Model of pair aggregation on the Bethe lattice

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We extend a recent model of aggregation of pairs of particles, analyzing the case in which the supporting framework is a Bethe lattice. The model exhibits a critical behavior of the percolation theory type. $[S1063-651X(97)03403-X]$

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I. INTRODUCTION

The continuing interest of the scientific community in disordered systems and aggregation processes is due to the widespread occurrence of these phenomena in nature and throughout the pure and applied sciences $[1–5]$. This has led to the development of theoretical models, which often put on equal footing problems quite distinct in appearance. Percolation theory (PT) [6] is a good example of a unifying conceptual framework for problems such as the spreading of infections $[7]$, fracture in heterogeneous materials $[8]$, sol-gel transition and polymerization [9], galactic structure $[10]$, dynamics of solar active regions $[11]$, recovery of oil from porous rocks $[12]$, hopping in semiconductors $[13]$, or thermal phase transitions $[14]$. Variants of the canonical models are explored to obtain insights and to accommodate the future theoretical demands of phenomenology.

With this aim, in Ref. $[15]$ we introduced a random model to simulate particle-pair aggregation. We used a lattice with each site occupied by one particle. Each particle has its partner and both are linked by a string no longer than a maximum length ℓ , which is an integer multiple of the basic lattice spacing. The spatial distance between the two partners is chosen at random between 1 and ℓ . When strings of different pairs intersect, they are assumed to become entangled. Thus disjoint clusters of pairs are formed. [This type of model may constitute an intermediate stage between the ordinary PT, in which single sites (or bonds) form aggregates, and other much more complex models involving clustercluster interactions, only accessible through very expensive numerical simulations. In one dimension there is no chance of forming a cluster of infinite pairs. Indeed, the distribution of clusters composed of *s* pairs decays exponentially with *s*. On the contrary, in two dimensions (square lattices), for $l \geq 4$, there appears a unique cluster connecting the limits of the underlying lattice. As the distance between the pairs is an integer number, the jump in the behavior between ℓ = 3 and 4 is drastic; in other words, there is no continuous parameter that could be adjusted to reach a critical point.

In this paper, we fill this gap with a model of this same type, located in another well-known framework: the Bethe lattice (BL). The criterion of clustering is simplified to render it tractable while retaining an interesting structure. In Sec. II, the model is presented. The cases ℓ = 2 and 3 are solved and we also calculate a mixed case where a random number p , between 0 and 1, fixes the respective probabilities of using $l = 2$ or 3 in building up clusters. In this mixed case, an interesting critical structure appears. In Sec. III, various moments of the size distribution are calculated that allow us to calculate some critical exponents. Finally, in Sec. IV, we carry out a comparison with standard PT on the BL $\lfloor 16,17 \rfloor$ and state our conclusions.

II. MODEL

BL's are characterized by their coordination number *Z*, but as the critical behavior that will emerge later is *Z* independent, we will analyze the most simple case $Z=3$. Occasionally, comments for other values of *Z* will also be made.

In the philosophy of our model, pairs of particles are located on different sites of a BL with $Z=3$. See Fig. 1(a). There, a pair is identified by a particle with a letter, for example, A , and its partner with A' . As we see in this figure, we agree that two pairs are linked if one of the particles of the pair is located on a site (elbow) left free by another pair along its string. In Fig. 1(a), for example, the pair AA' is

FIG. 1. Entanglements between particle pairs: (a) allowed entanglements and (b) forbidden entanglements.

linked to BB' and BB' to CC' and EE' . The pairs DD' and *FF'* are free and there is no chance of entanglement. As in our model, all sites are occupied by particles; the four free sites left unoccupied in Fig. $1(a)$ would be the origins of other clusters. Thus, what is drawn in Fig. $1(a)$ represents one cluster of four pairs and two clusters of one pair. The number of pairs forming a cluster will be denoted by *s*, and n_s will stand for the normalized probability of generating clusters of size *s*, departing from a given site.

