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COMMENT

Effects of dilution on the phase diagram of some non-equilibrium systems

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Abstract. The effects of site dilution on the phase diagram of the contact process and other related non-equilibrium systems is studied by use of the mean-field renormalisation group method. The variation of the critical kinetic parameter reflects the decrease of the effective dimensionality due to dilution.

1. Introduction

Among the simplest realisations of non-equilibrium systems whose steady states display a phase transition are certain stochastic lattice models when rates of creation and annihilation of particles depend on the local environment and on certain kinetic parameters.

One example is the 'contact process', which can be seen as a model of an epidemic with recovery or as a realisation of Schlögl's model of an autocatalytic reaction. This process has been exhaustively studied by different methods [1, 2] and shown to belong to the same universality class as directed percolation [3] and Reggeon field theory [4]. Other related models, such as the so-called A-model, which can be used to describe the poisoning of a catalytic surface have also been studied [2]. Whereas in most cases rather accurate estimates of critical dynamic parameters and critical exponents can be achieved by numerical methods (either Monte Carlo simulations or, in the case of one-dimensional systems, series expansions methods [2]) the analytic studies are still far behind: besides the rate approximation, which is essentially a site mean-field theory and gives rather poor estimates of the critical parameters, there are some results of the dynamic pair approximation [5] and, recently, of another finite cluster method which also incorporates the ideas of scaling, the mean-field renormalisation-group (MFRG) method [6]. The results of the latter are very close to those of the pair approximation when one compares one- and two-site clusters [7], whereas the consideration of bigger clusters is likely to improve the results considerably.

The possibility of spatial disorder by introducing randomness in the local reaction probabilities was first considered by Kinzel [3] and then developed by Noest [8] for the stochastic cellular automata of directed percolation. The emphasis of this numerical study is less on the concentration dependence of the critical parameters than on the determination of the critical exponents associated with a new universality class.

In this work, we use the MFRG method to study how dilution affects the critical kinetic parameters in some of these models with different local rules and dynamics. The method has the advantage of being an analytic one and is easily implemented

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with small clusters, even though the difficulty in treating bigger clusters, due to the extension of the algebra, precludes an accuracy comparable to the results of computer simulations, or a correct description in the vicinity of the percolation threshold.

In section 2 we consider the contact process with dilution. In section 3 we study a model with sequential dynamics and local rules identical to the ones of site-directed percolation; for comparison, the results for the same model with simultaneous updating in two interpenetrating sublattices are also presented. In section 4 we consider again the contact process but with a different type of disorder. We conclude in section 5 with a brief discussion of the results.

2. Contact process with dilution

This process is applied to lattice models such that to each site a binary variable $\sigma_i = 0$ or 1 is associated. $\sigma_i = 0$ (1) can represent a vacant (occupied) site on a process of adsorption-desorption on a surface; it can represent a healthy (ill) person in a population with low mobility subjected to an epidemic process, or a moderate (extremist) view in the propagation of public opinion. The local rules for this process are such that $\sigma_i = 1$ changes to $\sigma_i = 0$ at a rate $1/(1+\eta_i)$ whereas the rate for $\sigma_i = 0$ changing to $\sigma_i = 1$ is taken as $\eta_i/(1+\eta_i)$ times the fraction of 1's in 'influent' nearest-neighbour sites to i.

We consider here a model with quenched disorder such that $\eta_i = \eta$ in a fraction p of the sites and $\eta_i = 0$ in the remaining sites. In processes of desorption-adsorption this means that a fraction $(1-p)$ of the sites is not appropriate to adsorb particles, whereas in epidemic processes this means that a fraction $(1-p)$ of the population has been vaccinated and is therefore imune to catching illness again; and in the process of propagation of a public opinion we can also think of the effects of cutting the means of communication to a fraction of individuals chosen at random, therefore securing that this fraction cannot hold extremist views and has no possibility of influencing its neighbours.

