Structure of random fractals and the probability distribution of random walks

H. Eduardo Roman
Institut für Theoretische Physik, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany
(Received 7 June 1994; revised manuscript received 8 December 1994)

The structure of percolation clusters at criticality, described by the distribution of the end-to-end distance r between two cluster sites as a function of their minimal path length ℓ, $P(r,\ell)$, is discussed. Analytical expressions for the exponents describing the distribution for spatial dimensions $2 \leq d \leq 6$ are presented, and extensive numerical simulations in two and three dimensions are performed in support of these predictions.

PACS number(s): 05.40.+j, 05.60.+w, 66.30.−h

Percolation clusters at criticality represent useful models of random fractals with a variety of applications in many fields of science [1–3]. In many circumstances, a detailed knowledge of the cluster structure is required, as, for instance, in the study of transport phenomena on fractals [1,2,4]. In this context, random walks on fractals have attracted much attention in recent years. One of the reasons for this interest is the advent of new transport laws required to describe them and, secondly, because of their applications for modeling anomalous transport behavior commonly observed in many disordered materials [1–6].

Much effort has been devoted, therefore, to elucidating the form of the probability density $P(r,t)$ of random walks on self-similar structures. This central quantity represents the probability that a random walker is at distance r at time t from its starting point at $t = 0$. It is generally accepted that, on average,

$$P(r,t) \sim \frac{1}{t^{d_s/2}} \exp[-\text{const} \times (r/R)^u] \qquad (1)$$

when $t \to \infty$ and $r \gg R$. Here, $R^2 = \langle [\mathbf{r}(t) - \mathbf{r}(0)]^2 \rangle$ is the mean-square displacement of the random walk, $R \sim t^{1/d_w}$, and $d_w > 2$ is the anomalous diffusion exponent [1,5]. The spectral dimension [5] $d_s = 2d_f/d_w$, d_f is the fractal dimension of the structure, and the exponent $u = d_w/(d_w - 1)$. Since $d_w > 2$ on fractals, $u < 2$ and $P(r,t)$ is called a stretched Gaussian [7]. We note that (1) is consistent with the normalization condition $\int_0^\infty dr\ r^{d_f-1}\ P(r,t) = 1$.

Recent theoretical studies have indicated, however, that a more accurate expression for the asymptotic form of $P(r,t)$ is instead given by

$$P(r,t) \sim \frac{1}{t^{d_s/2}} (r/R)^\alpha \exp[-\text{const} \times (r/R)^u], \qquad (2)$$

containing a power-law correction term $(r/R)^\alpha$ to the usual stretched Gaussian law [8–10]. Equation (2) can be obtained analytically by considering a generalized diffusion equation on fractals of the form [9,10]

$$\frac{\partial^{1/d_w}\ P(r,t)}{\partial t^{1/d_w}} = -A \left(\frac{\partial\ P(r,t)}{\partial r} + \frac{\kappa}{r}\ P(r,t) \right), \qquad (3)$$

where the symbol $\partial^{1/d_w}/\partial t^{1/d_w}$ denotes a fractional temporal derivative of order $1/d_w$. The exact asymptotic solution of Eq. (3) then yields

$$\alpha = u \left(\frac{1}{2}(d_s - 1) - \kappa \right). \qquad (4)$$

Equation (3) reduces to its standard counterpart when $d_w = 2$ and $d_f = d$, the Euclidean dimension of the space. In this case, $\kappa = (d-1)/2$ and $\alpha = 0$. The exact value of κ on fractals is, however, not known at present. More recent theoretical arguments, based on the continuous time random walks formalism, have been presented suggesting that [11]

$$\kappa = \frac{1}{2}\ (d_f - 1). \qquad (5)$$

As we will see, Eqs. (2)–(4) are very useful since they permit us to estimate analytically the exponents describing the structure of the random fractal where the diffusion process takes place.

In this paper, we discuss in detail a simple derivation of the asymptotic form Eq. (2) from which analytical expressions for the exponents describing the structure of percolation clusters at criticality are obtained. These theoretical predictions are supported by extensive numerical simulations in two and three dimensions.

