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Dilute semi-infinite Potts model

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Abstract. — The influence of bond-dilution (which is assumed both on the surface and in the bulk) on the phase transitions of a semi-infinite d-dimensional q-state Potts model is investigated. Phase diagrams and critical exponents have been calculated within an exension of Migdal's approch to disordered systems. We find that the percolation effects in a semi-infinite system are characterised by phase diagrams of striking similarity to that of the pure system. Indeed, for the three-dimensional cubic lattice we observe four different phase transitions, irrespective of the number of Potts state, which can be designated using the same known terminology, namely the ordinary, surface, extraordinary, and special phase transitions.

1. Introduction.

Phase transitions and critical behaviour in semi-infinite systems have been the subject of much recent interest, and a detailled review article containing an extensive list of references has been published by Binder [1]. Such systems are important for their theoretical richness and experimental utility, besides various applications such as catalysis and corrosion. Most works have been devoted to non-random systems (pure Ising, q-state Potts, anisotropic Heisenberg models), which have been studied using a variety of approximations and mathematical techniques, such as the mean field approximation, the high-temperature series expansion method, Monte Carlo simulations and various real-space renormalisation-group (RG) schemes.

On the other hand, the diluted semi-infinite systems have not been studied as extensively as the pure systems, and the theory of surface with disordered magnetic composition seems to be far from complete, although some progress has been noted recently [2-9]. These studies have focused on the criticality corresponding to the particular case where dilution is assumed only on the surface, namely the free-surface problem (semi-infinite bulk). Almost no attempts are available in the literature concerning the more general problem, where we have to consider the presence of bond inhomogeneity both on the surface and in the bulk, which presents interesting features. It is our purpose to perform such a study and to check whether such systems can exhibits surface magnetism. We exhibit some rather simple calculations to study the criticality associated with the quenched bond-diluted q-state Potts ferromagnet model on a semi-infinite d-dimensional hypercubic lattice. We investigate the influence of bond-dilution on the phase diagrams, and we calculate the critical exponents using an approximate real-space renormalisation-group method based on the Migdal-Kadanoff (MK) [10, 11] recursion relations. We find that the percolation effects in a semi-infinite system are characterised by phase diagrams similar to that of the pure system. The results for the Ising model and bond percolation are recovered for $q = 2$ and $q = 1$, respectively.

The outline of this paper is as follows : In section 2 we introduce the model and derive the recursion relations. Sections 3 contains our main results and conclusion.

2. Model and recursion relations.

Consider a nearest-neighbor q-state Potts model on a semi-infinite d-dimensional hypercubic lattice and subject to randomly inhomogeneous pair coupling. The appropriate reduced Hamiltonian is

$$-\beta H = \sum_{\langle ij \rangle} K_{ij}(q\delta_{\sigma_i\sigma_j} - 1) ; \quad (\sigma_i = 1, 2, .., q ; \forall i \ ) \tag{1}$$

where the sum runs over all pairs of first-neighboring sites and K_{ij} is a random variable whose probability distribution is given by

$$\mathcal{P}_S(K_{ij}) = (1 - p_S)\,\delta(K_{ij}) + p_S\,\delta(K_{ij} - K_S) \tag{2a}$$

when both sites i and j belong to the surface. Otherwise the probability distribution reads

$$\mathcal{P}_B(K_{ij}) = (1 - p_B)\,\delta(K_{ij}) + p_B\,\delta(K_{ij} - K_B) \tag{2b}$$

with $K_S \geqslant 0$ (resp. $K_B \geqslant 0$) and $0 \leqslant p_S \leqslant 1$ (resp. $0 \leqslant p_B \leqslant 1$) are the reduced coupling constant and bond concentration on the surface (resp. in the bulk).

As is very common in the real-space renormalisation-group studies on the Potts model, we introduce the convenient variable

$$t = [1 - e^{-qK}][1 + (q - 1)\,e^{-qK}]^{-1} = f(K) \tag{3}$$

which defines t_S and t_B from K_S and K_B, respectively.

The renormalisation-group recursion relations are obtained using the usual bond-moving Migdal-Kadanoff approximation, which consists in successive contractions by a scale factors b along each of the d Cartesian directions, resulting in a volume contraction by an overall factor b^d. Each contraction involves a bond shifting perpendicular to the contraction and a decimation along the contraction.

