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Mean-field renormalisation group transformations for geometric phase transitions

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Abstract. It is shown that the mean-field renormalisation group technique of Indekeu *et al* may be applied directly to the self-avoiding walk (SAW) and percolation problems (without reference to the $n \to 0$ limit of interacting spin systems). Numerical results for the SAW and bond and site percolation (both directed and undirected) problems on the square lattice, obtained by using a variety of small cells, are reported. An isotropic transformation for the percolation problems on the d-dimensional hypercubic lattice is also discussed.

1. Introduction

Recently Indekeu *et al* (1982) have introduced a method for constructing the recursion equations which describe a real space renormalisation group transformation for interacting spin systems. They note that since the magnetisation per site $M = \partial f/\partial h$, where f is the free energy per site, the product $M\,\partial h$ should scale like the reciprocal of volume under a renormalisation group transformation. Indekeu *et al* define a renormalisation group transformation within the context of a mean-field calculation by applying the constraint

$$M' = (N/N')\lambda M \qquad \lambda = \partial h/\partial h' \tag{1.1}$$

where $M'(M)$ is the magnetisation per site in a system of $N'(N)$ spins. By considering small groups (cells) of spins and simulating the effect of an infinite system by applying a mean-field approximation on the boundary of the cell, Indekeu *et al* obtain recursion relations for the nearest-neighbour interaction parameter in the limit of zero external field ($h \to 0$).

The phase transitions which occur in spin systems may be termed thermal phase transitions since the probability that the system is in a given state is dependent on the temperature through a Boltzman factor. A second class of phase transitions are the geometric phase transitions typified by the self-avoiding walk (for a review see McKenzie 1976) and percolation problems (for a review see Essam 1980) in which the probability that the system is in a given 'state' is dependent only on the geometric properties of the lattice. The critical properties of these systems are, in general, analogous to those of interacting spin systems and various authors (e.g. Shapiro 1978, Malakis 1980, Young and Stinchcombe 1975, Reynolds *et al* 1977, 1978, Redner 1982) have applied real space renormalisation group techniques to these problems.

In this paper the application of the method of Indekeu *et al* (1982) to the self-avoiding walk (SAW) and the percolation (both directed and undirected) problems

is considered. A brief description of the method as formulated for these problems is given in § 2. Numerical results from small-cell calculations for the square lattice are presented in § 3. Results for the percolation problems with d (lattice dimensionality) >2, obtained using the smallest cell which allows an isotropic renormalisation group transformation of the hypercubic lattice are also presented in § 3. Section 4 contains a summary of results and concluding remarks.

2. Mean-field theory and recursion relations

In the bond (site) percolation problem bonds (sites) of the lattice are occupied with normalised probability p and the role of order parameter is played by the percolation probability $P(p)$, the probability that the site at the origin is the source of an infinite cluster. Here the interpretation of the 'external field' is that used by Reynolds *et al* (1977, 1978): the probability h that a given site is connected to a 'ghost site' which lies outside the lattice. In the directed percolation problem the flow of 'fluid' is restricted to one direction only along any bond. Here the term is used to denote that all parallel bonds in a hypercubic lattice are directed in the same sense.

The percolation probability may be expressed as

$$P(p) = 1 - \frac{\partial f}{\partial h} = 1 - \frac{\partial}{\partial h} \sum_s n_s(p)(1-h)^s \tag{2.1}$$

where $sn_s(p)$ is the probability that the origin is the source of a cluster of size s (for undirected percolation n_s is simply the mean number of clusters of size s per site) and f is the analogue of the free energy per site (Essam 1980). The requirement that the analogue of the total free energy be preserved under a renormalisation group transformation leads to the scaling requirement

$$P'(p) = (N/N')\lambda P(p) \tag{2.2}$$

where primed (unprimed) quantities refer to a system of N' (N) sites and $\lambda = \partial h/\partial h'$.

