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Partial and Random Lattice Covering Times in Two Dimensions

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The problems of the partial covering time (PCT) and of the random covering time (RCT) are studied in two dimensions using Monte Carlo simulations. We find that the PCT (RCT) presents a discontinuous transition at $f=1$ ($f=0$), where f is the fraction of visited sites by a random walker. An analysis of the time evolution of the surviving unvisited clusters reveals that they exhibit a time-dependent fractal-like structure.

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In the last few years the concept of random walkers (RW) has been used in an increasing number of new and interesting theoretical and practical problems in physics [1], biology [2], chemistry [3], ecology [4], economics [5], and technology [6]. RW have a large domain of applicability in these disciplines mainly due to the important role this concept plays in the subjects of polymer statistics and critical phenomena [7], diffusion [8] and noise theory [9], and fractals [10].

Recently a new RW problem, namely the lattice covering time problem (CT), was studied by Nemirovsky, Coutinho-Filho, and Mártin [11,12] in one through four dimensions, from the point of view of theory and computer simulations. The covering time, t_c, is the mean time for a lattice RW to visit all $N(N\rightarrow\infty)$ sites at least once. Besides its intrinsic theoretical interest, the CT problem presents interesting connections with the problems of the Grand Tour [12,13] and ergodicity [12,14]. In $d=1$ this problem reduces to a first visit problem and it is exactly solved. In particular, $t_c=\frac{1}{2}N(N-1)$ for periodic boundary conditions. However, for $d\geq 2$ the CT problem is not reducible to any of the well known lattice RW problems. In Ref. [12] based on MC results it was suggested that $t_c\simeq AN\ln^2 N(1+C/\ln N)$, $d=2$, and $t_c\simeq AN\ln N(1+C/\ln N)$, $d\geq 3$, where A is universal, i.e., not dependent on boundary conditions, while C is the magnitude of the leading scaling correction and does depend on the boundary condition. In $d=\infty$ it has been shown [11] that $A=1$. More recently, Brummelhuis and Hilhorst presented a very detailed theoretical analysis of a closely related problem, namely the "last-site problem." By identifying the characteristic time appearing in the latter problem, to leading order in N, with t_c, they confirmed the above predictions for t_c and found $A=1/\pi$, $d=2$ and $A=g_\infty(0)$, $d\geq 3$ where $g_\infty(0)$ [15] is a lattice-dependent parameter for $N\rightarrow\infty$, in very good agreement with the numerical values of the MC results [12].

In this Letter we investigate two problems of great practical and theoretical interest which are closely related to the CT problem. The first one is the partial covering time (PCT, t_p) problem, in which the RW stops after visiting a given fraction f of the N sites. The second problem is the random covering time (RCT, t_r) problem, which means to calculate the mean time the RW takes to visit a fraction f of sites *previously* chosen at random. The PCT can be applied to the Monte Carlo method [16] if one is interested in the speed at which configurations are sampled once equilibrium has been reached. In this case not all configurations (points in the phase space) are to be visited, but only some fraction of them. Here we investigate these dilute covering time problems using extensive Monte Carlo simulations on large lattices varying from $N=10^2$ to 1200^2 sites, requiring at least 50 statistical averages per point. A finite-size scaling analysis of the data suggests that the reduced times t_p/t_c and t_r/t_c of partial and random covering times display discontinuities at $f=1$ and $f=0$, respectively. In this work we restrict ourselves to $d=2$ where the effects of correlation are strong. Expressions for t_p/t_c and t_r/t_c near the transitions

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are suggested based on theory and simulations and, in particular, Montroll's result [17] for the problem of one-trap site is a special case of our expression for t_r. Moreover, we calculate the spatial structure of the set of unvisited sites at the time scale of t_c and develop a complete analysis of the fragmentation generated in these RW problems. We find that the average number of the unvisited sites in a time t within a ball of radius R centered in unvisited sites scales as $n \sim R^{d-t/t_c}$, in agreement with the suggestion of Brummelhuis and Hilhorst [18] that n has a time-dependent fractal-like structure.

A fragmentation analysis of the CT problem is important since it reveals interesting aspects of this highly correlated dynamics and also because the fragmentation induced by a single RW is reminiscent of many dynamic processes occurring in nature. As a first example we may cite failure in brittle materials. In this case the material fragments when cracks appear, grow, and propagate as a result of dynamical processes, such as in rock blasting [19]. Fragments are formed when the crack density is sufficiently high so as to fully surround pieces of matter. If the solid is homogeneous the first crack will propagate unstably and lead to complete fracture [20]. So, the covering time problem presents a formal resemblance with the fragmentation of brittle homogeneous materials if we assume that the RW simulates the crack evolution. The fragmentation analysis associated with the covering time can also be useful in many ecologic/epidemic/biological problems where a group of predators or caterpillars/disease/organism wanders in a plantation/region, or planet/culture medium generating at the time t a certain distribution $n(s,t)$ of disconnected unvisited regions or fragments of size (mass or area) s.