In what follows we specialize in the case which consists by first performing the decimation and then moving the bonds. Thus when the system is homogeneous the recursion relations are

$$t'_B = f[b^{d-1} f^{-1}(t_B^b)] \tag{4a}$$

$$t'_S = f\left[b^{d-2}\left\{f^{-1}(t_S^b) + \frac{(b-1)}{2} f^{-1}(t_B^b)\right\}\right]. \tag{4b}$$

For the bond-diluted semi-infinite Potts model the analogs of equations (4) determine each new local coupling $(t'_B)_{\alpha\beta}$ and $(t'_S)_{\alpha\beta}$ in terms of a set of original couplings $\{(t_B)_{ij}, (t_S)_{ij}\}$.

$$(t'_B)_{\alpha\beta} = f\left[\sum_{i=1}^{b^{d-1}} f^{-1}\left\{\prod_{j=1}^{b} (t_B)_{ij}\right\}\right] \tag{5a}$$

$$(t'_S)_{\alpha\beta} = f\left[\sum_{i=1}^{b^{d-2}} \left\{f^{-1}\left(\prod_{j=1}^{b} (t_S)_{ij}\right) + \frac{(b-1)}{2} f^{-1}\left(\prod_{k=1}^{b} (t_B)_{ik}\right)\right\}\right]. \tag{5b}$$

A straightforward but tedious analysis of all the possible values for the interactions taking into account their respective probabilities gives the expression for the renormalised probability distributions $\mathcal{P}'_{\mathrm{B}}(t'_{\alpha\beta})$ and $\mathcal{P}'_{\mathrm{S}}(t'_{\alpha\beta})$ which are not of the same form as the initial ones given by (2).

$$\mathcal{P}'_{\mathrm{B}}(t'_{\alpha\beta}) = \sum_{m=0}^{b^{d-1}} C_m^{b^{d-1}} (p_{\mathrm{B}}^b)^m (1 - p_{\mathrm{B}}^b)^{b^{d-1}-m} \delta [t'_{\alpha\beta} - f\{mf^{-1}(t_{\mathrm{B}}^b)\}] \tag{6a}$$

$$\mathcal{P}'_{\mathrm{S}}(t'_{\alpha\beta}) = \sum_{m,n=0}^{b^{d-2}} C_m^{b^{d-2}} C_n^{b^{d-2}} (p_{\mathrm{B}}^b)^m (1 - p_{\mathrm{B}}^b)^{b^{d-2}-m} \times$$
$$\times (p_{\mathrm{S}}^b)^n (1 - p_{\mathrm{S}}^b)^{b^{d-2}-n} \delta \left[t'_{\alpha\beta} - f\left\{nf^{-1}(t_{\mathrm{S}}^b) + \frac{m(b-1)}{2} f^{-1}(t_{\mathrm{B}}^b)\right\}\right]. \tag{6b}$$

To render the computations tractable we make an additional approximation at each iteration by forcing the transformed distributions back to a two-peak form. Namely,

$$(\mathcal{P}'_{\mathrm{B}})_{\text{approx}}(t'_{\alpha\beta}) = (1 - p'_{\mathrm{B}})\, \delta(t'_{\alpha\beta}) + p'_{\mathrm{B}}\, \delta(t'_{\alpha\beta} - t'_{\mathrm{B}}) \tag{7a}$$

$$(\mathcal{P}'_{\mathrm{S}})_{\text{approx}}(t'_{\alpha\beta}) = (1 - p'_{\mathrm{S}})\, \delta(t'_{\alpha\beta}) + p'_{\mathrm{S}}\, \delta(t'_{\alpha\beta} - t'_{\mathrm{S}}) \tag{7b}$$

Equating the zero and first moments of $\mathcal{P}'_{\mathrm{B}}(t'_{\alpha\beta})$ and $(\mathcal{P}'_{\mathrm{B}})_{\text{approx}}(t'_{\alpha\beta})$ on the one hand and of $\mathcal{P}'_{\mathrm{S}}(t'_{\alpha\beta})$ and $(\mathcal{P}'_{\mathrm{S}})_{\text{approx}}(t'_{\alpha\beta})$ on the other we obtain the recursion relations for the variables p_{B}, p_{S}, t_{B} and t_{S} within the two-peak approximation

