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Critical Exponents for Two-Dimensional Tracer Diffusion through a Changing Background at Concentration $c = c_p$

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We study the diffusion of a particle on the sites of a triangular lattice of which half the sites are occupied by a "background" of other particles. No two particles may occupy the same site. We carry out Monte Carlo simulations for the following model: At each Monte Carlo step the tracer attempts to move to a neighboring site, which it does if the site is unoccupied. At each step, each background particle attempts to desorb with probability γ. If a background particle desorbs, it is replaced at a randomly chosen site on the lattice. We define $\langle R_{tr}^2(t)\rangle/t = D_{tr}$. For the case $\gamma = 0$, we calculate $D_0 \sim t^k$ and find $k = 0.71 \pm 0.01$, where t is the number of Monte Carlo steps. When $\gamma > 0$, we calculate $D_{tr} \sim \gamma^{-w_{ad}}$ and find $w_{ad} = 0.24 \pm 0.02$. We compare this to the model in which the background particles are constrained to move to nearest neighbor sites and find $D_{tr} \sim \gamma^{-w_1}$ with $w_1 = 0.28 \pm 0.03$.

KEY WORDS: Critical exponents; tracer diffusion in 2D; Monte Carlo simulation.

1. INTRODUCTION

An understanding of the diffusion of a tracer particle in the presence of a background of other objects is of practical importance as well as being of intrinsic interest. A study of the movement of a tracer in two dimensions has applications to, for example, the distribution of proteins or other polymers in biological or model membranes.[1–4] Simplified models of these systems have been devised to study the diffusion of a tracer particle on the sites of a lattice which can also be occupied by "background" particles.[5,6]

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Of particular interest is the movement of the tracer particle at the static percolation limit, i.e., when the background particles have a concentration $c = c_p$. Here we will compare the results of computer simulations for the cases in which a tracer particle moves by jumping to an empty nearest neighbor site while the background particles move by either (a) jumping to an empty nearest neighbor site or (b) desorbing from the lattice while another particle is adsorbed onto the lattice. The concentration of background particles is maintained at $c = c_p$. Kehr *et al.*[7] derived an expression for the exponent w describing how the long-time diffusion coefficient goes to zero in case (a). Although they confirmed it by computer simulation for $d = 3$, they did not report a value for $d = 2$. This paper will be concerned with calculating values for this exponent in cases (a) and (b) for $d = 2$.

2. MODEL AND SIMULATION PROCEDURE

We used a triangular lattice of N sites with periodic boundary conditions. Half of the sites were occupied by background particles distributed randomly, and N_{tr} tracer particles, with $N_{tr} \ll N$, were placed at unoccupied sites. Probabilities 1 and $P \leqslant 1$ were assigned to the tracers and to the background particles, respectively. We performed a Monte Carlo simulation in order to calculate the diffusion coefficient of the tracer,

$$D_{tr} = \lim_{t \to \infty} \langle R_{tr}^2(t) \rangle_s / t \tag{1}$$

where t is the number of Monte Carlo steps elapsed and $R_{tr}^2(t)$ is the square of the vector distance moved by the tracer in that number of steps. $\langle \cdots \rangle_s$ indicates that the simulation was repeated a number of times s in order to obtain a value for D_{tr}.

At each Monte Carlo step all particles were visited in a random sequence. Each tracer particle attempted to move to a randomly chosen nearest neighbor site, which it did if that site was not occupied by a background particle. At each step, for each background particle, we selected a random number $0 \leqslant r < 1$. If $r > P$, then the background particle remained unmoved. If $r \leqslant P$, then that background particle could attempt to move as follows for the two cases: (a) For the same particle we chose one of the six nearest neighbor sites randomly. If this site was unoccupied, then we moved the background particle to that site. (b) We removed the background particle from the lattice. We then randomly chose a site on the lattice. If it was unoccupied, we placed a background particle there. If it was occupied, we searched in its neighborhood until we found an unoccupied site and placed a background particle there.

It is clear that case (b) is not simply the extension of case (a) to allow

steps of any range for the background particles. In case (a) we do not search for an empty nearest neighbor site. However, case (b) is a more realistic representation of objects adsorbing and desorbing while keeping $c = c_p$.