We start by considering the case of topologically one-dimensional random fractal structures generated by standard random walks on regular lattices (RW chains), for which the asymptotic solution for $P(r,t)$ can be obtained exactly. We are thus in a position to test the validity of the predictions Eqs. (4) and (5) in these cases. More important, from this analysis a remarkably simple relation is suggested which turns out to play a fundamental role in the present approach.

Random walk chains

In the case of RW chains, the random walker can only performs jumps to nearest-neighbor sites of the linear path which have been created sequentially by a previous random walk. Thus, although intersection of the path with itself actually occurs, the walker experiences just a one-dimensional path. The distance of the walker along the linear path from its starting point (center of

the chain) is denoted as the *chemical* distance [1], $\ell \geq 0$. In this topologically one-dimensional space, diffusion is normal and the corresponding probability is simply given by

$$P(\ell,t) \sim \frac{1}{t^{1/2}} \exp[-\text{const} \times (\ell/L)^2], \tag{6}$$

when $t > \ell$, where $L \sim t^{1/2}$. For RW chains [1], $d_f = 2$, the diffusion exponent $d_w = 2d_f = 4$, and $d_s = 1$.

To obtain the asymptotic behavior of $P(r,t)$, we employ the method already discussed in the literature [1,7,12], in which $P(\ell,t)$ and $P(r,t)$ can be related by

$$P(r,t) = \int_{\ell_{\min}}^{t} d\ell\ \Phi(\ell \mid r)\ P(\ell,t), \tag{7}$$

where $\Phi(\ell \mid r)$ gives the conditional probability that a site of the RW chain at a distance r from the center of the chain is at a chemical distance ℓ, and $\Phi(\ell \mid r) = 0$ when $\ell < r$. It is normalized according to $\int_{\ell_{\min}}^{\ell_\infty} d\ell\ \Phi(\ell \mid r) = 1$, where $\ell_{\min} \sim r$ (but a different r dependence may also take place [13]), and $\ell_\infty \to \infty$ in general.

The function $\Phi(\ell \mid r)$ is related to the structural function $P(r,\ell)$, the quantity of interest here, by $\Phi(\ell \mid r) = A_\ell(r)P(r,\ell)$. The latter represents the probability that a site of the RW chain has grown at distance r from the origin after ℓ steps, i.e.,

$$P(r,\ell) \sim \frac{1}{\ell^{d/2}} \exp(-\text{const} \times r^2/\ell) \tag{8}$$

when $\ell > r$, and is normalized according to $\int_0^\infty dr\ r^{d-1}\ P(r,\ell) = 1$. Finally, the proportionality factor $A_\ell(r)$ can be obtained from the normalization condition on $\Phi(\ell \mid r)$, yielding [14]

$$\Phi(\ell \mid r) \sim \frac{1}{\ell}\ (r/\ell^{1/2})^{d-2} \exp(-\text{const} \times r^2/\ell). \tag{9}$$

The asymptotic form for $P(r,t)$ can now be obtained by applying the method of steepest descents in Eq. (7). To be noticed is that the saddle [15] $\ell_* \sim (r^2 t)^{1/3}$, should occur in the interval $\ell_{\min} < \ell_* < \ell_{\max}$, where $\ell_{\max} \sim r^2$ gives the location of the maximum of $\Phi(\ell \mid r)$ [16]. The result has the form of Eq. (2), with $u = d_w/(d_w - 1) = 4/3$ and $\alpha = 2d/3 - 2$. The latter can be written as in Eq. (4), with $d_s = 1$ and

$$\kappa = \frac{1}{2}\ [(d_f + 2 - d) - 1]. \tag{10}$$

It is gratifying that the suggested value for κ in Eq. (5) coincides with the exact result in Eq. (10), at least in one particular case, i.e., when the embedding dimension $d = 2$.