$$p'_{\mathrm{B}} = 1 - (1 - p_{\mathrm{B}}^b)^{b^{d-1}} \tag{8a}$$

$$p'_{\mathrm{S}} = 1 - (1 - p_{\mathrm{B}}^b)^{b^{d-2}} (1 - p_{\mathrm{S}}^b)^{b^{d-2}} \tag{8b}$$

$$p'_{\mathrm{B}}\, t'_{\mathrm{B}} = \sum_{m=0}^{b^{d-1}} C_m^{b^{d-1}} (p_{\mathrm{B}}^b)^m (1 - p_{\mathrm{B}}^b)^{b^{d-1}-m} f[mf^{-1}(t_{\mathrm{B}}^b)) \tag{9a}$$

$$p'_{\mathrm{S}}\, t'_{\mathrm{S}} = \sum_{m,n=0}^{b^{d-2}} C_m^{b^{d-2}} C_n^{b^{d-2}} (p_{\mathrm{B}}^b)^m (1 - p_{\mathrm{B}}^b)^{b^{d-2}-m} (p_{\mathrm{S}}^b)^n (1 - p_{\mathrm{S}}^b)^{b^{d-2}-n} \times$$
$$\times f\left[nf^{-1}(t_{\mathrm{S}}^b) + \frac{m(b-1)}{2} f^{-1}(t_{\mathrm{B}}^b)\right]. \tag{9b}$$

The correlation lenght exponents ν can be calculated at all the relevant fixed points by calculating the Jacobian matrix for the recursion relations (8) and (9).

$$M = \frac{\partial(t'_{\mathrm{B}}, t'_{\mathrm{S}}, p'_{\mathrm{B}}, p'_{\mathrm{S}})}{\partial(t_{\mathrm{B}}, t_{\mathrm{S}}, p_{\mathrm{B}}, p_{\mathrm{S}})} \tag{10}$$

whose eigenvalues can be written as $(\lambda_{t_{\mathrm{B}}}, \delta_{t_{\mathrm{S}}}, \lambda_{p_{\mathrm{B}}}, \lambda_{p_{\mathrm{S}}})$. The correlation length exponents are then calculated from

$$\nu_\alpha = \frac{\ln(b)}{\ln(\lambda_\alpha)} \tag{11}$$

3. Results and conclusion.

The MK recursion relations have been established for the dilute semi-infinite Potts model for arbitrary d, b, and q. Notice that it is well known that this scheme yields a continuous bulk transition for all finite q and $d > 1$. A discontinuous bulk transition is obtained only in the many component limit $q \to \infty$ [12]. However, it is known exactly that this bulk transition is discontinuous for $q > 4$ in $d = 2$ [13]. In addition, both field theoretic RG calculations [14] and position-space RG calculations for diluted Potts model [15] indicate that the three-dimensional bulk transition is discontinuous for $q > 3$. Therefore we will mainly focus on the cases ($d = 2$; $b = 2$; $q = 1, 2, 3, 4$) and ($d = 3$; $b = 2$; $q = 1, 2$), (from which the Ising model and bond percolation are recovered for $q = 2$ and $q = 1$, respectively), where the MKRG scheme yields the correct nature of the bulk transition.

For the pure semi-infinite Potts model, by iterating the RG equations (4) one obtains the qualitative phase diagrams displayed in figure 1 for the following cases : (a) $d = 2$, $b = 2$ and (b) $d = 3$, $b = 2$. For the cubic lattice, which presents interesting features, there are three different phases : paramagnetic (PM), surface ferromagnetic (SF) where the surface is ferromagnetic but the bulk is disordered, and bulk ferromagnetic (BF) where the bulk and the surface both are ordered. These phases are separated by various types of transitions. The point O represents the so-called ordinary transition where the surface and the bulk magnetisations vanish simultaneously. E is the point characterising the « extraordinary transition » when the bulk magnetisation vanishes and the surface continues ordered. S corresponds to the surface transition, characterising the phase transition of a two-dimensional system. The special transition is described by the point Sp, where the surface goes ferromagnetic before the bulk.