We defined $\gamma = 1/P$ and searched for an exponent such that (see, e.g., ref. 5)

$$D_{\rm tr} \sim \gamma^{-w} \tag{2}$$

where $w = w_1$ for case (a) and $w = w_{\rm ad}$ for case (b). Equivalently, if the tracer and background particles moved at average rates of Γ' and Γ, respectively, then $\Gamma'/\Gamma = \gamma$. Kehr *et al.*[7] performed computer simulations and calculated $w_1 = 0.56 \pm 0.02$ for $d = 3$, in essential agreement with the expression[7]

$$w_1 = \mu/(2\nu - \beta + \mu) \tag{3}$$

3. RESULTS

We studied the behavior of $D_{\rm tr}$ in both cases for $N = (200)^2$, $N_{\rm tr} = 40$, and for t equal to 1000, 2000, and 4000 Monte Carlo steps in order to identify asymptotia. For $t = 4000$ [case (a)] and $t = 2000$ [case (b)] we fitted $\langle R_{\rm tr}^2(t)\rangle_s$ to the form[8]

$$\langle R_{\rm tr}^2(t)\rangle_s \sim A + B \log t + D_{\rm tr} t \tag{4}$$

and plotted $\langle R_{\rm tr}^2(t)\rangle_s/t$ against $\log t/t$, ignoring the term in A/t, to obtain a value for $D_{\rm tr}$. We also plotted $\langle R_{\rm tr}^2(t)\rangle_s/t$ against t, ignoring the terms in A and $B \log t$, and obtained another value for $D_{\rm tr}$. We compared the results of these two methods and found them to be consistent. We used $s = 32$, i.e., 32 samples each containing 40 tracers. We confirmed that the ratio of the average rate of movement Γ'/Γ was equal to $\gamma = 1/P$.

We checked our procedures in the case for which the background particles are static ($P = 0$) and found that

$$\langle R_{\rm tr}^2(t)\rangle_s \sim t^k, \qquad k = 0.71 \pm 0.01 \tag{5}$$

for short times (up to $t = 1000$), in accord with previous results.[5]

For longer times (from $t = 1000$ to $t = 4000$), we found that

$$k = 0.66 \pm 0.01 \tag{6}$$

From this value we calculated μ using the expression

$$\mu = (2\nu - \beta)(1 - k)/k \tag{7}$$

and found that

$$\mu = 1.30 \pm 0.04 \tag{8}$$

when the values of $\beta = 5/36$ and $\nu = 4/3$[9] for $d = 2$ are substituted.

Figure 1 shows plots of $\log(D_{tr})$ against $\log(\gamma)$ for case (a) (Fig. 1A) and case (b) (Fig. 1B). The slopes of these plots yield $-w_1$ and $-w_{ad}$, respectively. From the first we found that

$$w_1 = 0.28 \pm 0.03 \tag{9}$$

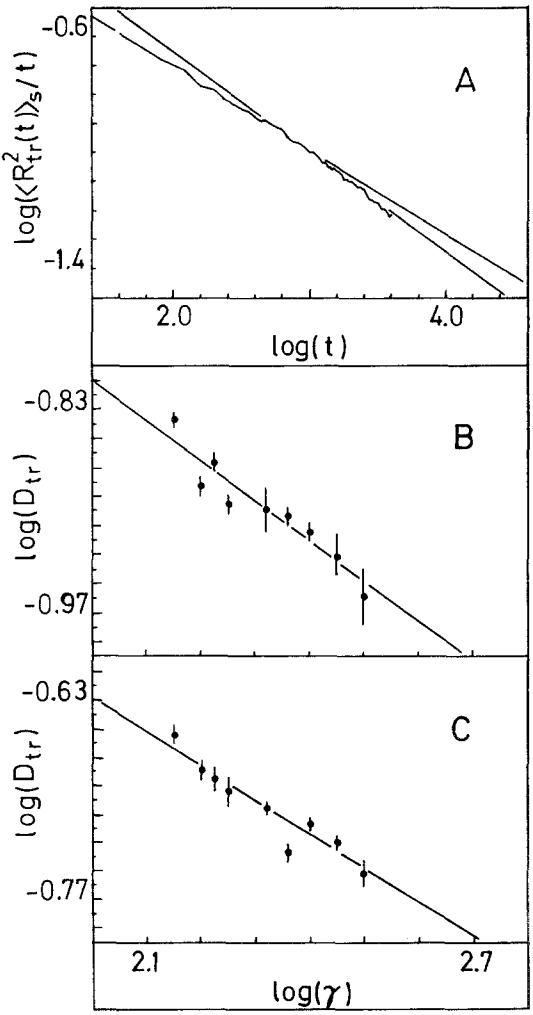

Fig. 1. (A) $\log(\langle R_{tr}^2(t)\rangle_s/t)$ vs. $\log(t)$ for $P = 0$. The slope is $k^{-1} = -0.29$ for $\log(t)$ up to 3. For $\log(t)$ from 3 to 3.6, $k^{-1} = -0.34$. (B, C) $\log(D_{tr})$ vs. $\log(\gamma)$. The slopes give (B) $w_1 = 0.28$ and (C) $w_{ad} = 0.24$.

which is essentially in accord with that given by (3), $w_1 = 0.30 \pm 0.01$, when the values of $\beta = 5/36$, $\nu = 4/3$,[9] and $\mu = 1.10 \pm 0.05$[10] for $d = 2$ are substituted. From the second we found that

$$w_{ad} = 0.24 \pm 0.02 \tag{10}$$

which is expected to be different from w_1.

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