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A First Passage Time Problem for Random Walk Occupancy

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Two recent studies of diffusion and flow properties of polymers in a melt have suggested the problem of finding the average time for m Brownian particles to leave a sphere for the first time, given that exited particles can also reenter the sphere. We prove that the asymptotic density (as $m \to \infty$) for the time to first emptiness of the sphere for zero-mean Brownian motion is a delta function, characterized by the exit time $a(m/\ln m)^{2/D}$, a being a constant and D being the dimension. The presence of a field leaves the delta-function form for the density, but changes the time dependence to $a \ln m$, with only the constant a depending on the dimension. Simulations of the process suggest that the value of m needed for the validity of the asymptotic result is orders of magnitude greater than 1000.

KEY WORDS: Brownian motion; random walk occupancies; reptation times; first passage times.

1. INTRODUCTION

When a stress is applied to a polymer melt, one observes a crossover from an elastic to a plastic viscosity response. The polymer physicist is interested in determining how the characteristic time τ for this crossover to occur

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scales with the chain mass M. Experimental results suggest that the dependence of τ on M goes like

$$\tau \sim M^{3+\alpha} \tag{1}$$

where the parameter α has been found to lie in the interval (0.3, 0.4). There are a number of theoretical analyses of this problem, most of which suggest that the correct dependence of τ on M is of the form given in Eq. (1) with $\alpha = 0$, in contrast with the experimental results. Doi[1] and Graessley[2] suggest that the correct dependence of τ on M is indeed $\alpha = 0$, and that the observed dependence is an intermediate state. More recently, Scher and Shlesinger[3] have suggested a theoretical picture that allows for the possibility $\alpha > 0$, although their model does not give an exact value for this parameter. This model was reconsidered by Weiss *et al.*,[4] whose analysis suggests that $\alpha = 1/3$ is indeed the correct theoretical result.

In the framework of the Scher–Shlesinger model the determination of the proper exponent in Eq. (1) depends on the solution of a mathematical problem that does not seem to have appeared either in the mathematical or physical literature. Its solution, therefore, is of some interest outside of its particular application in polymer physics and is the subject of the present paper. The problem may be posed in terms of the occupancy of a D-dimensional sphere, initially populated by m uniformly distributed point particles, each of which moves, independently of the others, by a Brownian motion process. At $t = 0$ the particles are released and allowed to diffuse throughout all space, the boundary of the sphere posing no obstacle, so that the particles can both exit and reenter the sphere. The problem so stated is a variant of the occupancy problem for Brownian motion particles first studied by Darling and Kac.[5]

In the present formulation the number of particles in the sphere at time t, $n(t)$, is a random variable. The solution to the physical problem suggested by the Scher–Shlesinger model can be shown to be equivalent to finding the dependence on $n(0) = m$ of the expected value of the random variable t_m, defined as

$$t_m = \inf\{t \mid n(t) = 0\} \tag{2}$$

Weiss *et al.*[4] have shown by a simple argument that in three dimensions

$$\langle t_m \rangle \leqslant m^{2/3} \tag{3}$$

Based on this inequality, they conjectured that $\langle t_m \rangle$ is exactly of the order of $m^{2/3}$, which can be shown to be equivalent, in the terms of the original problem, to $\tau_m \sim M^{10/3}$, in good agreement with the experimentally found dependence.

In the present paper we will find the exact asymptotic dependence of $\langle t_m \rangle$ on m, as well as the complete probability distribution in the $m = \infty$ limit. In particular, it will be shown that for zero-mean Brownian motion in D dimensions the scaling behavior of $\langle t_m \rangle$ takes the form

$$\langle t_m \rangle \sim (m/\ln m)^{2/D}, \qquad m \to \infty \tag{4}$$

which satisfies the inequality in Eq. (3). Furthermore, the effect of the logarithmic term is probably unobservable experimentally unless measurements are made over an unrealistically large range in M. The analysis of Section 2 leads to the conclusion that the limiting form of the probability density for the random variable t_m is a delta function. However, the analysis gives almost no clue as to how large m must be in order for the resulting form to be a good approximation. In the final section we address this question by means of computer simulations of the process. It is interesting to note from Eq. (4) that $\langle t_m \rangle$ decreases with increasing dimension. This is a consequence of the recurrence properties of the random walk considered as a function of dimension. A practical result of this phenomenon is that it is easier to do simulations for three-dimensional as compared to one-dimensional systems.