First we study the average fraction of unvisited sites at time t, $N_{nv}(t)/N$, where $N_{nv}(t)$ is defined in terms of the distribution function $n(s,t)$ of the preceding paragraph as

$$N_{nv}(t) = \sum_s n(s,t)s \,. \tag{1}$$

In the inset of Fig. 1 we show the dependence of $N_{nv}(t)/N$ with t/t_c for lattices of $N=500^2$, 800^2, and 1200^2 sites. It suggests that $\ln[N_{nv}(t)/N] = \gamma t/t_c$. Figure 1 exhibits a plot of γ versus N for lattice sizes varying from $N=400^2$ to $N=1200^2$. The straight line refers to the best fit $\gamma = (0 \pm 0.1) - (1.00 \pm 0.08)\ln N$, leading to $N_{nv}(t)/N \simeq N^{-t/t_c}$, first derived in Ref. [18]. As the fraction f of visited sites at time t is given by $f = 1 - N_{nv}(t)/N$, the last expression can be solved for t/t_c giving the reduced PCT,

$$t_p/t_c \simeq -\ln(1-f)/\ln N \,, \tag{2}$$

which fits very well the data of Fig. 2 for lattices of 10^2 to 100^2 sites. It also shows that, in the thermodynamic limit ($N \to \infty$), the reduced PC time displays a discontinuous transition: $t_p/t_c \to 0$, for $0 \le f < 1$ and $t_p/t_c \to 1$, for $f=1$ [take $f = 1 - 1/N$ in (2)]. In the CT problem the cost of time, t_c, for the RW to visit all lattice sites is mainly due to the cost to visit the small $(1-f) = (m/N) \to 0$ fraction of the last unvisited sites.

Moreover, a detailed examination of the data of Fig. 2 suggests that, in the thermodynamic limit, the following complementarity relation between the RCT and the PCT holds:

$$(t_r/t_c)_f \leftrightarrow 1 - (t_p/t_c)_{1-f} \,, \tag{3}$$

i.e., the reduced time needed to visit $m = fN (N \to \infty)$ sites previously chosen at random is equal to 1 minus the reduced time needed to visit the complementary number $(1-f)N (N \to \infty)$ of sites. It means that for $N \to \infty$,

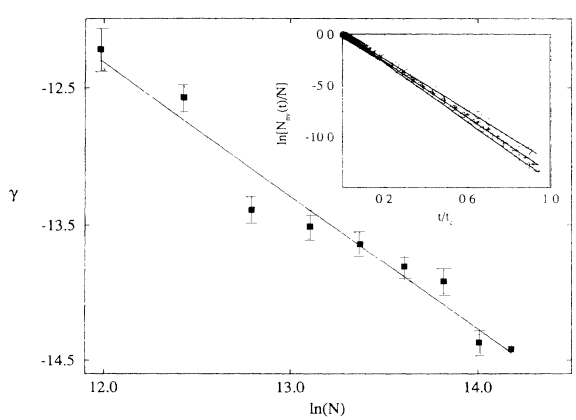

FIG. 1. Average fraction of unvisited sites, $N_{nv}(t)/N$, at time t, for lattices of $N=500^2$ (○), 800^2 (*), and 1200^2 (△) sites (inset), and the dependence of γ with N (see text, fifth paragraph).

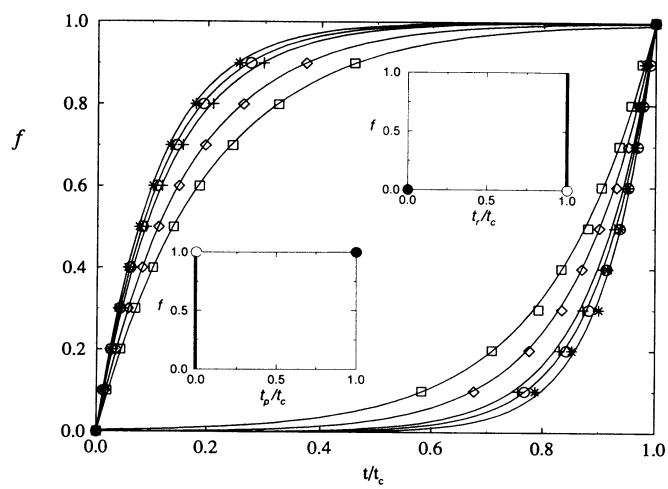

FIG. 2. Fraction f (held fixed) of visited sites at time t for lattices of 10^2 (□), 20^2 (◇), 50^2 (+), 70^2 (○), and 100^2 (*) sites. The curves on the left (right) refer to the PCT (RCT) problem. The insets illustrate schematically the discontinuous transitions in the thermodynamic limit.