Self-avoiding random walk chains

In the following, we are going to test our result Eq. (10) on a more complex linear fractal for which the structural function $P(r,\ell)$ is also known, i.e., chains generated by self-avoiding random walks (SAW chains). For these chains, the structural function reads [17]

$$P(r,\ell) \sim \frac{1}{\ell^{\nu d}}\ (r/\ell^\nu)^{\tilde{t}}\ \exp[-\text{const} \times (r/\ell^\nu)^\delta] \tag{11}$$

when $r/\ell^\nu \gg 1$, and

$$P(r,\ell) \sim \frac{1}{\ell^{\nu d}}\ (r/\ell^\nu)^g \tag{12}$$

when $r/\ell^\nu \ll 1$. Now, $\nu \cong 3/(d+2)$, $\delta = 1/(1-\nu)$, $\tilde{t} = \delta\ [d(\nu - 1/2) - (\gamma - 1)]$, and $g = (\gamma - 1)/\nu$. For SAW chains, $d_f = 1/\nu = (d+2)/3$ and $d_w = 2d_f$, similarly as for RW-chains [1].

The exponent γ (≥ 1) is called the enhancement factor and is not known exactly (except when $d = 2$) [17]. Despite several attempts, such an accurate and simple expression for γ, as for its counterpart ν (the Flory result) valid for all d, has not been derived yet [6].

For SAW chains, Eq. (9) is changed to $\Phi(\ell \mid r) \sim (1/\ell)\ (r/\ell^\nu)^{d-1/\nu+\tilde{t}}\ \exp[-\text{const} \times (r/\ell^\nu)^\delta]$, when $r/\ell^\nu > 1$ [which is the relevant range for the asymptotic case in Eq. (2)], and displays a maximum at $\ell_{\max} \sim r^{1/\nu}$. The asymptotic behavior of $P(r,t)$ can be obtained from Eq. (7), where again the saddle [16] $\ell_{\min} < \ell_* < \ell_{\max}$, $\ell_* \sim (tr^\delta)^{1/(1+\delta)}$. The result has the form of Eq. (2), with $\alpha = -u\ \kappa$, and

$$\kappa = \frac{1}{2}\ [(d_f + \Delta d_f) - 1] \tag{13}$$

where $\Delta d_f = d_f - 2(d + \tilde{t})/\delta$. To get deeper insight into this result, we will assume that the correction term found in Eq. (10) holds here too, i.e., $\Delta d_f \cong 2 - d$. This yields a prediction for γ which reads

$$\gamma = 1 + \frac{4-d}{6}. \tag{14}$$

This simple result agrees remarkably well with the best numerical estimates presently available [17] ($\gamma = 1.33 \pm 0.003$, $\gamma_{\text{exact}} = 43/32$ when $d = 2$, and $\gamma = 1.1663 \pm 0.003$ when $d = 3$). Note that $\gamma = 1$ when $d = 4$, as expected [17].

Encouraged by these results, we apply the same ideas to percolation clusters at criticality, where, however, no analytical expressions for the analogous exponents $\tilde{t}$ and g are known so far.

Percolation clusters at criticality

Accurate numerical results on percolation clusters at criticality [1,18] have indicated that the structural function $P(r,\ell)$ can be well described by a form similar to Eq. (11), for an appreciable range of values of the scaling variable $x = r/\ell^\nu$, including values $x < 1$. However, some discrepancies have been observed when $x \ll 1$ [18].

In the following, we assume that for percolation clusters, $P(r,\ell)$ actually obeys the scaling forms Eqs. (11) and (12), when $x > 1$ and $x < 1$, respectively, and suggest expressions for the corresponding exponents $\tilde{t}$ and g. In addition, we assume that $\delta = 1/(1-\nu)$.

For percolation, values of ν are known in the literature [1,2], with $\nu = 1/2$ when $d \geq 6$. From Eq. (11) we obtain the conditional function $\Phi(\ell \mid r)$, which is