Let us exemplify the rules of this process on a square lattice. Consider the neighbourhood of site i, as shown in figure 1(a). In this case, all the nearest neighbours of i are 'influent' sites (η_i is non-zero for all of them, so there is the possibility of 0's becoming 1's in a subsequent time interval); the rate for site i going from $\sigma_i = 0$ to $\sigma_i = 1$ is then $\frac{2}{4}\eta/(1+\eta)$; $\frac{2}{4}$ being the ratio of the number of 1's in nearest-neighbour sites (=2) and the number of influent sites (=4). Now consider the configuration displayed in figure 1(b), where the site labelled by $\times$ is a non-influent site (i.e. $\eta_j = 0$); in a steady situation the configuration of that site will always be $\sigma_j = 0$, since there is no possibility for 0 to change to 1 since this site has been prevented from communicating

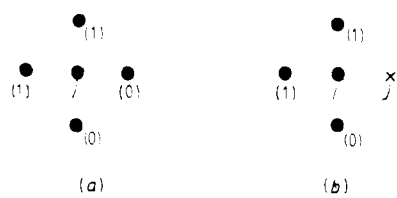

Figure 1. Possible configurations for the neighbours of site i. (a) Four 'influent' neighbours, two of which are in state (1); (b) three 'influent' neighbours, two of which are in state (1).

with others. In this case the rate for site i going from $\sigma_i = 0$ to $\sigma_i = 1$ is now $\frac{2}{3}\eta/(1+\eta)$, i.e. the influence of the two active neighbours is larger than in the previous case because the number of 'influent' sites has decreased.

We now apply the MFRG method to this model, following the procedure in [6]. We start by writing the time evolution of the probabilities for a cluster of two influent sites, ij:

$$\frac{dP_{(00)}}{dt} = -P_{(00)}\left(\frac{\eta}{1+\eta}\right)\left(\frac{E}{E+1}+\frac{D}{D+1}\right)x + (P_{(01)}+P_{(10)})\frac{1}{1+\eta}x + O(x^2)$$

$$\frac{dP_{(01)}}{dt} = P_{(11)}\frac{1}{1+\eta} - P_{(01)}\left(\frac{1}{1+\eta}+\frac{\eta}{1+\eta}\frac{1}{E+1}\right) + P_{(00)}\left(\frac{\eta}{1+\eta}\right)\left(\frac{D}{D+1}\right)x + O(x^2)$$

where x is the probability of an influent site outside the cluster to be occupied (x is arbitrarily small in the vicinity of the transition) and E (D) is the number of influent neighbours to i (j) other than j (i). For brevity we have omitted similar equations for $dP_{(10)}/dt$ and $dP_{(11)}/dt$.

In the steady state and averaging over all possible configurations of the neighbours one gets for $P_{II} = P_{(11)} + \frac{1}{2}(P_{(10)} + P_{(01)})$:

$$\begin{aligned} P_{II} = x[&p^6 f(\eta,3,3) + 6p^5(1-p)f(\eta,3,2) + 6p^4(1-p)^2 f(\eta,3,1) + 9p^4(1-p)^2 f(\eta,2,2) \\ &+ 2p^3(1-p)^3 f(\eta,3,0) + 18p^3(1-p)^3 f(\eta,1,2) + 6p^2(1-p)^4 f(\eta,2,0) \\ &+ 9p^2(1-p)^4 f(\eta,1,1) + 6p(1-p)^5 f(\eta,1,0)] + O(x^2) \end{aligned}$$

where $f(\eta, E, D) = P_{(11)}(\eta, E, D) + \frac{1}{2}[P_{(10)}(\eta, E, D) + P_{(01)}(\eta, E, D)]$

$$P_{(11)}(\eta, E, D) = \frac{D/[(D+1)(E+1+\eta)] + E/[(E+1)(D+1+\eta)]}{(E+1)/(E+1+\eta) + (D+1)/(D+1+\eta)}\eta^2$$

$$P_{(10)}(\eta, E, D) = \frac{E+1}{E+1+\eta}\left(P_{(11)}(\eta, E, D) + \frac{\eta D}{D+1}\right)$$

$$P_{(01)}(\eta, E, D) = \frac{D+1}{D+1+\eta}\left(P_{(11)}(\eta, E, D) + \frac{\eta E}{E+1}\right).$$

