here we again use $|i-j| > 1$ which allows us to decouples the problem.) Now for any configuration of $b_{i'}$'s, the distribution of $b_i$ is given by a density function that can be bounded above and below independent of the $b_{i'}$. Hence, for the event $b_i < \varepsilon$ we obtain a constant times $\varepsilon$ and similarly at the site $j$. Thus, all in all, we have

$$\langle s_i^{[X]} s_j^{[X]} \rangle + \text{const}\,.\,\varepsilon^6 \geqslant \varepsilon^2 T_{i,j}\,. \tag{4.10}$$

The result follows by setting $\varepsilon^6 = \langle s_i^{[X]} s_j^{[X]} \rangle$. □

*Corollary.* Let $\mathbb{X}^*$ denote the expected size of the connected Wolff cluster in any translation invariant and spin rotation invariant state $\langle - \rangle^*$ that arises as a limit of the finite volume states discussed and let $\chi_u^*$ denote the corresponding untruncated susceptibility:

$$\chi_u^* = \sum_i \langle s_0^{[X]} s_j^{[X]} \rangle^*\,.$$

Then $\chi_u^*$ is finite if and only if $\mathbb{X}^*$ is finite.

*Proof.* Under the conditions stated, to within factors of 2, we may replace $\langle \boldsymbol{s}_i \cdot \boldsymbol{s}_j \rangle^*$ with $\langle s_i^{[X]} s_j^{[X]} \rangle^*$ and vice versa. In these systems, by means of a Simon inequality [47],

if $\chi_u^*$ is finite then the decay of correlations is exponential. Hence, using the lower bound of Lemma 4.2, there is also exponential decay of the connectivity function $T_{i,j}$ and hence $\mathbb{X}^*$ is finite. On the other hand, if $\chi_u^*$ is infinite then according to the upper bound, so is $\mathbb{X}^*$. Thus, in general one anticipates the onset of ordering – or near ordering – in the $XY$ systems to correspond to percolation – or "incipient percolation" – in the Wolff measure providing a distinctive geometric signature of the transition out of the high temperature state. □

*Note added.* Recently, the connection between phase transitions in $XY$-systems and percolation in their associated Wolff representation has been sharpened. For example, the percolation density has been proved to be equal (modulo uniform constants) to the spontaneous magnetization. Details to appear in Ref. [22]. Similar results have also been established for the isotropic $O(3)$ – model in Ref. [23].

## References


[1] L. Chayes, J. Machta, Graphical representations and cluster algorithms. I. Discrete spin systems, Physica A 239 (1997) 542–601.

[2] C.M. Fortuin, P.W. Kasteleyn, On the random cluster model I. Introduction and relation to other models, Physica 57 (1972) 536–564.

[3] R.H. Swendsen, J.S. Wang, Nonuniversal critical dynamics in Monte Carlo simulations, Phys. Rev. Lett. 58 (1987) 86.

[4] R.G. Edwards, A.D. Sokal, Generalization of the Fortuin–Kasteleyn–Swendsen–Wang representation and Monte Carlo algorithm, Phys. Rev. D 38 (1988) 2009–2012.

[5] J. Machta, Y.S. Choi, A. Lucke, T. Schweizer, L.V. Chayes, Invaded cluster algorithm for equilibrium critical points, Phys. Rev. Lett. 75 (1995) 2792–2795.

[6] J. Machta, Y.S. Choi, A. Lucke, T. Schweizer, L.M. Chayes, Invaded cluster algorithm for Potts models, Phys. Rev. E 54 (1996) 1332–1345.

[7] W. Klein, Potts-model formulation of continuum percolation, Phys. Rev. B 26 (1982) 2677–2678.

[8] J.A. Givens, G. Stell, The Kirkwood–Salsburg equation for random continuum percolation, J. Stat. Phys. 59 (1980) 981–1018.

[9] U. Wolff, Collective Monte Carlo updating for spin systems, Phys. Rev. Lett. 62 (1989) 361.

[10] D. Kandel, E. Domany, General cluster Monte Carlo dynamics, Phys. Rev. B 43 (1991) 8539–8548.

[11] M. Aizenman, J.T. Chayes, L. Chayes, C.M. Newman, Discontinuity of the magnetization in one-dimensional $1/|x-y|^2$ Ising and Potts models, J. Stat. Phys. 50 (1988) 1–40.

[12] J.T. Chayes, L. Chayes, R. Kotecký, The Analysis of the Widom–Rowlinson model by stochastic geometric methods, Commun. Math. Phys. 172 (1995) 551–569.

[13] G. Giacomin, J.L. Lebowitz, C. Maes, Agreement percolation and phase coexistence in some Gibbs systems, J. Stat. Phys. 22 (1995) 1379–1403.

[14] The present work.

[15] O. Häggström, M.N.M. Lieshout, J. Møller, Characterization results and Markov chain Monte Carlo algorithms including exact simulation for some spacial point processes, preprint, 1996.

[16] H.-O. Georgii, O. Häggström, Phase transition in continuum Potts models, Commun. Math. Phys. 181 (1996) 507–528.