now normalized according to $\int_{\ell_{\min}}^{\ell_\infty} d\ell\ \ell^{d_\ell - 1}\ \Phi(\ell \mid r) = 1$, where $d_\ell = \nu d_f > 1$ is the fractal dimension in ℓ-space (topological dimension) [1]. It is, however, convenient to incorporate the factor $\ell^{d_\ell - 1}$ into the definition of $\Phi(\ell \mid r)$, such that it still preserves the simple scaling form $(1/\ell)\phi(r/\ell^\nu)$ as in the previous examples, i.e., $\Phi(\ell \mid r) \sim (1/\ell)\ (r/\ell^\nu)^{d-1/\nu+\tilde{t}-\Delta\tilde{t}}\ \exp[-\text{const} \times (r/\ell^\nu)^\delta]$ when $r/\ell^\nu > 1$, and $\Phi(\ell \mid r) \sim (1/\ell)\ (r/\ell^\nu)^\beta$ when $r/\ell^\nu < 1$, with $\beta = d - 1/\nu + g - \Delta\tilde{t}$, where $\Delta\tilde{t} = (d_\ell - 1)/\nu$. The resulting normalization is then $\int_{\ell_{\min}}^{\ell_\infty} d\ell\ \Phi(\ell \mid r) = 1$, and the relation Eq. (7) does not carry any additional factor in the integrand.

Because of the presence of loops and dangling ends on all length scales, diffusion in chemical space is anomalous on percolation clusters [1,2], and the form of the probability density $P(\ell, t)$ is not known exactly. Extensive numerical studies have indicated, however, that to a good approximation [1,7],

$$P(\ell, t) \sim \frac{1}{t^{d_s/2}}\ \exp[-\text{const} \times (\ell/L)^v], \tag{15}$$

where $L \sim t^{1/d_w^\ell}$, $d_w^\ell = \nu d_w$ is the diffusion exponent in ℓ-space, and $v = d_w^\ell/(d_w^\ell - 1)$, similarly as in r-space [cf. Eq. (1)] [1,2].

From our previous discussions, however, a power-law correction term of the form $(\ell/L)^{\alpha_\ell}$, as in Eq. (2), may be present also in ℓ-space. To understand this point better, notice that for fractals such as Sierpinski gaskets, both ℓ- and r-spaces are equivalent, and the same power-law correction term, if existing, should be present in both spaces. But percolation clusters are not deterministic fractals and a different situation may actually occur, yet such correction terms in ℓ-space for percolation are essential as we will see below. Therefore we expect in Eq. (15) also a power-law correction term described by the exponent

$$\alpha_\ell = v\left(\frac{1}{2}(d_s - 1) - \kappa_\ell\right), \tag{16}$$

where κ_ℓ remains to be determined.

We proceed with the evaluation of Eq. (7). Now, the saddle $\ell_* \sim (r^\delta t^{v/d_w^\ell})^{1/(\delta+v-1)}$, and the final result for $P(r, t)$ can be written in the form of Eq. (2), with α given by Eq. (4), and $\kappa = (d_f + \Delta d_f - 1)/2$, where

$$\Delta d_f = d_s - d_f - \frac{2}{\delta}(d + \tilde{t} - \Delta\tilde{t}) + \frac{2}{\nu\delta} - \frac{2\alpha_\ell}{v} + 1. \tag{17}$$

We now see the important role played by α_ℓ [Eq. (16)]: It cancels out the term d_s, containing the dynamical exponent d_w, in Eq. (17), and Δd_f is given by static exponents only, as is reasonable to expect.

Finally, assuming that $\Delta d_f = 2 - d$ holds here too, we obtain a closed expression for $\tilde{t}$. Since we expect that $\tilde{t}$ should vanish when $d = 6$, because percolation clusters become similar to regular random walks when $d \geq 6$, we finally impose this condition to $\tilde{t}$ to obtain $\kappa_\ell = 0$. This surprising result corresponds to an effective topological dimension $d_\ell^{\text{eff}} = 1$ if one naively assumes $\kappa_\ell = (d_\ell^{\text{eff}} - 1)/2$. The origin of such special behavior of diffusion in ℓ-space, obtained here for percolation clusters for which $d_\ell > 1$, remains to be understood [19].

Our final estimate for the structural exponent $\tilde{t}$ on percolation clusters at criticality now reads

$$\tilde{t} = \delta\ (d - d_f)\ (\nu - 1/2), \tag{18}$$

which is the main result of this work. Notice that, when $d = 6$, $\nu = 1/2$, and $\tilde{t} = 0$, as required. If we write Eq. (18) in a form similar to that for SAW chains, i.e., $\tilde{t} = \delta\ [d(\nu - 1/2) - (\gamma - 1)]$, we find $\gamma = 1 + d_f(\nu - 1/2)$. These results generalize the previous ones for RW and SAW chains, as can be easily verified.