2. ANALYSIS

We consider m particles, which perform independent Brownian motions in D space with covariance matrix equal to the identity matrix and a drift vector μ. The position of the ith particle at time t is denoted by $X_i(t)$. Thus, for given $X_i(0) = x_i$, the density of $X_i(t)$ is

$$p(x, t) = \left(\frac{1}{2\pi t}\right)^{D/2} \exp\left(-\frac{1}{2t}\|x - x_i - t\mu\|^2\right) \tag{5}$$

where $\|\cdot\|$ denotes the Euclidean norm. Most of our attention will be focused on the case of zero drift ($\mu = 0$), but for contrast we also give some results for the case $\mu \neq 0$. Throughout we assume that the initial positions x_i of the particles are fixed and lie in the unit ball B. Thus

$$\|X_i(0)\| = \|x_i\| \leqslant 1, \qquad 1 \leqslant i \leqslant m \tag{6}$$

It will turn out that our estimates are uniform in the x_i under the restrictions specified in Eq. (6). Thus, we could equally well choose the x_i random according to any distribution for which Eq. (6) holds (e.g., the x_i

could be chosen independent and uniform on B, which is appropriate for the original physical problem). We define

$$V = V_D = \text{volume of the unit ball in } D \text{ space}$$

With this definition, we shall prove the following theorem.

Theorem 1. Assume $\mu = 0$. Let

$$\alpha_D = \frac{1}{2\pi}\left(\frac{D}{2} V_D\right)^{2/D}$$

Then

$$\left(\frac{\ln m}{m}\right)^{2/D} t_m \to \alpha_D \text{ in probability, as } m \to \infty \tag{7}$$

and for every $k \geq 1$

$$\langle t_m^k \rangle \sim \alpha_D^k \left(\frac{m}{\ln m}\right)^{2k/D}, \qquad m \to \infty \tag{8}$$

These results are equivalent to an asymptotic delta-function density for the variable t_m. It is interesting to observe that there is no difference between transient and recurrent Brownian motion in the present context.

The behavior of t_m for the case with drift is rather different, as shown by the next theorem.

Theorem 2. Assume $\mu \neq 0$. Then

$$\frac{1}{\ln m} t_m \to \frac{2}{\|\mu\|^2} \text{ in probability, as } m \to \infty$$

In fact,

$$P\left\{\frac{1}{\|\mu\|^2}[2 \ln m - (D+3) \ln \ln m] \leq t_m \leq \frac{1}{\|\mu\|^2}[2 \ln m + (D-2) \ln \ln m]\right\} \to 1, \qquad \text{as} \quad m \to \infty \tag{9}$$

Also, for $k \geq 1$

$$\langle t_m^k \rangle \sim \left(\frac{2 \ln m}{\|\mu\|^2}\right)^k, \qquad m \to \infty$$

The proofs are based on consideration of the events

$$E_i(t) := \{ \|X_i(t)\| > 1 \}$$
$$= \{ i\text{th particle is outside } B \text{ at time } t \}$$

and

$$E(t) := \bigcap_{i=1}^{m} E_i(t) = \{ n(t) = 0 \}$$

Thus, $\{t_m \leqslant T\}$ is the same event as $\{E(t)$ occurs for some $t \leqslant T\}$. We estimate the probability of the last event by applying Chebyshev's inequality to the amount of time during $[0, T]$ for which $E(t)$ occurs. More specifically, we define

$$\rho(T) = |\{t \leqslant T\colon E(t) \text{ occurs}\}|$$

($|\cdot|$ denotes Lebesgue measure), and estimate $\langle \rho(T) \rangle$ and

$$\operatorname{var}[\rho(T) - \rho(T/2)]$$
$$:= \langle [\rho(T) - \rho(T/2)]^2 \rangle - [\langle \rho(T) - \rho(T/2) \rangle]^2$$

To carry out the details, we must actually consider the slightly more general problem, in which B is replaced by a ball of radius r with r not necessarily equal to 1. We write $B(r)$ for the ball of radius r,

$$E_i^r(t) = \{ \|X_i(t)\| > r \}$$

and define $E^r(t)$, $\rho^r(T)$ in the obvious way.