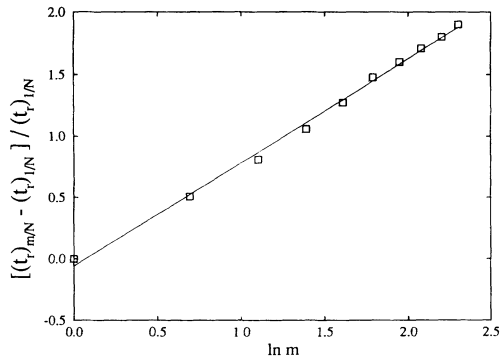

FIG. 3. Numerical checking of the average RCT [Eq. (5)] on a two-dimensional lattice of 200^2 sites with "m traps."

$t_r/t_c \to 1$ for $0 < f \leq 1$, and $t_r/t_c \to 0$ for $f=0$. In the RCT problem the cost of time, t_r, to visit any finite fraction of previously selected sites is of the same order as the cost t_c to visit *all* lattice sites.

We can now work further on this analogy by assuming that, to leading order, the counterpart of Eq. (2) for RCT can be written in the form

$$t_r/t_c \simeq 1 + \frac{\ln f^*}{\ln N^*}, \tag{4}$$

where f^* and N^* are effective fraction and number of sites to be determined by fitting the data of Fig. 2 and satisfying other theoretical constraints. A major theoretical constraint follows by matching Eq. (4) to Montroll's exact result for the "one-trap" problem [17]. Since $t_c \simeq AN\ln^2 N$ in $d=2$, with $A=0.30 \pm 0.03$, this matching results, effective if one places $f^* = ef$ and $N^* = N$, in (4) to obtain

$$t_r = \left(\frac{1}{\pi}\right) N \ln N (1 + \ln m) + O(N). \tag{5}$$

Notice that $A = 1/\pi$, which confirms the suggestion of Brummelhuis and Hilhorst [18] and in agreement with our MC data [12]. An independent numerical checking of Eq. (5) is shown in Fig. 3 for a lattice of 200^2 sites.

From the above discussion it is clear that Eq. (5) is valid only for $f = (m/N) \to 0$. For $0 < f \leq 1$, a good fitting of the data of Fig. 2 is obtained for $f^* = f$ and $N^* \simeq N^{1.2}$, i.e., the complementarity relation (4) between the RCT and PCT is obtained after a proper lattice scale transformation is performed in the former problem under a constant fraction of sites to be visited.

In Fig. 4 we show the dependence of the average size $\bar{s}$ of unvisited regions as a function of the reduced time t/t_c for large systems with 400^2 to 1200^2 sites. This quantity exhibits a clear power-law dependence when t/t_c varies by a factor near 10^2. It indicates that in the scaling region $\ln\bar{s} = (0.15 \pm 0.01) - (1.20 \pm 0.05)\ln(t/t_c)$. We thus conjecture that

$$\bar{s} = (\pi/e)(t/t_c)^{-(\pi/e)}. \tag{6}$$

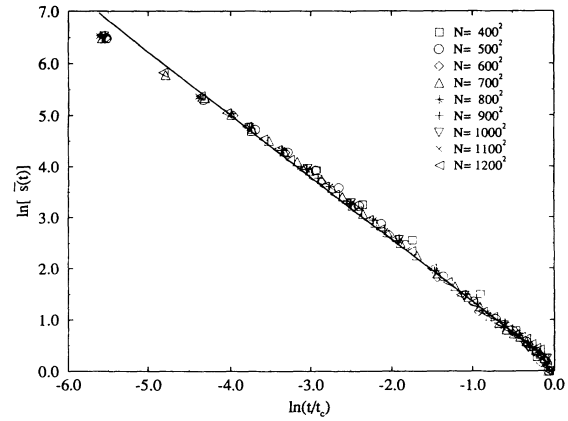

FIG. 4. Average size $\bar{s}$ of unvisited regions as a function of the reduced time t/t_c for lattices of 400^2 to 1200^2 sites.