From what has been said in the previous paragraphs, we deduce that there is a restriction in the location process. The restriction consists in assuming that there can be only one string running along any bond of the lattice. In Fig. $1(b)$, the bond between B and A' has two strings, one belonging to the pair AA' and the other to the pair BB' . Also in Fig. 1(b), the bond between C' and D' has two strings, both belonging to the pair CC' . Therefore, these two entanglements are forbidden.

Thus, by allowing only insertions on the free elbows of the type in Fig. $1(a)$, we respect the basic branching structure of the Cayley tree. This also leads to a great simplification: any configuration formed by *s* linked pairs is characterized by the number of free sites *n*, where insertions are possible. These configurations, for ℓ fixed, will be called V_n . Obviously, if $n=0$, we have a closed cluster already inaccessible to growth by new pair additions.

A. Case $\ell = 2$

The case $l = 1$ is trivial: $n_1(l = 1) = 1$. For $l = 2$, and always supposing $Z=3$, one observes that after locating one of the particles of the pair and heading in one direction, its partner has three possibilities of location (one of them at distance 1 and two at distance 2). Hence we find the probability $\frac{1}{3}$ of having a configuration V_0 and $\frac{2}{3}$ of having configurations V_1 . This can be expressed by the vector

$$
\mathbf{V}^{(1)} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}^{(1)}.
$$
 (2.1)

Hence n_1 (ℓ = 2) = $V_0^{(1)} = \frac{1}{3}$. The addition of a new pair to the first will be represented by the action of a matrix on $V^{(1)}$. In this sense we follow the strategy used in Ref. $[15]$ for one dimension. The first component of $V^{(1)}$, which stands for V_0 , is closed and, as a consequence, cannot grow. The configuration V_1 (second component) can either be closed by a new addition (probability $\frac{1}{3}$) or give birth to a new configuration V_1 (probability $\frac{2}{3}$). Thus, by inspection, we find that the form of the relevant transfer matrix is

$$
\begin{pmatrix} 0 & \frac{1}{3} \\ 0 & \frac{2}{3} \end{pmatrix} \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}^{(1)} = \begin{pmatrix} \frac{2}{9} \\ \frac{4}{9} \end{pmatrix}^{(2)}.
$$
 (2.2)

Thus, in our notation, the superscript in the vectors denotes the number of pairs entangled in a cluster and the values of the respective components are the probabilities of having none or one free elbow. Therefore, in Eq. (2.2) the first component of the vector $(s=2)$ is the probability of generating a closed configuration V_0 and hence $n_2(\ell=2)=\frac{2}{9}$. For $\ell=2$, it is clear that the process repeats itself identically because the transfer matrix is always the same. This implies that

$$
\mathbf{V}^{(s+1)} = \begin{pmatrix} 0 & \frac{1}{3}(\frac{3}{2})^{s-1} \\ 0 & (\frac{2}{3})^s \end{pmatrix} \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}^{(1)} = \begin{pmatrix} \frac{1}{3}(\frac{2}{3})^s \\ (\frac{2}{3})^{s+1} \end{pmatrix}^{(s+1)}
$$
(2.3)

and, as a consequence, n_s , i.e., the probability of generating a cluster of size *s*, is

$$
n_s = \frac{1}{3} \left(\frac{2}{3}\right)^{s-1} \quad (\ell = 2, \ Z = 3). \tag{2.4}
$$

Thus n_s is a mere geometric progression. Its sum is

$$
S = \sum_{s=1}^{\infty} n_s = \frac{1}{3} \frac{1}{1 - \frac{2}{3}} = 1.
$$
 (2.5)