We concentrate on the proof of Theorem 1. Lemmas 1–4 all deal with the case $\mu = 0$.

Lemma 1. Let $\mu = 0$ and set

$$\beta = \frac{2}{D} (\alpha_D)^{D/2} = \left(\frac{1}{2\pi}\right)^{D/2} V_D$$

For all $\varepsilon > 0$ there exists a constant $c = c(\varepsilon, D)$ such that, uniformly on $1/2 \leqslant r \leqslant 2$, $mT^{-D/2} \geqslant c$, $T \geqslant c$, $\|x_i\| \leqslant 1$,

$$\langle \rho^r(T) \rangle \leqslant (1 + 2\varepsilon) \frac{2}{\beta D r^D} \frac{1}{m} T^{1 + D/2}$$
$$\times \exp[-(1 - \varepsilon) \beta r^D m T^{-D/2}] \tag{10}$$

Also, uniformly on $1/2 \leqslant r \leqslant 2$, $mT^{-D/2} \geqslant c$, $T \geqslant c$, and for all x_i [not necessarily satisfying (6)]

$$\langle \rho^r(T) - \rho^r(T/2) \rangle \geqslant (1 - 2\varepsilon) \frac{2}{\beta\, Dr^D} \frac{1}{m} T^{1 + D/2} \times \exp[-(1+\varepsilon)\, \beta r^D m T^{-D/2}] \qquad (11)$$

Proof. Let $I(t, r)$ denote the indicator function of $E^r(t)$. Then

$$\langle \rho^r(T) \rangle = \left\langle \int_0^T I(t, r)\, dt \right\rangle = \int_0^T \langle I(t, r) \rangle\, dt$$

$$= \int_0^T P\{E^r(t)\}\, dt = \int_0^T \prod_{i=1}^m P\{E_i^r(t)\}\, dt$$

$$= \int_0^T \prod_{i=1}^m [1 - P\{\|X_i(t)\| \leqslant r\}]\, dt$$

From Eq. (5) with $\mu = 0$ we immediately see that for any given $\varepsilon > 0$ there exists an $a = a(\varepsilon)$ such that for $t \geqslant a(\varepsilon)$ and uniformly in $\|x_i\| \leqslant 1$ and $r \leqslant 2$

$$(1 - \varepsilon)\, \beta r^D t^{-D/2} \leqslant P\{\|X_i(t)\| \leqslant r\} \leqslant \beta r^D t^{-D/2} \qquad (12)$$

By taking $a(\varepsilon)$ larger, we may then even write

$$\exp[-(1+\varepsilon)\, \beta r^D t^{-D/2}] \leqslant P\{E_i^r(t)\} \leqslant \exp[-(1-\varepsilon)\, \beta r^D t^{-D/2}], \qquad t \geqslant a(\varepsilon) \qquad (13)$$

In fact, the right-hand inequality of Eq. (12), and hence the left-hand inequality of Eq. (13), holds uniformly in *all* x_i.