[17] J. Salas, A.D. Sokal, Dynamic critical behavior of a Swendsen–Wang-type algorithm for the Ashkin–Teller model, J. Stat. Phys. 85 (1996) 297–361.

[18] C.E. Pfister, Y. Velenik, Random cluster representation of the Ashkin–Teller model, J. Stat. Phys. 88 (1997) 1295–1331.

[19] S. Wiseman, E. Domany, Cluster method for the Ashkin–Teller model, Phys. Rev. E 48 (1993) 4080–4090.

[20] A. Patrascioiu, E. Seiler, Phase structure of two-dimensional spin models and percolation, J. Stat. Phys. 69 (1992) 573.
[21] M. Aizenman, On the slow decay of $O(2)$ correlations in the absence of topological excitations: remark on the Patrascioiu–Seiler model, J. Stat. Phys. 77 (1994) 351–359.
[22] L. Chayes, Discontinuity of the spin-wave stiffness in the two-dimensional $XY$ model, submitted.
[23] M. Campbell, L. Chayes, The isotropic O(3) model and the Wolff representation, J. Phys. A: Math. Gen., to appear.
[24] L. Chayes, R. Kotecký, S.B. Shlosman, Aggregation and intermediate phases in dilute spin-systems, Commun. Math. Phys. 171 (1995) 203–232.
[25] G. Johnson, H. Gould, J. Machta, L.K. Chayes, Monte Carlo study of the Widom–Rowlinson fluid using cluster methods, preprint, 1997.
[26] J. Machta, J. Jiang, L.X. Chayes, in preparation.
[27] B. Bollobás, G. Grimmett, S. Janson, The random cluster model on the complete graph, Probab. Theory Related Fields 104 (1996) 283–317.
[28] F.Y. Wu, Dilute Potts model, duality and site-bond percolation, J. Phys. A: Mathe. Gen. 14 (1981) L39–L44.
[29] J.T. Chayes, L. Chayes, The correct extension of the Fortuin–Kasteleyn result to plaquette percolation, Nucl. Phys. B [FS] 235 (1984) 19–23.
[30] G. Grimmett, Potts models and random-cluster processes with many-body interactions, J. Stat. Phys. 75 (1994) 67–121.
[31] M. Blume, V.J. Emery, R.B. Griffths, Ising model for the $\lambda$ transition and phase separation in $^3$He–$^4$He mixtures, Phys. Rev. A 4 (1971) 1071–1077.
[32] M. Aizenman, C.M. Newman, Commun. Math. Phys. 107 (1986) 611–647.
[33] B. Widom, J.S. Rowlinson, New model for the study of liquid-vapor phase transitions, J. Chem. Phys. 52 (1970) 1670–1684.
[34] J.L. Lebowitz, J.L. Monroe, Inequalities for higher order Ising spins and for continuum fluids, Commun. Math. Phys. 28 (1972) 301–311.
[35] K.S. Alexander, L. Chayes, Non-perturbative criteria for Gibbsian uniqueness, Commun. Math. Phys., to appear.
[36] L. Chayes, R. Kotecký, An intermediate phase for a classical continuum model, Phys. Rev. B 54 (1996) 9221–9224.
[37] L. Chayes, D. Klein, A generalization of Poisson convergence to "Gibbs convergence" with applications to statistical mechanics, Helv. Phys. Acta 67 (1994) 30–42.
[38] See Ref. [36].
[39] C. Heneley, preprint, 1996.
[40] E. Domany, D. Mukamel, A. Schwimmer, Phase diagram of the $\mathbb{Z}(5)$ model on the square lattice, J. Phys. A: Math. Gen. 13 (1980) L311–L320.
[41] B. Nienhuis, Coulomb gas formulation of two-dimensional phase transitions, in: C. Domb, J.L. Lebowitz (Eds.), Phase Transitions and Critical Phenomena, vol. 11, Academic Press, London, 1987.
[42] D.B. Abraham, C.M. Newman, Wetting in a three-dimensional system: an exact solution, Phys. Rev. Lett. 61 (1988) 1969–1972.
[43] H.G. Evertz, M. Hasenbusch, M. Marcu, K. Pinn, S. Solomon, Stochastic cluster algorithms for discrete Gaussian (SOS) models, Phys. Lett. B 254 (1991) 185–191.
[44] M. Hasenbusch, G. Lana, M. Marcu, K. Pinn, Cluster algorithms for a solid-on-solid model with constraints, Phys. Rev. B 46 (1992) 10 472–10 475.
[45] J.S. Wang, R.H. Swendsen, R. Kotecký, Antiferromagnetic Potts models, Phys. Rev. Lett. 63 (1989) 109–112.
[46] J.S. Wang, R.H. Swendsen, R. Kotecký, 3-state antiferromagnetic Potts models – a Monte Carlo study, Phys. Rev. B 42 (1990) 2465–2474.
[47] V. Rivasseau, Lieb's correlation inequality for plane roters, Commun. Math. Phys. 77 (1980) 145–147.