In a similar way, one gets for a one-site cluster

$$P_I = \eta'[1-(1-p)^4]x' + O(x'^2).$$

Applying now the MFRG main assumption that in the vicinity of the transition P_I and P_{II} must scale like x' and x, one is led to the RG fixed-point equation $\eta_c = \eta_c(p)$. This relation is displayed in figure 2 for $p^* < p < 1$; p^* is the site-percolation concentration, below which there is no possibility of an infinite cluster of influent sites, and therefore no steady state with non-zero fraction of occupied sites can be attained.

For $p = 1$, one recovers the pure contact process; for this one knows [6] that comparison of one-site and two-site clusters within MFRG just gives $\eta_c = 2d/(2d-1)$, d being the dimensionality, and therefore $\eta_c(p=1) = \frac{4}{3}$. The inclusion of non-influent sites has the effect of increasing η_c; however η_c never reaches the value $\eta_c = 2$ predicted for a one-dimensional system within the same approximation. The estimate obtained for η_c at the percolation concentration $\eta_c(p^*) = 1.46$ corresponds here to an effective dimensionality $D = 1.6$, in agreement with the sparse structure characteristics of the backbone [8].

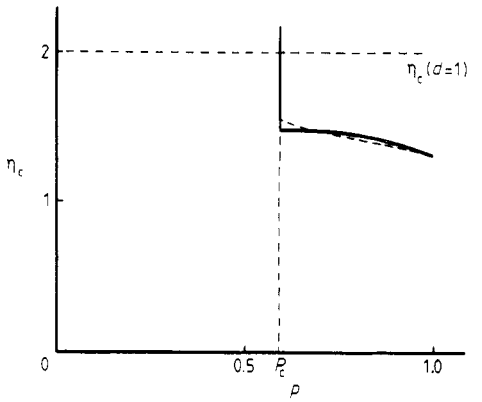

Figure 2. Phase diagram for the contact process with dilution. Results of the MFRG method by counting all the configurations of neighbours and then averaging (full curve). Results of the MFRG method by considering the average effect of dilution on dynamic rules (broken curve). Also indicated is $\eta_c(d=1)$, as given by the MFRG method, again by comparison of one- and two-site clusters.

An alternative way to take into consideration the change in the local rules introduced by dilution is, instead of counting all the possible configurations of neighbours and then averaging, as we have done above, to enter beforehand with the average effect dilution has on these dynamic rules. This means giving different weights to the sites when calculating the fraction of occupied influent sites: sites outside the cluster enter with weight $\bar{\eta} = p\eta$, whereas the influent sites of the cluster considered enter with weight η. This means, for example, for the two-site cluster considered before, that the rate at which $P_{(01)}$ changes to $P_{(11)}$, for vanishingly small x, is now $[\eta/(1+\eta)]/[\eta/(3\bar{\eta}+\eta)]$ and the rate for P_{00} changing to P_{01} is now $3\,[\eta/(1+\eta)]/[\bar{\eta}x/(3\bar{\eta}+\eta)]$.

With these changes, the MFRG equation, when clusters of the same size as above are considered, becomes

$$\frac{3p}{3p+1}\left(\frac{\eta_c}{3p+1}\right)-1=0$$

i.e. $\eta_c=(3p+1)/3p$.

The result of this approximation is also represented in figure 2. Consideration of bigger clusters is certainly required for better accuracy if one wants to compare these estimates with results of simulation studies, even though we are not aware that they exist in this case; however, the algebra involved becomes increasingly tedious and we have not attempted that here. We think that, apart from this limitation, the present approximation is able to give the correct picture of the concentration dependence of the critical kinetic parameter in this process.