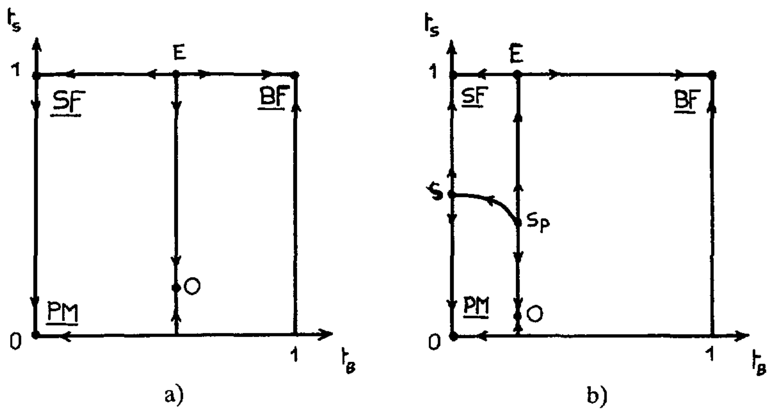

Fig. 1. — Flow diagrams in the (t_B, t_S) space of the pure semi-infinite Potts model. (a) $d = 2$, $b = 2$; (b) $d = 3$, $b = 2$.

As we vary q the critical lines are displaced but the overall picture is the same. Thus, the qualitative phase diagrams obtainedd are similar for any number of Potts state, and in the particular case $q = 2$ we recover the results obtained for the Ising model.

In addition to that analysis we iterated the recursion relations numerically, and identified the locations of the non-trivial fixed points, their eigenvalues, and their associated critical exponents. The numerical results are summarised in table I and II for the square and cubic lattices, respectively.

For the bond-diluted semi-infinite Potts model, equations (8) and (9) give the RG recurrence in the (t_B, t_S, p_B, p_S) space. Flows in a four-dimensional parameter space are not easy to visualise. To get a better understanding we shall consider some invariant subspaces.

* Subspace $p_B = 1$, $p_S = 1$. This corresponds to the pure system and recursion relations (9) reduce, in this case to (4).

Table I. — *Fixed points, eigenvalues and critical exponents of a pure semi-infinite two-dimensional Potts model.*

Potts state	Fixed points	Eigenvalues	Exponents
$q = 1$	(E) $t_B = 0.618$	$\lambda_{t_B} = 1.528$	$\nu_{t_B} = 1.635$
	$t_S = 1$	$\lambda_{t_S} = 1.572$	$\nu_{t_S} = 1.531$
	(O) $t_B = 0.618$	$\lambda_{t_B} = 1.528$	$\nu_{t_B} = 1.635$
	$t_S = 0.272$	$\lambda_{t_S} = 0.427$	
$q = 2$	(E) $t_B = 0.544$	$\lambda_{t_B} = 1.678$	$\nu_{t_B} = 1.338$
	$t_S = 1$	$\lambda_{t_S} = 1.474$	$\nu_{t_S} = 1.784$
	(O) $t_B = 0.544$	$\lambda_{t_B} = 1.678$	$\nu_{t_B} = 1.338$
	$t_S = 0.184$	$\lambda_{t_S} = 0.356$	
$q = 3$	(E) $t_B = 0.5$	$\lambda_{t_B} = 1.777$	$\nu_{t_B} = 1.205$
	$t_S = 1$	$\lambda_{t_S} = 1.414$	$\nu_{t_S} = 2$
	(O) $t_B = 0.5$	$\lambda_{t_B} = 1.717$	$\nu_{t_B} = 1.205$
	$t_S = 0.144$	$\lambda_{t_S} = 0.310$	
$q = 4$	(E) $t_B = 0.469$	$\lambda_{t_B} = 1.852$	$\nu_{t_B} = 1.124$
	$t_S = 1$	$\lambda_{t_S} = 1.370$	$\nu_{t_S} = 2.200$
	(O) $t_B = 0.469$	$\lambda_{t_B} = 1.852$	$\nu_{t_B} = 1.124$
	$t_S = 0.119$	$\lambda_{t_S} = 0.279$	

* Subspace $p_B = 0$. This corresponds to the two-dimensional dilute system.
* Subspace $t_B = 1$, $t_S = 1$. The recursion relations reduce to (8a) and (8b) which describe the percolation effects in a semi-infinite system. The corresponding flow diagrams represented in figure 2, for the square and cubic lattices, shows a striking similarity to that of the pure system (Fig. 1). For the three-dimensional cubic lattice there four non-trivial fixed points characterising four different phase transitions, which can be designated using the same terminology as for pure Potts model. Even if p_B is less than the three-dimensional percolation threshold, the flow diagram shows that an infinite cluster connected to the surface exists if p_S, being less than the two-dimensional threshold, is however sufficiently large. The coordinates of the fixed points with the corresponding eigenvalues and critical exponents are given in table III.
* Subspace $p_B = p_S = p$. In this case bond concentrations on the surface and in the bulk are equal. As $p_B = 1$ is an invariant subspace, the t_B – and t_S-coordinates of the non-trivial fixed points listed in table I and II are not modified and for all these fixed points the bond concentration p is not a relevant scaling field. The coordinates, eigenvalues and critical exponents of the new fixed points characterising the percolation behaviour are listed in table IV.