This result holds for any Z . Thus n_s declines exponentially with *s* and there cannot exist any clusters of infinite size because the probability of generating finite clusters saturates the total probability. For later use, let us calculate $T = \sum_{s=1}^{\infty} s n_s$, which provides the mean size of the finite clusters. Rewriting Eq. (2.4) as $n_s = \frac{1}{2}a^{s-1}$, $a = \frac{2}{3}$, we have

$$
T = \frac{1}{3} \sum_{s} s a^{s-1} = \frac{1}{3} \sum_{s} \frac{d}{da} (a^{s}) = \frac{1}{3} \frac{d}{da} \left(\sum_{s} a^{s} \right)
$$

$$
= \frac{1}{3} \frac{d}{da} \left(\frac{a}{a-1} \right) = 3. \tag{2.6}
$$

B. Case $\ell = 3$

Let us analyze the case $\ell = 3$ (Z=3). Using arguments similar to those used for ℓ = 2, we see that

$$
\mathbf{V}^{(1)} = \begin{pmatrix} \frac{1}{7} \\ \frac{2}{7} \\ \frac{4}{7} \end{pmatrix}^{(1)},
$$
 (2.7)

i.e., a first pair of particles can give rise to configurations V_0 (probability $\frac{1}{7}$), V_1 (probability $\frac{2}{7}$), and V_2 (probability $\frac{4}{7}$). Thus n_1 ($\ell = 3$) = $\frac{1}{7}$. $\mathbf{V}^{(2)}$ is constructed by observing the configurations that can arise from those of $V^{(1)}$ after adding a new pair. In fact, there is an important difference with respect to the case ℓ = 2. Now the configuration *V*₂ can give rise to configurations V_1 , V_2 , and V_3 , i.e., the size of $V^{(2)}$ has one component more than $\mathbf{\bar{V}}^{(1)}$. This implies that the corresponding transfer matrix is no longer a square matrix. In this initial step we would have

$$
\begin{pmatrix} 0 & \frac{1}{7} & 0 \\ 0 & \frac{2}{7} & \frac{1}{7} \\ 0 & \frac{4}{7} & \frac{2}{7} \\ 0 & 0 & \frac{4}{7} \end{pmatrix} \begin{pmatrix} \frac{1}{7} \\ \frac{2}{7} \\ \frac{4}{7} \end{pmatrix}^{(1)} = \begin{pmatrix} \frac{1}{7} \times \frac{2}{7} \\ (\frac{2}{7})^2 + \frac{4}{7^2} \\ 2 \times \frac{4}{7} \times \frac{2}{7} \\ (\frac{4}{7})^2 \end{pmatrix}^{(2)}
$$
(2.8)

Hence $n_2(\ell=3) = \frac{2}{49}$. As we can easily see, the transfer matrix to pass from the stage (*s*) to $(s+1)$ is an $(s+3)\times(s+2)$ matrix of the form

Once **M** is known, n_s (ℓ = 3) can be calculated for any *s*. When the sum $\sum n_k$ for $\ell = 3$ is made we obtain

$$
S(\ell=3) = \frac{1}{4},\tag{2.10}
$$

i.e., only 25% of probability corresponds to generate finite clusters and the other 75% to generate infinite clusters. Performing this analysis for $\ell = 3$ and arbitrary *Z*, we obtain

$$
S(\ell=3,\mathbb{Z})=\frac{1}{(\mathbb{Z}-1)^2}.
$$

C. Mixed case of $\ell = 2$ and 3

The results obtained for ℓ = 2 and 3 make it plausible to think that a combination of the two cases will generate a model where the probability of generating infinite clusters will start from zero in the way that occurs in standard percolation [6]. With this aim, let us define the probability p of using pairs taken from the pure case $\ell = 3$, and a probability $q=1-p$, of using pairs of $l=2$.

The calculation of the new $S(p) \equiv \sum_{s} n_s$ can be done selfconsistently $[6]$. As any reference point is totally equivalent to any other, in order to generate finite clusters we can state the following equation for *S*:

$$
S = \left(\frac{1-p}{3} + \frac{p}{7}\right) + 2\left(\frac{1-p}{3} + \frac{p}{7}\right)S + \frac{4p}{7}S^2 \quad (Z = 3). \tag{2.11}
$$

The two solutions of this second-order algebraic equation in *S* are

$$
S = 1, \quad S = \frac{7 - 4p}{12p}.
$$
 (2.12)

The second solution is valid for $S \le 1$, i.e., $16p \le 7$; thus there is a transition at a critical value of *p*, $p_c = \frac{7}{16} = 0.4375$. For $p < p_c$, $S=1$ (this includes the case $p=0$, i.e., $l=2$); for $p > p_c$, $S = (7-4p)/12p$; and for $p=1$, $S = \frac{1}{4}$, calculated by summing up explicitly the successive $n_s(l=3)$. These results are shown in Fig. 2.