3. Effects of dilution in other processes

We now consider the effects of dilution in a process with sequential dynamics and probability P_i that site i appears in state 1 given that any of its nearest neighbours is in state 1 one time step before. As can be seen in [3], the use of this same rule and simultaneous updating of sites in two sublattices leads to the cellular automatum that describes site-directed percolation.

The time evolution of the probabilities for a cluster of two sites is now, to leading order in x

$$\frac{dP_{(00)}}{dt} = -2PP_{(00)}x + (P_{(01)} + P_{(10)})$$

$$\frac{dP_{(11)}}{dt} = -2P_{11}(1-P) + (P_{(01)} + P_{(10)})P.$$

Incorporating now the possibility of site dilution, i.e. considering that P_i takes the value P in a fraction p of the sites and is zero in the remaining sites, leads, when comparison of the two smallest clusters is considered, to the following concentration dependence of the critical parameter: $P_c = 1/(3p+1)$. This is plotted in figure 3 together with the results of the MFRG when four-site clusters are also used in the comparison. As can be seen P_c increases monotonically with $(1-p)$; however, even in the vicinity of the percolation threshold, P_c is still far below the value obtained within a comparable approximation for a one-dimensional system (a MFRG with one- and two-site clusters gives in this case $P_c = \frac{1}{2}$). It would be interesting to be able to compare these results with those of numerical simulations: the present approximation is again expected to give a good qualitative prediction of the concentration dependence of the critical parameter, although, as in the pure system, one would have to go to bigger clusters and lengthier algebra to extract more accurate estimates.

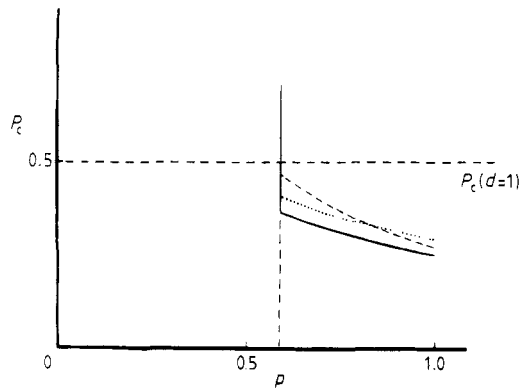

Figure 3. Results of the MFRG method for the other process considered. Sequential dynamics, comparison of one- and two-site clusters (full curve); sequential dynamics, comparison of one- and four-site clusters (broken curve); simultaneous updating, comparison of one- and two-site clusters (dotted curve). Also indicated are the values of $P_c(d=1)$ and $P_c(d=2)$ as given by the MFRG method by comparison of one- and two-site clusters.

Very accurate numerical data certainly do exist [9] for this process with simultaneous updating, i.e. directed percolation. Noest [8] has studied this model with dilution but also numerical methods seem to face certain difficulties in determining accurately the full phase diagram. Our study here is therefore meant as a comparison to what has been done above for the process with sequential dynamics and to the qualitative picture drawn in figure 1 of [8].

The MFRG method is therefore now applied to the simultaneous updating in two interpenetrating sublattices, as referred to in [3]. Taking now as a time unit the time

for updating in one sublattice followed by updating in the other, one has, for the rate of change of (01) into (10), $P(1-P)$. The rates of change of (σ_i, σ_j) into (σ_i', σ_j') are indicated in table 1, again for a square lattice and in the vicinity of the transition.