The remainder of this proof is devoted to the proof of Eq. (10). We leave the proof of Eq. (11) to the reader. Given $a(\varepsilon)$, there exists a $b = b(\varepsilon) > 0$ such that $P\{E_i^r(t)\} \leqslant e^{-b}$, uniformly in $1/2 \leqslant r \leqslant 2$, $\|x_i\| \leqslant 1$, and $t \leqslant a(\varepsilon)$. Consequently, for $T \geqslant a(\varepsilon)$

$$\langle \rho^r(T) \rangle \leqslant a(\varepsilon) \exp[-mb(\varepsilon)] + \int_0^T \exp[-(1-\varepsilon)\, m\beta r^D t^{-D/2}]\, dt$$

The integral here equals

$$\frac{2}{D} [(1-\varepsilon)\, \beta r^D]^{2/D}\, m^{2/D} \int_{(1-\varepsilon) m\beta r^D T^{-D/2}}^{\infty} e^{-s} s^{-1-2/D}\, ds$$

and one integration by parts shows that

$$\int_A^\infty e^{-s} s^{-p}\, ds \sim A^{-p} e^{-A}, \qquad A \to \infty \tag{14}$$

Equation (10) follows from this, and the proof of Eq. (11) is similar. ∎

As an immediate corollary, we obtain "one-half" of Theorem 1.

Lemma 2. Let $\mu = 0$. For small $\varepsilon > 0$ and large m

$$P\left\{t_m \leqslant (1-5\varepsilon)\,\alpha_D \left(\frac{m}{\ln m}\right)^{2/D}\right\} \leqslant m^{-\varepsilon/2} (\ln m)^{-2/D}$$

Proof. Take $r = 1 - \varepsilon$ and set

$$\Delta = \Delta(m, \varepsilon) = \varepsilon^2 (4D^2 \ln m)^{-1}$$

If at a certain time τ there are no particles in $B = B(1)$, then the conditional probability of there being no particles in $B(r)$ during the whole time interval $[\tau, \tau + \Delta]$ is at least

$$1 - P\{\text{at least one particle has a displacement} \geqslant \varepsilon \text{ during } [\tau, \tau+\Delta]\}$$

$$\geqslant 1 - \frac{2mD}{(2\pi\Delta)^{1/2}} \int_{\varepsilon/D}^\infty e^{-s^2/2\Delta}\, ds$$

$$\geqslant \frac{1}{2} \quad \text{for large enough } m$$

Consequently,

$$\left\langle \int_\tau^{\tau+\Delta} I(t, r)\, dt \,\middle|\, n(\tau) = 0 \right\rangle \geqslant \frac{1}{2} \Delta$$

We now take for τ the (Markov) time t_m. Then, by the (strong) Markov property of the Brownian motion (I_A denotes the indicator function of A)

$$\langle \rho^r(T+\Delta) \rangle \geqslant \left\langle \int_{t_m}^{t_m+\Delta} I(t, r)\, dt \cdot I_{[t_m \leqslant T]} \right\rangle$$

$$\geqslant P\{t_m \leqslant T\} \frac{1}{2} \Delta$$

Combined with Eq. (10), this yields

$$P\{t_m \leqslant T\} \leqslant \frac{2}{\Delta} \langle \rho^r(T+\Delta) \rangle$$

$$\leqslant C_1 \frac{\ln m}{\varepsilon^2} \frac{1}{m} (T+1)^{1+D/2} \exp[-(1-\varepsilon)^{D+1} \beta m (T+1)^{-D/2}]$$

for some constant C_1, when $mT^{-D/2} \geqslant c$, and m and T large enough. Lemma 2 follows by substituting $T = (1-5\varepsilon)\,\alpha_D(m/\ln m)^{2/D}$. ∎

We continue with the proof of the other half of Theorem 1. The restriction in Eq. (6) is not necessary for this part. In addition, we only need to take $r=1$ in Lemmas 3 and 4. Accordingly, we drop the r from the notation [e.g., we write $I(s)$ instead of $I(s, 1)$]. For the upper bound for t_m we derive a bound for

$$\begin{aligned}
&\operatorname{var}[\rho(T) - \rho(T/2)] \\
&\quad = \operatorname{var}\left[\int_{T/2}^{T} I(s)\,ds\right] \\
&\quad = \int_{T/2}^{T} ds \int_{T/2}^{T} dt\,[\langle I(s)\,I(t)\rangle - \langle I(s)\rangle\langle I(t)\rangle]
\end{aligned} \tag{15}$$