Thus, in this model, at $p < p_c$ the BL is completely occupied by finite clusters and at p_c there appears the onset of

FIG. 2. Sum of probabilities of generating finite clusters *S* versus *p* in the mixed model.

infinite clusters. Thus one expects the usual scaling properties near p_c . This is indeed what occurs. From Eq. (2.12) , we find

$$
1 - S\infty (p = p_c)^{\beta}, \quad (p \rightarrow p_c, \ p > p_c), \tag{2.13}
$$

with $\beta=1$, and, therefore, in our model, the probability of generating infinite clusters vanishes linearly when *p* tends to p_c from above.

Equation (2.12) expresses the total probability of generating finite clusters as a function of *p*. The individual probability of generating a cluster of size *s*, at a given *p*, follows lines similar to those explained for $l=2$ and 3. In this case, for arbitrary *p*, the first vector $V^{(1)}$ would be

$$
\mathbf{V}^{(1)} = \begin{pmatrix} \frac{q}{3} + \frac{p}{7} \\ \frac{2q}{3} + \frac{2p}{7} \\ \frac{4p}{7} \end{pmatrix}^{(1)} = \begin{pmatrix} \frac{7 - 4p}{21} \\ \frac{14 - 8p}{21} \\ \frac{12p}{21} \end{pmatrix}^{(1)} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}.
$$
 (2.14)

As usual, the first component of the vector corresponds to n_1 , i.e., the probability of generating a closed cluster formed by one pair. Now we are going to organize the calculation in an equivalent but more compact way. For the moment, we leave $V^{(1)}$ aside and proceed to multiply the transfer matrices, denoting their products by $\mathbf{X}(i)$, i.e., $\mathbf{X}(2) \equiv \mathbf{M}^{(2)}$, $X(3) \equiv M^{(3)}M^{(2)}$, $X(4) \equiv M^{(4)}M^{(3)}M^{(2)}$, etc. The dimension of **X**(2) is 4×3, that of **X**(3) is 5×3, the next 6×3, and so on. Thus, each of these matrices $X(i)$ is composed of three columns and $(i+2)$ rows, the first column formed by 0's, the second column is a vector $A(i)$, of $(i+2)$ components denoted by $(A_1, A_2, ..., A_{i+2})$, and the third column again is a vector $\mathbf{B}(i)$, composed of $(B_1, B_2, ..., B_{i+2})$; i.e., we have

$$
\mathbf{X}(i) = \begin{bmatrix} 0 & A_1 & B_1 \\ 0 & A_2 & B_2 \\ 0 & A_3 & B_3 \\ \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots \\ 0 & A_{i+2} & B_{i+2} \end{bmatrix} .
$$
 (2.15)

 is recurrently calculated from $**X**(i)$ **. Denoting the** next order by primed letters, one finds that

$$
A'_{1} = aA_{2},
$$

\n
$$
A'_{2} = bA_{2} + aA_{3},
$$

\n
$$
A'_{j} = cA_{j-1} + bA_{j} + aA_{j+1} \quad (2 < j < i+2) \quad (2.16)
$$

\n
$$
A'_{i+2} = cA_{i+1} + bA_{i+2},
$$

\n
$$
A'_{i+3} = cA_{i+2}.
$$

With the exchange $A \leftrightarrow B$ the coefficients for the *B*'s are obtained by using relations identical to Eqs. (2.16) . Returning now to $V^{(1)}$, the first component of the vector obtained by acting $\mathbf{X}(i)$ on $\mathbf{V}^{(1)}$ will be $n_i(p)$, i.e.,

$$
n_i(p) = bA_1(i) + cB_1(i). \tag{2.17}
$$

The small-*s* cases can be computed explicitly by inspection, giving

$$
n_1 = a
$$
, $n_2 = ab$, $n_3 = a(b^2 + ac)$,...