The MFRG equation is now, for the model with dilution and when the smallest clusters are considered,

$$\frac{p}{(1-P_c)(1+2P_c)}\left[P_c+(P_c+1)\left(3+\frac{P_c}{-P_c^2+P_c+1}\right)\right]+3(1-p)=4$$

and the respective plot is also included in figure 3. For the pure one-dimensional system the same approximation gives $P_c=\frac{1}{2}$, considerably above the value obtained for $P_c(p^*)\simeq 0.39$. Of course these estimates represent just a qualitative picture of the concentration dependence, once the values obtained within this approximation for the pure system do not distinguish between site and bond dilution and are still far from accurate values for bond-directed percolation: $P_c(d=1+1, \text{square lattice})=0.705$ [3], $P_c(d=2+1, \text{BCC})=0.287$ [9]. The consideration of bigger clusters involves in this case more tedious algebra and we have not done that here.

Table 1

(σ_i, σ_j)	(σ_i', σ_j')	Rates
(00)	(11)	$3P^2x$
(00)	(10)	$3P(1-P)x$
(00)	(01)	$3P(1-P)x$
(01)	(11)	P^2
(01)	(00)	$1-P$
(01)	(10)	$P(1-P)$
(10)	(11)	P^2
(10)	(00)	$1-P$
(10)	(01)	$P(1-P)$
(11)	(00)	$1-P$
(11)	(10)	$P(1-P)$
(11)	(01)	$P(1-P)$

It still remains to investigate whether the different values of P_c for the process with sequential or simultaneous dynamics are just a result of the approximation or whether they are intrinsic to the models; there is, in principle, no reason why different dynamics should lead to the same critical kinetic parameters, even in cases where the same critical exponents are encountered.

4. Contact process with a different type of disorder

We again consider the contact process where the rates of change are again $1/(1+\eta_i)$ and $\eta_i/(1+\eta_i)$ times the fraction of 1's in nearest-neighbour sites, but now we assume that, independently of the site, there is a probability p that $\eta_i=\eta$ and a probability $(1-p)$ that $\eta_i=0$. This process can describe the situation when members of the population undergo temporary and random isolation such that at a given time they have a certain probability of behaving as non-influent.

The time evolution of the probabilities is now, for a two-site cluster on a square lattice,

$$\frac{dP_{(00)}}{dt} = -\tfrac{3}{2}P_{(00)}\left((1-p)\frac{\eta}{1+\eta}\right)^{x} + (P_{(10)}+P_{(01)})\left((1-p)\frac{1}{1+\eta}+P\right)+O(x^2)$$

$$\frac{dP_{(11)}}{dt} = -2P_{(11)}\left((1-p)\frac{1}{1+\eta}+p\right)+\tfrac{1}{4}(P_{(10)}+P_{(01)}\left((1-p)\frac{\eta}{1+\eta}\right)+O(x^2)$$

and the MFRG method applied to this process gives a transition at $\eta_c = 4/(-4+7p)$. When $p = 1$ one recovers the estimate $\eta_c = \frac{4}{3}$ for the pure system. However, the transition disappears for $p < \bar{p} = \frac{4}{7}$, $\bar{p}$ playing here the role of a percolation threshold, even though this problem is conceptually different from quenched dilution (where translation invariance is broken); also here $1/\eta_c$ goes to zero when p approaches $\bar{p}$, contrary to what happens in the quenched dilution case, as we have seen above.

5. Conclusions

In conclusion, we have shown that the interest of the present method as an analytic tool to deal with phase transitions in non-equilibrium systems extends to situations where the local dynamic rules present some type of spatial disorder.

The implementation of the method by using small clusters presents some limitations. The estimates it gives for the critical exponents are usually poorer than the ones for the critical parameters; for example, υ is always estimated from above ($d\upsilon$ is above 2 in the present cases and this prevents us from checking the extension of the Harris criterion to non-equilibrium systems [8], with the occurrence of new critical exponents associated with the disorder); the use of small clusters also misses important details in the vicinity of the percolation threshold. However, a considerable improvement of the results by considering bigger clusters is bound to involve rather lengthy calculations.

Despite these limitations we think that the method is useful for a qualitative description of the effects of disorder on the phase diagram of these systems; the processes involved have interest on their own and it would be useful to have results, numerical or otherwise, to compare with the present ones.

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