The RG flow diagram associated with the three-dimensional Ising model in the (t_B, t_S, p) space is described in figure 3. Three phases are observed characterised by trivial

Table II. — *Fixed points, eigenvalues and critical exponents of a pure semi-infinite three-dimensional Potts model.*

Potts state	Fixed points	Eigenvalues	Exposents
$q = 1$	(O) $t_B = 0.282$	$\lambda_{t_B} = 1.759$	$\nu_{t_B} = 1.227$
	$t_S = 0.096$	$\lambda_{t_S} = 0.352$	
	(S) $t_B = 0$	$\lambda_{t_B} = 0$	
	$t_S = 0.618$	$\lambda_{t_S} = 1.528$	$\nu_{t_S} = 1.635$
	(E) $t_B = 0.282$	$\lambda_{t_B} = 1.759$	$\nu_{t_B} = 1.227$
	$t_S = 1$	$\lambda_{t_S} = 0$	
	(Sp) $t_B = 0.282$	$\lambda_{t_B} = 1.759$	$\nu_{t_B} = 1.227$
	$t_S = 0.545$	$\lambda_{t_S} = 1.410$	$\nu_{t_S} = 2.014$
$q = 2$	(O) $t_B = 0.255$	$\lambda_{t_B} = 1.917$	$\nu_{t_B} = 1.065$
	$t_S = 0.077$	$\lambda_{t_S} = 0.306$	
	(S) $t_B = 0$	$\lambda_{t_B} = 0$	
	$t_S = 0.544$	$\lambda_{t_S} = 1.678$	$\nu_{t_S} = 1.338$
	(E) $t_B = 0.255$	$\lambda_{t_B} = 1.917$	$\nu_{t_B} = 1.065$
	$t_S = 1$	$\lambda_{t_S} = 0$	
	(Sp) $t_B = 0.255$	$\lambda_{t_B} = 1.917$	$\nu_{t_B} = 1.065$
	$t_S = 0.464$	$\lambda_{t_S} = 1.526$	$\nu_{t_S} = 1.639$

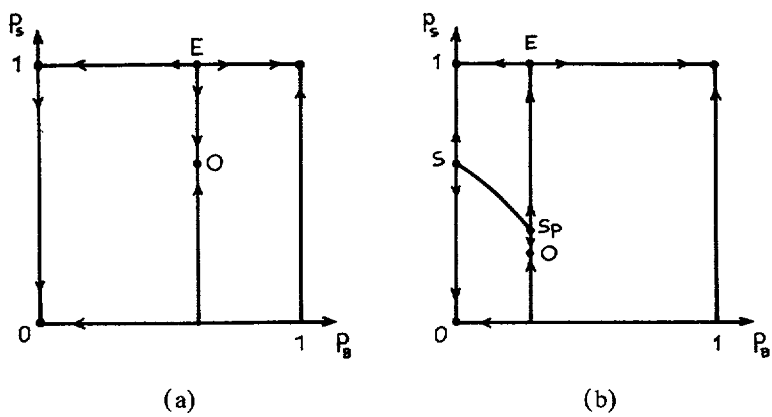

Fig. 2. — Flow diagrams in the (p_B, p_S) space of a semi-infinite d-dimensional hypercubic lattice. (a) $d = 2$, $b = 2$; (b) $d = 3$, $b = 2$.