The first \bf{A} and \bf{B} vectors used to feed recursion (2.16) at the level $i=3$ are

$$
\mathbf{A}(3) = (ab, b^2 + ac, 2bc, c^2, 0),
$$

$$
\mathbf{B}(3) = (a^2, 2ab, 2ac + b^2, 2bc, c^2).
$$
 (2.18)

From Eq. (2.18) the recursion relations (2.16) provide any desired $n_s(p)$. Calculating the individual n_s 's, and hence *S*(*p*), one reproduces Fig. 2 exactly.

The mean size of the finite clusters $T(p)$, for $p \leq p_c$, can also be calculated in a self-consistent way, in a form similar to that used for S [6]. As the mean size of a branch must be identical to that of a subbranch, we can formulate the following self-consistent equation for *T*:

$$
T = \sum_{s=1}^{\infty} s n_s = \left(\frac{q}{3} + \frac{p}{7}\right) + 2\left(\frac{q}{3} + \frac{p}{7}\right)(T+1) + \frac{4p}{7}(2T+1) \quad (p < p_c, \ Z = 3). \tag{2.19}
$$

which leads to

$$
T = \frac{\frac{21}{16}}{\frac{7}{16} - p}.
$$
 (2.20)

For $p=0$ (i.e., $l=2$), $T=3$, as we calculated in Eq. (2.6). For $p > p_c$, Eq. (2.19) has no solution because of the existence of

FIG. 3. Numerical fit of the σ exponent using data on both sides of the critical point. The solid line has a slope equal to 2.

the infinite clusters. Beyond p_c one must take into account the nontrivial denominators $T = \sum_{s} s n_s / \sum_{s} n_s$ because they no longer are unity. We find a completely symmetric behavior on both sides of p_c :

$$
T \propto \frac{1}{|p - p_c|^{\gamma}}, \quad \gamma = 1. \tag{2.21}
$$

III. OTHER RESULTS OF THE MIXED MODEL

As at $p=0$ (i.e., $l=2$) n_s fulfills relation (2.4), we have

$$
n_s(p=0) \propto e^{-1.986}.\tag{3.1}
$$

Recalling other critical phenomena, at $p=p_c$ a power-law behavior for $n_s(p_c)$ vs *s* is expected. This is indeed the result. We obtain that for large *s*

$$
n_s(p_c) \propto \frac{1}{s^{\tau}}, \quad \tau = \frac{3}{2}.
$$
 (3.2)

Near p_c we fit the ratio $v_s \equiv n_s(p)/n_s(p_c)$ by a scaling function of the form $[6]$

$$
v_s(p) = f(z) = e^{-cz^{1/\sigma}} = e^{-c(p-p_c)^{1/\sigma_s}}, \tag{3.3}
$$

where $z = (p - p_c)s^{\sigma}$, with *c* and σ constants.

If Eq. (3.3) is correct, it follows that a plot of log_v^{*s*} against *s*, for *p* fixed, should be a straight line, with a slope $-c(p-p_c)^{1/\sigma}$. This has been checked on both sides of p_c . Furthermore, if Eq. (3.3) is valid, then $log[-(log v_s)/s]$ versus $\log|p-p_c|$ should be a straight line with slope $1/\sigma$ and an intercept equal to $log(c)$. This is shown in Fig. 3 for $s=2^{16}$. The continuous line drawn here represents a straight line of slope 2. From this figure one deduces that $\sigma \approx 0.5$ and $c=4$. Once *c* and σ are known, we can illustrate Eq. (3.3) by plotting v_s against z_s for different values of s_s . As scaling holds, all the curves for different *s* should collapse on the same Gaussian. Figure 4 shows the scaling function $v_s(p)$

FIG. 4. Test of the scaling assumption for the clustering numbers. Note the data collapsing for various cluster sizes, represented by different symbols.

obtained for six different clusters sizes *s* (from $s=2^{10}$ to 2^{15}). Each symbol in Fig. 4 corresponds to an interval of one unit in the exponent. Note that $f_{\text{max}} = \nu_s(z_{\text{max}}) = 1$, which coincides with the standard percolation result on the BL.