We now follow Indekeu *et al* (1982) by determining $P(p)$ within a 'mean-field' calculation (the formal application of mean-field approximations to percolation problems has been discussed extensively by De'Bell and Essam 1981, 1983a) in which the connectivity within a cell of n sites is treated exactly and the probability that a site adjacent to the cell is connected to the infinite cluster is set to b. Hence if the cell consists of a single site

$$(1 - P(b, h)) = (1-h)(1-pb)^z \tag{2.3}$$

where z is the coordination number of the lattice (setting $b = P$ in (2.3) we obtain the usual mean-field theory equation). (Our approach differs slightly from that of Indekeu *et al* in that we determine $P(p)$ at the origin and only use cells symmetric about the site at the origin. This is equivalent to treating every site in an infinite system by the same mean-field approximation. Indekeu *et al* averaged the magnetisation over all sites in a cell. While our method is more appropriate to the problems treated here, the differences in the two methods are essentially surface effects and should be negligible in the large-cell limit.) Since b is an effective percolation probability it must obey the same scaling condition as P:

$$b' = (N/N')\lambda b. \tag{2.4}$$

In the percolation problem, the percolation probability approaches zero as p approaches p_c and h approaches zero from above. Solving to leading order in b and h, the equation resulting from the substitution of (2.4) into (2.3) yields a recursion relation for p which is expected to be valid in the critical region.

The critical behaviour of the observables for the SAW problem is analogous to that found in interacting spin and percolation problems (e.g. McKenzie 1976): indeed there is a formal equivalence between the SAW observables and those of an n-vector model in the limit $n \to 0$ (de Gennes 1972). However, the interpretation of the ordered phase in the SAW problem is not clear. The SAW has been used as a model of polymers in the dilute region and the magnetisation and external field of the $n \to 0$ n-vector model do have a physical interpretation for polymers in the semi-dilute phase (Des Cloizeaux 1975, Daoud *et al* 1975); however, this does not provide a simple order parameter for the SAW problem. Redner and Reynolds (1981) have suggested that the order parameter for an isolated SAW is the fraction of monomers in an infinite SAW; however, their approach does not preserve the analogy with the magnetic system and in particular does not yield the value of the exponent γ expected from the magnetic analogy.

In this paper, it is assumed that a 'mean-field theory' for SAWS may be constructed by direct analogy with the percolation problem. We recall that the mean-field equation for the pair connectedness in the percolation problem reduces to a random-walk approximation in the region $P = 0$ ($p \leq p_c$, $h = 0$) (De'Bell and Essam 1981, equation (2.14)) and note that within the mean-field approximation the percolation probability in the region $p \leq p_c$ may be represented to leading order in h by a sum over finite clusters:

$$P(p) = \sum_{c \in C} W(c, p)h + O(h^2) \tag{2.5}$$

where C is the set of finite clusters with source at the origin and a single bond directly connecting a site of the cluster to the ghost site and $W(c, p)$ is the weight factor determined by the number of bonds (sites) in the cluster and its perimeter.

The SAW quantity analogous to the pair connectedness is the sum over all walks between the origin and site of $\boldsymbol{r}$, with weight p associated with each step of a walk. Within the random-walk approximation this may be written

$$W(\boldsymbol{r}) = \sum_{\boldsymbol{r}' \in \Omega(0)} pW(\boldsymbol{r} - \boldsymbol{r}') \qquad (W(0) = 1) \tag{2.6}$$

where $\Omega(0)$ is the set of sites adjacent to the origin. By analogy with the percolation problem, the mean-field order parameter (for $p < p_c$) is assumed to be

$$P_s(p) = \sum_{\boldsymbol{r}} \sum_{n} W_n(\boldsymbol{r}) p^n h + O(h^2) \tag{2.7}$$

where $W_n(\boldsymbol{r})$ is the number of n-step walks from the origin to $\boldsymbol{r}$ and h is the external field. The terms in the sum of (2.7) are a sum over all walks which pass through $\boldsymbol{r}$ and terminate with a step from a lattice site to the ghost site. Clearly the derivative of P_s with respect to the field is the analogue of the percolation mean size (or magnetic susceptibility):

$$\left.\frac{\partial P_s}{\partial h}\right|_{h=0} = \sum_{\boldsymbol{r}} \sum_{n} W_n(\boldsymbol{r}) p^n = \sum_{n} W_n p^n. \tag{2.8}$$

Consider now a mean-field calculation of P_s in which the effective value of P_s calculated at sites neighbouring the origin is taken to be b; then equations (2.6) and (2.7) lead to

$$P_s(p, h) = h + zpb + O(h^2, hb, b^2) = h' + O(h'^2) \tag{2.9}$$

(which is just equation (2.3) to leading order). Clearly this interpretation of the effective field h' may be extended to the case where walks within a cell are treated exactly (i.e. the self-avoiding constraint is applied) and walks outside the cell are treated by a mean-field approximation.