Using this scaling relation and that for $N_{nv}(t)/N$, we can obtain the total number of unvisited disconnected regions or fragments generated by the RW dynamics at time t, defined by

$$F = \sum_s n(s,t) = N_{nv}(t)/\bar{s}(t), \tag{7}$$

in the scaling form

$$(F/N) \simeq (t/t_c)^{\alpha} N^{-t/t_c}, \quad \alpha = \pi/e. \tag{8}$$

This function is plotted in Fig. 5 for a 600^2 lattice. F/N clearly exhibits a maximum at a time $t_f/t_c = \alpha/\ln N$, which can be easily found from the condition $[d(F/N)/d\tau]_{t_f/t_c} = 0$, $\tau \equiv (t/t_c)$. Thus the critical exponent α appearing in the scaling of $\bar{s}$ with t/t_c is simply the prod-

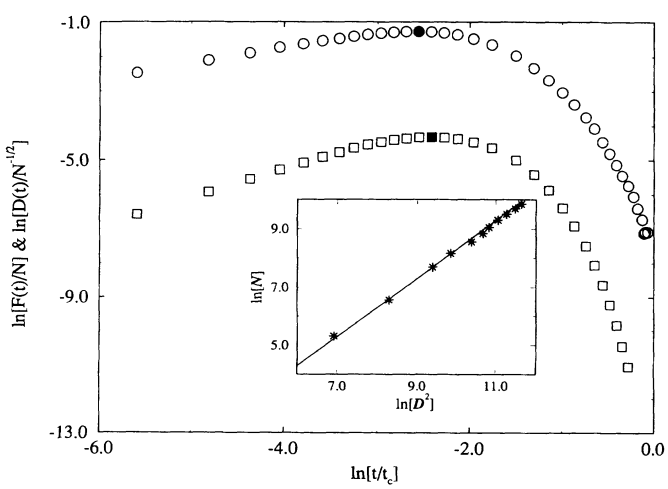

FIG. 5. Total number of unvisited disconnected regions or fragments (○) and the diversity of fragments (□) as a function of time for a lattice of 600^2 sites. Full circle (square) denotes the time of maximal number $\mathcal{N}$ (diversity $\mathcal{D}$) of fragments. (See text, tenth and eleventh paragraphs.) The inset shows the scaling relation between $\mathcal{N}$ and $\mathcal{D}$.

uct of the reduced time t_f/t_c times $\ln N$. As a consequence, for *any* given lattice there is a constant fraction f_0 ($\simeq 0.703$), given by $(t_p/t_f) \simeq -(e/\pi)\ln(1-f_0)=1$, for which the PCT, Eq. (2), coincides with the time of maximal fragmentation. For $f > f_0$, $t_p > t_f$, for $f < f_0$, $t_p < t_f$. Using the asymptotic expression [12] for the CT in $d=2$ we argue that the time t_f of maximal fragmentation is given by

$$t_f = (1/e) N \ln N + O(N) . \tag{9}$$

In Fig. 5 we also exhibit a plot of the diversity of fragments as a function of t/t_c. The diversity,

$$D(t) = \sum_s \{1 - \delta_{n(s,t),0}\} , \tag{10}$$

measures the number of different sizes of unvisited regions present at time t. $D(t)$ has a maximum almost coincident with that of $F(t)$. Then, a maximum number of length (size) scales coexist in the PCT problem at the critical time $t_{\rm crit} \approx t_f$. In the inset of Fig. 5 we show that the maximum of $F(t)$, $\mathcal{N}$, and the maximum of $D(t)$, $\mathcal{D}$, present the simple scaling relation $\mathcal{N} \sim \mathcal{D}^{2\pm 0.1}$. A careful analysis of our data together with the conjecture $\alpha = \pi/e$ suggest that the maximum number of disconnected unvisited regions (fragments), $\mathcal{N} = F(t_f)$, and the average (fragment) size at the same (critical) time, $\bar{s}(t_f)$, assume the asymptotic values