The consistency of these results with the previously calculated critical behavior is clear. *T* is a divergent quantity at p_c ; by substituting the sum by an integral [6] we find

$$
T \approx \int_0^\infty \frac{1}{s^{\tau - 1}} e^{-c|p - p_c|^{1/\sigma_s}} ds.
$$
 (3.4)

With the change of variable $x = c|p-p_c|^2 s$, we obtain

$$
T \propto |p - p_c|^{(\tau - 2)/\sigma} \int_0^\infty \frac{1}{x^{\tau - 1}} e^{-x} dx \propto \frac{1}{|p - p_c|^{\gamma}}, \quad (3.5)
$$

i.e., the value $\gamma=1$ fits with $\tau=\frac{3}{2}$ and $\sigma=\frac{1}{2}$.

IV. COMPARISON WITH THE STANDARD PERCOLATION THEORY AND CONCLUSIONS

From the results above presented one deduces that this pair model has the same scaling behavior that PT exhibits on the BL. But in order not to create any confusion, we want to emphasize certain points. In this paper, n_s is the probability of generating clusters of size *s*, departing from a point. If instead of calculating n_s by multiplying matrices as done here, we had made a numerical simulation that n_s would be, for each *p*, the ratio between the obtained number of clusters of size *s* and the total number of clusters (which varies with p). In PT, the normalization of n_s is made by dividing the number of clusters of size *s* by the total number of sites in the lattice, which is a constant. As a consequence, in our model $T = \sum_{s} s n_{s} / \sum_{s} n_{s}$ is the mean cluster size, while in PT, $T = \sum_{s} s^2 n_s / \sum_{s} s n_s$. The critical exponents are equal to those in standard PT, except τ , which is one unit less. As in our model the occupation fraction is unity (the whole board is full of particles), it seems that the successive momenta of the distributions of n_s are one unit advanced with respect to standard PT and hence our $\tau=3/2$ is consistent with $\gamma=\beta=1$ $=2\sigma$, which are the same critical exponents of PT, but there $\tau=5/2$. The exponent $\tau=3/2$ in power laws is typical in mean-field descriptions of the size of avalanches in selforganized critical phenomena (see, for example, Ref. $[18]$).

To conclude, let us recall that we have formulated a model of particle pairs on a BL. This choice has been done for reasons of simplicity. (In ordinary non-tree-like lattices one has to deal, from the start, with numerical simulations and the results are not so transparent.) This has been implemented by reducing the process of clustering to insertions respectful of the underlying branching geometry of the BL. The successive probabilities of passing from n_s to n_{s+1} are calculated by means of transfer matrices. Only for $l=2$, these matrices are square and *s* independent. $S(l=2)=1$. For $l=3$ the matrices are no longer square. They grow with *s*, and at each level of *s* a new configuration is opened. This leads to the fact that $S(l=3)$ <1, which means that the probability of generating infinite clusters is not null.

A mixed model between $l=2$ and 3, with a tuning parameter $0 \leq p \leq 1$ to fix the proportion between the two *l*'s, allows the appearance of a critical point p_c . At p_c , $n_s \propto 1/s^{\tau}$ with $\tau=3/2$. Near the critical point $n_s = n_s(p_c)e^{-c|p-p_c|^2s}$, with $c=4$. The probability of generating infinite clusters starts at $p > p_c$ with an exponent $\beta=1$. The mean size of finite clusters diverges at p_c with a critical exponent $\gamma=1$.

If instead of building a mixed model between $l=2$ and 3 we take, for instance, $l=2$ and 4 $(Z=3)$, Eq. (2.20) , for example, adopts the form $T = \frac{15}{24} / (\frac{5}{24} - p)$, i.e., there is a shift to the left of the critical point, now at $p_c = \frac{5}{24}$, but again $\gamma = 1$. Thus the universality of the critical exponents is maintained.

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