In order to apply the method of Indekeu *et al* to the self-avoiding walk problem we assume the mean-field order parameter in the region $p > p_c$ to be defined by (2.9) (or the corresponding equation for larger cells) and that it obeys the same scaling relation as the percolation probability (equation (2.2)) close to the critical point. Solving (2.2) to leading order in b then yields the zero-field recursion relation for p, as described for the percolation problems.

3. Numerical results

3.1. Self-avoiding walks on the square lattice

The technique described in § 2 has been applied to the SAW problem on the square lattice. The cells used belong to two classes, square cells and cross-shaped cells, and are shown in figure 1. By solving equation (2.2) for various pairs of cells, recursion relations for several different values of the length rescaling factor $l = (N/N')^{1/d}$ have been obtained. The fixed points and corresponding thermal exponents $y_t = \ln(\partial p'/\partial p)/\ln l$ and field exponents $y_h = \ln(\partial h'/\partial h)/\ln l$ are presented in table 1.

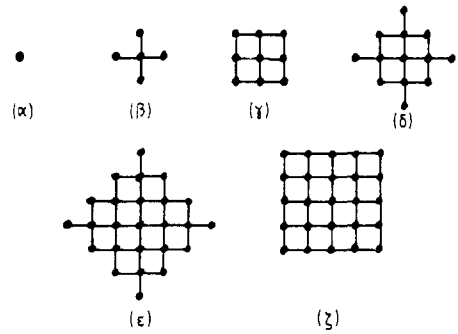

Figure 1. Labelling of cells used for the SAW and undirected percolation problems.

The fixed points and exponents of table 1 show a clear tendency to approach the expected values as the cell size is increased and are consistent with the prediction of Indekeu *et al* (1982) that application of the technique to cells of ever-increasing size should yield convergent sequences of results. (Convergent sequences would be obtained by comparing cells of similar shape. For completeness results obtained by comparing a square cell with a cross-shaped cell are included in table 1. These are in the same region as those obtained by comparing cells of similar shape but are clearly not part of the same sequences.)

3.2. Percolation on the square lattice

Using the technique described in § 2, recursion relations for the bond and site percolation problems on both the directed and undirected square lattices have been obtained. The fixed points and exponents are presented in table 1. Our results for

Table 1. Fixed points (p^*: first row of each label) and exponents (y_t: second row of each label; y_h: third row of each label) of the SAW. (*a*) undirected site percolation; (*b*) undirected bond percolation; (*c*) directed site percolation; (*d*) and directed bond percolation; (*e*) square lattice problems. The labels $\alpha, \beta, \ldots, \zeta$ for the SAW and undirected percolation problems refer to figure 1 and denote cells of linear dimension (L) 1, $\sqrt{5}$, 3, $\sqrt{13}$, 5, 5, respectively. The labels (1, 3, 5, ...) for the directed problems refer to square cells of linear dimension (L) 1, 3, 5, ... (see text).

(*a*)	L/L'	α	β	γ	δ
	β	0.333			
		0.86			
		1.53			
	γ	0.349	0.366		
		0.98	1.35		
		1.62	1.89		
	δ	0.346	0.355	0.333	
		0.95	1.10	0.80	
		1.58	1.68	1.38	
	ε	0.353	0.359	0.356	0.363
		0.99	1.14	1.02	1.18
		1.61	1.70	1.59	1.72
	ζ	0.357	0.364	0.363	0.370
		1.03	1.21	1.14	1.38
		1.64	1.77	1.70	1.89

Expected values: $p_c = 0.3790$, $y_t = 1.33$, $y_h = 1.88$ (McKenzie 1976)

(*b*)	L/L'	α	β	γ
	β	0.382		
		0.767		
		1.58		
	γ	0.427	0.500	
		0.804	0.979	
		1.61	1.69	
	δ	0.436	0.500	0.500
		0.765	0.770	0.435
		1.60	1.63	1.55

Expected values: $p_c = 0.593$, $y_t = 0.75 \pm 0.01$, $y_h = 1.93 + 0.07$ (Reynolds *et al* 1978, Essam 1980).

(*c*)	L/L'	α	β
	β	0.347	
		0.808	
		1.40	
	γ	0.372	0.405
		0.880	1.121
		1.48	1.82

Expected values: $p_c = 0.5$, $y_t = 0.75 \pm 0.01$, $y_h = 1.93 \pm 0.07$ (Essam 1980)

Table 1—continued.