Lemma 3. Let $\mu = 0$. Then there exist constants $d = d(D)$ and $C = C(D)$ such that for all $T/2 \geqslant \gamma \geqslant d$ and all x_i

$$\begin{aligned}
\operatorname{var}[\rho(T) - \rho(T/2)] \leqslant{}& 2\gamma\langle\rho(T) - \rho(T/2)\rangle \\
&+ Cm(T\gamma)^{-D/2}\exp[Cm(T\gamma)^{-D/2}]\,[\langle\rho(T) - \rho(T/2)\rangle]^2
\end{aligned}$$

Proof. We note that

$$\begin{aligned}
\langle I(s)\,I(t)\rangle &= P\{E(s) \text{ and } E(t)\} \\
&= \prod_{i=1}^{m} [1 - P\{\|X_i(s)\| \leqslant 1\} - P\{\|X_i(t)\| \leqslant 1\} \\
&\qquad + P\{\|X_i(s)\| \leqslant 1,\ \|X_i(t)\| \leqslant 1\}]
\end{aligned}$$

while

$$\begin{aligned}
\langle I(s)\rangle\langle I(t)\rangle = \prod_{i=1}^{m} &[1 - P\{\|X_i(s)\| \leqslant 1\} - P\{\|X_i(t)\| \leqslant 1\} \\
&+ P\{\|X_i(s)\| \leqslant 1\}\,P\{\|X_i(t)\| \leqslant 1\}]
\end{aligned}$$

For any numbers $0 \leqslant a_i, b_i \leqslant 1$ one has

$$\prod_{i=1}^{m} (1 - a_i) - \prod_{i=1}^{m} (1 - b_i) \leqslant \sum_{i=i}^{m} [b_i - a_i]^+ \prod_{j \neq i} (1 - a_j \wedge b_j) \tag{16}$$

where $c^+ = \max(0, c)$ and $a \wedge b = \min(a, b)$. We take

$$a_i = P\{\|X_i(s)\| \leqslant 1\} + P\{\|X_i(t)\| \leqslant 1\} - P\{\|X_i(s)\| \leqslant 1, \|X_i(t)\} \leqslant 1\}$$

$$b_i = P\{\|X_i(s)\| \leqslant 1\} + P\{\|X_i(t)\| \leqslant 1\} - P\{\|X_i(s)\| \leqslant 1\} P\{\|X_i(t)\| \leqslant 1\}$$

Note that the formula for the Gaussian density shows that

$$a_i, b_i \leqslant [(2\pi s)^{-D/2} + (2\pi t)^{-D/2}] V_D = \beta[s^{-D/2} + t^{-D/2}]$$

and for $s < t$

$$\begin{aligned}|b_i - a_i| &\leqslant \int_{\|x\| \leqslant 1} P\{X_i(s) \leqslant 1\}\, dx \\ &\quad \times |P\{\|X_i(t-s) - x\| \leqslant 1\} - P\{\|X_i(t)\| \leqslant 1\}| \\ &\leqslant \left(\frac{1}{2\pi}\right)^D V_D^2 \left[\frac{1}{s(t-s)}\right]^{D/2} \qquad (17)\end{aligned}$$

Moreover, there exists a constant $d = d(D)$ such that, for $s \geqslant d$, $t - s \geqslant d$, one has $a_i, b_i \leqslant 1/2$, and hence

$$\begin{aligned}\prod_{j \neq i} (1 - a_j \wedge b_j) &\leqslant 2 \prod_{j=1}^{m} (1 - a_j \wedge b_j) \\ &\leqslant 2 \prod_{j=1}^{m} (1 - b_j) \prod_{j=1}^{m} [1 + 2(b_j - a_j)^+] \\ &\leqslant 2\left[\prod_{j=1}^{m} (1 - b_j)\right] \exp\left[\sum_{j=1}^{m} 2(b_j - a_j)^+\right]\end{aligned}$$