Table III. — *Fixed points, eigenvalues and critical exponents characterising bond percolation behaviour of a semi-infinite two and three-dimensional cubic lattices.*

Dimension	Fixed points	Eigenvalues	Exponents
2	(E) $p_B = 0.618$	$\lambda_{p_B} = 1.528$	$\nu_{p_B} = 1.635$
	$p_S = 1$	$\lambda_{p_S} = 1.236$	$\nu_{p_S} = 3.270$
	(O) $p_B = 0.618$	$\lambda_{p_B} = 1.528$	$\nu_{p_B} = 1.635$
	$p_S = 0.618$	$\lambda_{p_S} = 0.764$	
3	(O) $p_B = 0.282$	$\lambda_{p_B} = 1.759$	$\nu_{p_B} = 1.228$
	$p_S = 0.282$	$\lambda_{p_S} = 0.879$	
	(S) $p_B = 0$	$\lambda_{p_B} = 0$	
	$p_S = 0.618$	$\lambda_{p_S} = 1.528$	$\nu_{p_S} = 1.635$
	(E) $p_B = 0.282$	$\lambda_{p_B} = 1.759$	$\nu_{p_B} = 1.228$
	$p_S = 1$	$\lambda_{p_S} = 0$	
	(Sp) $p_B = 0.282$	$\lambda_{p_B} = 1.759$	$\nu_{p_B} = 1.228$
	$p_S = 0.384$	$\lambda_{p_S} = 1.109$	$\nu_{p_S} = 6.708$

Table IV. — *Fixed points, eigenvalues and critical exponents characterising percolation behaviour of a bond-diluted semi-infinite two and three-dimensional Potts model.*

Dimension	Fixed points	Eigenvalues	Exposents
2	$t_B = 0$	$\lambda_{t_B} = 0$	
	$t_S = 0$	$\lambda_{t_S} = 0$	
	$p = 0.618$	$\lambda_p = 1.528$	$\nu_p = 1.635$
	$t_B = 1$	$\lambda_{t_B} = 1.528$	$\nu_{t_B} = 1.635$
	$t_S = 1$	$\lambda_{t_S} = 0.764$	
	$p = 0.618$	$\lambda_p = 1.528$	$\nu_p = 1.635$
3	$t_B = 0$	$\lambda_{t_B} = 0$	
	$t_S = 0$	$\lambda_{t_S} = 0$	
	$p = 0.282$	$\lambda_p = 1.759$	$\nu_p = 1.226$
	$t_B = 1$	$\lambda_{t_B} = 1.759$	$\nu_{t_B} = 1.226$
	$t_S = 1$	$\lambda_{t_S} = 0.88$	
	$p = 0.282$	$\lambda_p = 1.759$	$\nu_p = 1.226$

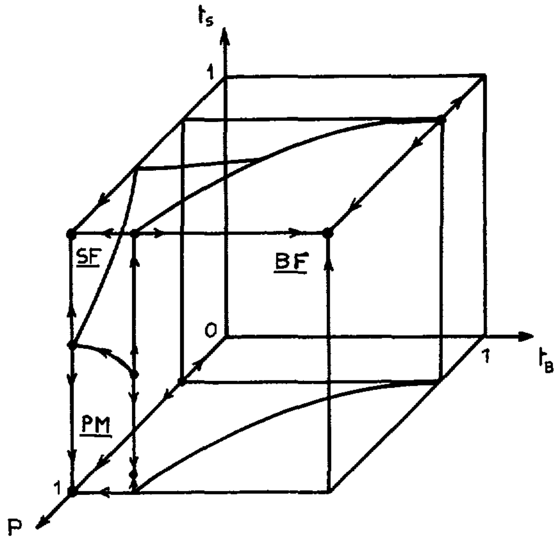

Fig. 3. — RG flow diagram in the (t_B, t_S, p) space of the diluted semi-infinite Ising model $(q = 2)$. PM, BF and SF, respectively denote the paramagnetic, bulk ferromagnetic and surface ferromagnetic phases.

fixed points, namely the paramagnetic [PM, $(t_B, t_S, p) = (0, 0, 1)$], bulk ferromagnetic [BF, $(t_B, t_S, p) = (1, 1, 1)$], and surface ferromagnetic [SF, $(t_B, t_S, p) = (0, 1, 1)$] phases. The PM-BF, SF-BF and SF-PM critical surfaces correspond to the so-called ordinary, extraordinary and surface phase transitions, while the PM-BF-SF critical line corresponds to the special transition.

Conclusion.

We have studied the critical behaviour and phase transitions of the quenched bond-diluted semi-infinite q-state Potts model on a d-dimensional hypercubic lattice. The real-space renormalisation-group method within the Migdal-Kadanoff scheme was applied. Various types of phases and phase transitions were observed. For the percolation behaviour in a semi-infinite system we find phase diagrams similar to that of the pure systems.

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