(*d*)	L/L'	1	3	5	7	9
	3	0.555				
		0.748				
		1.426				
	5	0.578	0.604			
		0.765	0.793			
		1.455	1.513			
	7	0.592	0.615	0.626		
		0.773	0.794	0.796		
		1.471	1.524	1.541		
	9	0.602	0.622	0.632	0.639	
		0.776	0.794	0.794	0.793	
		1.479	1.531	1.546	1.553	
	11	0.610	0.628	0.637	0.643	0.647
		0.778	0.794	0.793	0.791	0.789
		1.486	1.536	1.550	1.555	1.560
Expected values: $p_c = 0.705$, $y_t = 0.581 \pm 0.007$ (De'Bell and Essam 1983a)						
(*e*)	L/L'	1	3	5	7	9
	3	0.525				
		0.767				
		1.422				
	5	0.540	0.558			
		0.781	0.805			
		1.449	1.508			
	7	0.551	0.566	0.575		
		0.786	0.803	0.799		
		1.464	1.520	1.536		
	9	0.558	0.572	0.580	0.586	
		0.787	0.800	0.796	0.792	
		1.473	1.527	1.541	1.550	
	11	0.564	0.577	0.584	0.589	0.593
		0.787	0.797	0.793	0.788	0.785
		1.481	1.531	1.546	1.553	1.558
Expected values: $p_c = 0.645$, $y_t = 0.581 \pm 0.007$						

undirected percolation are restricted to rather small cells but are comparable with those of other RSRG calculations of similar difficulty. In the case of directed percolation results have been obtained for square cells of between 1 and 121 sites.

In all of the problems considered the values of p^* show a clear (if slow) tendency to approach the expected value with increasing cell size. The values of y_t show an initial upward trend with increasing cell size, the expected downward trend only appearing in the results for the directed problems obtained from the largest cells used. In the directed percolation problems there are two characteristic divergent lengths: $\xi_\parallel \sim |p_c - p|^{-\nu_\parallel}$ and $\xi_\perp \sim |p_c - p|^{-\nu_\perp}$, respectively the connectedness lengths parallel and perpendicular to the direction in which the system first percolates (Kinzel and Yeomans 1981). Only $\xi_\parallel$ rescales like a simple length scale under the type of lattice transformation described here, and the values of y_t reported in table 1 are approximations to $1/\nu_\parallel$ (Redner 1982). The difference between $\nu_\parallel$ and $\nu_\perp (\nu_\parallel > \nu_\perp)$ is a reflection of the

highly anisotropic nature of the large clusters which exist close to p_c. The initial values of y_t obtained for directed percolation are close to those obtained for the undirected isotropic problem and it seems probably that the anisotropic nature of the directed problems is not clearly distinguished in the small-cell calculations. The values of y_h for the undirected problems show an improvement with cell size similar to that found in the SAW problem. The estimates of y_h for the directed problems also appear to form well behaved sequences and would be consistent with a value of $y_h > 1.56$. This would indicate that the directed exponents do not obey the usual scaling law $y_h = \Delta y_t$ ($\simeq 1.47$: Blease 1977, De'Bell and Essam 1983a).

3.3. *Percolation on the hypercubic lattices*

Indekeu *et al* (1982) have applied the mean-field renormalisation group method to a q-state Potts model on the d-dimensional hypercubic lattice by using a cell of only two sites (renormalised to a single site). Using their expression for the nearest-neighbour interaction fixed point

$$K^* = \frac{q-1}{q} \ln\left(\frac{q+2(d-1)}{2(d-1)}\right) \tag{3.1}$$

and the relation between the critical probability p_c for undirected bond percolation and the critical point of the $q \to 1$ Potts model (Kasteleyn and Fortuin 1969)

$$p^*_{\lim_{q\to 1}} = 1 - \exp[-K^*/(q-1)] \tag{3.2}$$

we obtain

$$p^* = 1/(2d-1) \tag{3.3}$$

which is exactly the solution of the recursion relations for undirected bond percolation obtained using the technique described in § 2 with a two-spin cell.