$$\mathcal{N} \simeq (\pi/e^2)(N/\ln N) , \tag{11}$$

and

$$\bar{s}(t_f) \simeq (\pi/e)^{2-\pi/e} \ln N . \tag{12}$$

Finally, we calculate the correlation function

$$C(R) = \sum_{i=1}^{N_{nv}} n(R_i)/N_{nv}(t) , \tag{13}$$

on lattices of 600^2 sites, for $0.15 \le t/t_c \le 0.50$, where $n(r_i)$ is the number of unvisited sites within a ball of radius R_i centered at an unvisited site i. We find that $C(R) \sim R^\beta$, $\beta = (1.52 \pm 0.05) - (1.0 \pm 0.1)(t/t_c)$, for $R \le 5$, see Fig. 6, the time dependence being in excellent agreement with the prediction of Brummelhuis and Hilhorst [18] for $\ln R/\ln cN \ll 1$, $c \approx 1.85$, where c is a lattice parameter. The constant part of β deviates from $d=2$, expected in the continuum limit, because of lattice effects. In fact, by defining the number of sites inside the area, $A(R=1)$, of a ball of $R=1$ as the unit area, we have, for a square lattice, the following scaling relation: $A(R)/A(1) = R^x$, where the exponent x varies from 1 to ≈ 1.86 as $1 \le R \le 5$. For $R \to \infty$, $x \to d=2$.

From the conceptual point of view this Letter deals with very interesting phenomena, such as the discontinuous transitions for the PCT at $f=1$ and the RCT at $f=0$ as well as the time dependence of the fractal-like structure observed for the surviving unvisited clusters at the time scale of t_c. Besides representing a basic problem in RW statistics on its own, the subject of this Letter has direct or indirect implication in a number of problems in physics, biology, and technology.

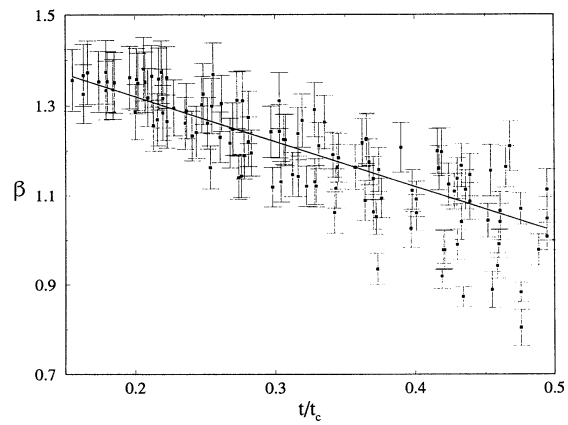

FIG. 6. Time-dependent exponent β associated with the correlation function [Eq. (13)] between unvisited sites.

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[1] J. W. Haus and K. W. Kehr, Phys. Rep. **150**, 253 (1987).
[2] J. D. Murray, *Mathematical Biology,* Springer Series in Biomathematics Vol. 19 (Springer, New York, 1989).
[3] A. K. Roy and A. Blumen, Physica (Amsterdam) **38D**, 291 (1989).
[4] A. Okubo, *Diffusion and Ecological Problems: Mathematical Models*, Springer Series in Biomathematics Vol. 10 (Springer, New York, 1980); S. A. Levin, in *Mathematical Ecology*, edited by Thomas G. Hallam and S. A. Levin (Springer, New York, 1986).
[5] B. B. Mandelbrot, Rev. Economics Stat. **LIII**, 225 (1971).
[6] P. G. Doyle and J. L. Snell, *Random Walks and Electric Networks* (The Mathematical Association of America, Washington, DC, 1984).
[7] P.-G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, 1979).
[8] S. Havlin and D. Ben-Avraham, Adv. Phys. **36**, 695 (1987).
[9] J. Feder, *Fractals* (Plenum, New York, 1988).
[10] B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, New York, 1983); R. Rammal, Phys. Rep. **103**, 151 (1984).
[11] A. M. Nemirovsky and M. D. Coutinho-Filho, Physica (Amsterdam) **177A**, 233 (1991).
[12] A. M. Nemirovsky, H. O. Mártin, and M. D. Coutinho-Filho, Phys. Rev. A **41**, 761 (1990).
[13] D. Asimov, SIAM J. Sci. Stat. Comput. **6**, 128 (1985).
[14] See, e.g., A. Münster, *Statistical Thermodynamics* (Springer-Verlag, Berlin, 1969), Vol. I.

[15] D. J. Aldous, Z. Wahrscheinlichkeitstheorie verw. Gebiete **62**, 361 (1983).

[16] See, e.g., K. Binder and D. Stauffer, in *Applications of Monte Carlo Method in Statistical Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1987).

[17] E. W. Montroll, J. Math. Phys. **10**, 753 (1969).

[18] M. J. A. M. Brummelhuis and H. J. Hilhorst, Physica (Amsterdam) **176A**, 387 (1991).

[19] R. Englman, N. Rivier, and Z. Jaeger, Philos. Mag. **56B**, 751 (1987).

[20] X. Z. Hu, B. Cotterell, and Y. W. Mai, Philos. Mag. Lett. **57**, 69 (1988).