Combining this with Eqs. (16) and (17), we find for our a_i, b_i, and $s \geqslant d$, $t - s \geqslant d$, and a suitable constant C_2

$$\begin{aligned}&\langle I(s)\, I(t)\rangle - \langle I(s)\rangle\langle I(t)\rangle \\ &= \prod_{j=1}^{m} (1 - a_j) - \prod_{j=1}^{m} (1 - b_j) \\ &\leqslant 2m \left(\frac{1}{2\pi}\right)^D V_D^2 [s(t-s)]^{-D/2} \prod_{j=1}^{m} (1 - b_j) \\ &\quad \times \exp\left\{2m \left(\frac{1}{2\pi}\right)^D V_D^2 [s(t-s)]^{-D/2}\right\} \\ &\leqslant C_2 m [s(t-s)]^{-D/2} \exp\{C_2 m [s(t-s)]^{-D/2}\} \langle I(s)\rangle\langle I(t)\rangle\end{aligned}$$

Trivially, we have also for all s, t

$$\langle I(s)\, I(t)\rangle - \langle I(s)\rangle\langle I(t)\rangle \leqslant \langle I(s)\rangle \wedge \langle I(t)\rangle$$

so that by Eq. (15)

$$\begin{aligned}
&\operatorname{var}[\rho(T)-\rho(T/2)]\\
&\quad = 2\int_{T/2}^{T} ds \int_{T/2}^{T} dt\, [\langle I(s)\, I(t)\rangle - \langle I(s)\rangle\langle I(t)\rangle]\\
&\quad \leqslant 2\int_{T/2}^{T} ds \int_{s}^{s+\gamma} dt\, \langle I(s)\rangle\\
&\qquad + 2\int_{T/2}^{T} ds \int_{s+\gamma\leqslant t\leqslant T} dt\, C_2 m[s(t-s)]^{-D/2}\\
&\qquad \times \exp[C_2 m s(t-s)]^{-D/2}\, \langle I(s)\rangle\langle I(t)\rangle\\
&\quad \leqslant 2\tau\langle \rho(T)-\rho(T/2)\rangle + 2C_2 m(T\gamma/2)^{-D/2}\\
&\qquad \times \exp[C_2 m(T\gamma/2)^{-D/2}][\langle \rho(T)-\rho(T/2)\rangle]^2 \quad \blacksquare
\end{aligned}$$

Lemma 4. For small $\varepsilon > 0$, large m and integral ν

$$P\left\{t_m \geqslant (1+5\varepsilon)\,\nu\alpha_D\left(\frac{m}{\ln m}\right)^{2/D}\right\} \leqslant m^{-\nu\varepsilon D/(2+D)} \tag{18}$$

uniformly in all x_i.

Proof. By virtue of the Markov property,

$$\begin{aligned}
&P\left\{t_m \geqslant (1+5\varepsilon)\,\nu\alpha_D\left(\frac{m}{\ln m}\right)^{2/D}\right.\\
&\qquad \left. 0 \leqslant t \leqslant (1+5\varepsilon)(\nu-1)\,\alpha_D\left(\frac{m}{\ln m}\right)^{2/D},\ 1\leqslant i\leqslant m\right\}\\
&\qquad \leqslant \sup_{x_i} P\left\{t_m \geqslant (1+5\varepsilon)\,\alpha_D\left(\frac{m}{\ln m}\right)^{2/D}\right\}
\end{aligned}$$

on the set

$$\left\{t_m > (1+5\varepsilon)(\nu-1)\,\alpha_D\left(\frac{m}{\ln m}\right)^{2/D}\right\}$$

It therefore suffices to prove the lemma for $\nu = 1$. For $\nu = 1$ we take

$$T = (1+5\varepsilon)\,\alpha_D \left(\frac{m}{\ln m}\right)^{2/D} \tag{19}$$

Then, by virtue of Chebyshev's inequality,

$$\begin{aligned} P\left\{t_m > (1+5\varepsilon)\,\alpha_D \left(\frac{m}{\ln m}\right)^{2/D}\right\} &\leqslant P\left\{\rho(T) - \rho\left(\frac{T}{2}\right) = 0\right\} \\ &\leqslant \frac{\operatorname{var}[\rho(T) - \rho(T/2)]}{[\langle \rho(T) - \rho(T/2)\rangle]^2} \end{aligned} \tag{20}$$