Unfortunately the two-spin cell transformation is anisotropic for $d > 1$. To study the percolation problems for general d we have constructed recursion relations using the smallest cell which provides an isotropic transformation for general d. That is a cell consisting of the site at the origin and its $2d$ nearest neighbours. The recursion relations for general d may readily be written down: for example, for undirected site percolation

$$p' = (2d-1)p^2 - (d-1)p^3 \tag{3.4}$$

with fixed point at

$$p^* = \{(2d-1) - [(2d-1)^2 - 4(d-1)]^{1/2}\}/2(d-1). \tag{3.5}$$

The fixed points and exponents for various values of d are given in table 2. In all of the problems considered the estimates of p^* improve with increasing dimensionality and the recursion relations have fixed points at the expected mean-field value in the large-d limit (i.e. $p^* = 1/2d$ for the undirected problems and $p^* = 1/d$ for directed problems). The exponents for the undirected problems show the expected variation with dimensionality below the critical dimension $d_c(=6)$ and approach (within the accuracy of the present calculation) the mean-field values at d_c. The dimensional dependence of the exponents continues for $d > d_c$ and this may be attributed to the

Table 2. Fixed points and exponents for the undirected (*a*) and directed (*b*) percolation problems on the *d*-dimensional hybercubic lattice. In all cases cells of $(2d+1)$ sites were used. Figures in brackets are reliable estimates of p_c (Reynolds *et al* 1978, Sur *et al* 1977, Kirkpatrick 1976, Blease 1977, De'Bell and Essam 1983a, b). The expected values of y_t and y_h are based on the exponent estimates obtained by other authors (Essam 1980, Blease 1977, De'Bell and Essam 1983a, b) and the relation $y_t = 1/\nu$, $y_h = \frac{1}{2}[d + (\gamma/\nu)] = \Delta/\nu$.

(*a*)	Site problem			Bond problem			Expected results	
d	p^*	y_t	y_h	p^*	y_t	y_h	y_t	y_h
2	0.382(0.593)	0.77	1.58	0.347(0.500)	0.81	1.54	0.75 ± 0.01	1.93 ± 0.07
3	0.219(0.312)	0.99	2.15	0.203(0.312)	1.04	2.11	1.18 ± 0.07	2.59 ± 0.25
4	0.153	1.20	2.73	0.144(0.198)	1.25	2.70		
5	0.117	1.39	3.31	0.112(0.141)	1.43	3.28		
6	0.095	1.57	3.89	0.091(0.106)	1.61	3.87	2	4
7	0.080	1.74	4.47	0.077	1.79	4.45	2	4
8	0.069	1.91	5.05	0.067	1.95	5.03	2	4

(*b*)	Site problem			Bond problem			Expected results
d	p^*	y_t	y_h	p^*	y_t	y_h	y_t
2	0.586(0.705)	0.75	1.48	0.539(0.645)	0.76	1.45	0.58
3	0.383(0.432)	0.95	2.09	0.347(0.383)	1.00	2.05	0.79 ± 0.01
4	0.279	1.15	2.68	0.256(0.268)	1.22	2.64	
5	0.219	1.34	3.27	0.203(0.209)	1.41	3.23	1
6	0.180	1.53	3.86	0.169(0.171)	1.59	3.82	1
7	0.153	1.70	4.44	0.144(0.146)	1.77	4.40	1

implicit assumption of hyperscaling (as noted by Inedkeu *et al* 1982). As noted previously in § 2.2 the exponents for directed percolation are close to the undirected values, and this may be assumed to be a small-cell effect.

4. Summary

It has been shown that the mean-field renormalisation group method recently introduced by Indekeu *et al* (1982) may be directly applied to the self-avoiding walk and percolation problems. Though no explicit use has been made of the relations between these models and the $n \to 0$ limits of interacting spin models, the analogies between the geometric and thermal models have been preserved (i.e., the defining equations of the renormalisation group transformation are the exact analogues of those for interacting spin systems).

Results for the square lattice have been obtained by the use of a variety of small cells (table 1). The values of p^*, y_h and, in the case of the SAW problem, y_t all show an improvement with increasing cell size similar to that found by Indekeu *et al* for the square lattice Ising model, and are consistent with the suggestion of Indekeu *et al* that the results should be convergent and hence that extrapolation techniques should be applicable to large-cell calculations. In this respect the initial movement of y_t for the percolation problems away from its expected value is disappointing; however, the results for directed percolation indicate that this behaviour may be

associated with small cells only. We note that initial results for y_t in the undirected site percolation problem by the method of Reynolds *et al* (1978) showed some oscillatory behaviour, while results based on larger cells appeared convergent.

Finally calculations for percolation problems on a d-dimensional hypercubic lattice (table 2) indicate that the estimates of p^* become increasingly accurate with increasing d. The exponents show the expected dimensional dependence for $d < d_c$; however, this dependence continues when $d > d_c$ due to the implicit assumption of hyperscaling.

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