Unfortunately, the exponent g describing the range $r/\ell^\nu < 1$ of $P(r, \ell)$, cannot be derived following lines similar to those leading to Eq. (18). However, we attempt to estimate it by using $g = (\gamma - 1)/\nu$, as for SAW chains [Eq. (12)]. Employing the above result for γ, we obtain

$$g = d_f\ (\nu - 1/2)/\nu \tag{19}$$

yielding $\beta = d - d_f/2\nu$, describing $\Phi(\ell \mid r)$ when $r/\ell^\nu < 1$.

In order to test the predictions Eqs. (18) and (19), we have calculated $P(r, \ell)$ numerically in two and three dimensions, as shown in Fig. 1. To estimate $\tilde{t}$ numeri-

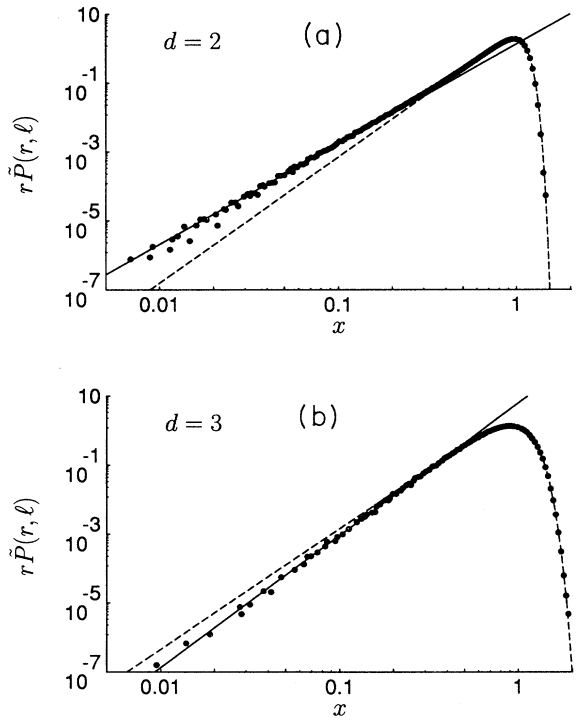

FIG. 1. The structural function for percolation clusters at criticality. Plotted is the function $r\tilde{P}(r, \ell)$ vs $x \equiv r/\ell^\nu$, where $\tilde{P}(r, \ell) = r^{d-1}P(r, \ell)$, and $r\tilde{P}(r, \ell) = x^d f(x)$. In $d = 2$, $\nu \cong 0.88$, and $\ell = 250$, 500, 750, and 1000 were used, and averages over 10^6 clusters, grown up to $\ell = 10^3$ chemical shells, were performed on a square lattice of $(2000)^2$ sites. In $d = 3$, $\nu \cong 0.75$, and $\ell = 100$, 200, 300, and 500 were used, and averages over 2.5×10^5 clusters, grown up to $\ell = 500$ chemical shells, were performed on a cubic lattice of $(300)^3$ sites. None of the clusters touched the boundaries. The lines represent the numerical fits as described in Table I.

cally, the data were fitted using the scaling function $f(x)$ (times x^d) described in Table I, for values of x around and above the maximum of $r\tilde{P}(r,\ell) = r^d P(r,\ell)$ (cf. Fig. 1). The exponent g was obtained by fitting a power law for small x. The resulting exponents are summarized in Table I. In two dimensions, the fitted $\tilde{t}$ turns out to be much larger than in Eq. (18), while g is consistent with Eq. (19). In three dimensions, the agreement with the theoretical predictions is remarkably good. The apparent discrepancy in $d = 2$ may be an indication that the true asymptotic behavior described by $\tilde{t}$ is reached for values of x well beyond the maximum of $f(x)$. In both cases, the actual nature of the crossover remains to be understood.

In summary, we have studied the structure of percolation clusters on d-dimensional lattices at criticality, and estimated analytically the corresponding exponents describing their asymptotic shape. The predicted (approximate) values for the exponents are in very good agreement with the numerical simulations in two and three dimensions. Nevertheless, many questions are still open and further theoretical and numerical work is required to clarify them.

TABLE I. The fitting parameters describing the scaling function $f(x)$ (Fig. 1) for percolation clusters at criticality: $f(x) = A\ x^{\tilde{t}}\ \exp(-B\ x^{\delta})$, when $x > 0.4$ (dashed lines), and $f(x) = C\ x^{g}$, when $x < 0.4$ (continuous lines). Here, $\delta = 1/(1-\nu)$, and d is the spatial dimensionality. The theoretical values expected from Eqs. (18) and (19) are indicated in parentheses.

d	A	B	C	$\tilde{t}$	g
2	3.10	0.53	1.30	1.65± 0.10 (0.33)	0.90± 0.10 (0.822)
3	4.55	1.27	6.16	0.50± 0.10 (0.50)	0.83± 0.10 (0.833)

[1] S. Havlin and D. Ben-Avraham, Adv. Phys. **36**, 695 (1987).

[2] *Fractals and Disordered Systems*, edited by A. Bunde and S. Havlin (Springer-Verlag, Heidelberg, 1991).

[3] *Fractals in Science*, edited by A. Bunde and S. Havlin (Springer-Verlag, Heidelberg, 1994).

[4] J.P. Bouchaud and A. Georges, Phys. Rep. **195**, 127 (1990).

[5] S. Alexander and R. Orbach, J. Phys. Lett. **43**, L625 (1982).

[6] *Fractals in Physics*, edited by L. Pietronero and E. Tosatti (North-Holland, Amsterdam, 1986).

[7] A. Bunde, S. Havlin, and H.E. Roman, Phys. Rev. A **42**, 6274 (1990).

[8] J. Klafter, G. Zumofen, and A. Blumen, J. Phys. A **24**, 4835 (1991).

[9] H.E. Roman and M. Giona, J. Phys. A **25**, 2107 (1992).

[10] M. Giona and H.E. Roman, Physica A **185**, 87 (1992).

[11] H.E. Roman and P.A. Alemany, J. Phys. A **27**, 3407 (1994).

[12] A. Bunde, H.E. Roman, St. Russ, A. Aharony, and A.B. Harris, Phys. Rev. Lett. **69**, 3189 (1992).

[13] A. Bunde and J. Dräger, Physica A **202**, 371 (1994); Philos. Mag. B (to be published).

[14] For RW chains, the integral $\int_{\ell_{\min}}^{\ell_\infty} d\ell\ \Phi(\ell \mid r)$ diverges when $\ell_\infty \to \infty$ and $d = 2$. In this case, we take ℓ_∞ finite, but sufficiently large in order to ensure a suitable normalization of $\Phi(\ell \mid r)$.

[15] H.E. Roman, Physica **191**, 379 (1992).

[16] A different dependence in the exponential decay of $P(r,t)$ is obtained when $\ell_* < \ell_{\min}$, depending on the number of configurations over which the average of $P(r,t)$ is performed [13]. In such cases, however, the resulting expression for $P(r,t)\ t^{d_s/2}$ is not a scaling function of the variable r/R alone, as, e.g., in Eq. (2), and the exponent α cannot be defined. We are not interested in such situations in this work.

[17] J. des Cloizeaux and G. Jannink, *Polymers in Solution: Their Modelling and Structure* (Clarendon Press, Oxford, 1990); P.G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, 1979).

[18] U.A. Neumann and S. Havlin, J. Stat. Phys. **52**, 203 (1988).

[19] The result $\kappa_\ell = 0$, i.e., $\alpha_\ell = v\ (d_s - 1)/2$, seems to be consistent with numerical calculations recently reported for Sierpinski gaskets [8], where diffusion indeed occurs in ℓ-space, since no distinction bewteen ℓ- and r-spaces effectively takes place for these deterministic fractals. The question whether $\kappa_\ell = 0$ actually holds in general remains open.