But for the T specified in Eq. (19), the result in Eq. (11) with $r = 1$ shows that

$$\langle \rho(T) - \rho(T/2)\rangle \geqslant C_3 m^{2\varepsilon} (\ln m)^{-1-2/D} \tag{21}$$

for a suitable constant C_3 [recall that $\beta(\alpha_D)^{-D/2} = 2/D$]. On the other hand. Lemma 3 with T as in Eq. (19) shows that for some constant C_4 (independent of τ, m)

$$\begin{aligned} &\operatorname{var}[\rho(T) - \rho(T/2)] \\ &\quad \leqslant 2\gamma \langle \rho(T) - \rho(T/2)\rangle \\ &\quad \times C_4 \gamma^{-D/2} (\ln m) \exp(C_4 \gamma^{-D/2} \ln m)\, [\langle \rho(T) - \rho(T/2)\rangle]^2 \end{aligned} \tag{22}$$

By choosing

$$\gamma = m^{4\varepsilon/(2+D)}$$

we obtain the result of Eq. (18) with $\nu = 1$ from Eqs. (20)–(22). ▮

The proof of Theorem 1 is now easily completed. Equation (7) is implied by Lemma 2 and Eq. (18) with $\nu = 1$. The result in Eq. (8) follows from Eq. (7) plus the uniform (in m) integrability of

$$\left\{\left(\frac{\ln m}{m}\right)^{2/D} t_m\right\}^k$$

implied by Eq. (18).

The proof of Theorem 2 is far easier. We restrict ourselves to a few remarks. In this case

$$P\{E_i^r(t)\} = 1 - \frac{1}{(2\pi t)^{D/2}} \int_{\|x\| \leqslant r} \exp\left(-\frac{1}{2t} \|x - x_i - t\mu\|^2\right) dx$$

and one easily sees that for $t \geqslant 1$, $r \leqslant 1$, and $\|x_i\| \leqslant 1$ the last integral lies between

$$r^D V_D \exp(-\tfrac{1}{2} t \|\mu\|^2 - 2 \|\mu\| - 2)$$

and

$$r^D V_D \exp(-\tfrac{1}{2} t \|\mu\|^2 + 2 \|\mu\|)$$

Consequently, for t greater than some $t_0(\mu)$,

$$\begin{aligned} \exp\left[-2m\left(\frac{r^2}{2\pi t}\right)^{D/2} V_D \exp\left(-\frac{t}{2} \|\mu\|^2 + 2\|\mu\|\right)\right] & \\ \leqslant P\{E^r(t)\} & \\ = \prod_{i=1}^{m} P\{E_i^r(t)\} & \\ = \langle I(r, t) \rangle & \\ \leqslant \exp\left[-2m\left(\frac{r^2}{2\pi t}\right)^{D/2} V_D \exp\left(-\frac{t}{2} \|\mu\|^2 - 2\|\mu\| - 2\right)\right] & \end{aligned}$$

In particular, for

$$T_1 = \|\mu\|^{-2} [2 \ln m - (D-2) \ln \ln m]$$

we have

$$\begin{aligned} P\left\{t_m > \frac{2 \ln m}{\|\mu\|^2} - \frac{D-2}{\|\mu\|^2} \ln \ln m\right\} & \\ \leqslant 1 - P\{E^1(T_1)\} = O[(\ln m)^{-1}] \to 0 & \end{aligned}$$

Also, with

$$T_2 = \|\mu\|^{-2} [2 \ln m - (D+2) \ln \ln m]$$

we obtain for $1/2 \leqslant r \leqslant 2$ and some constant $C_5 > 0$

$$\langle \rho^r(T_2) \rangle = \int_0^{T_2} \langle I(r, t) \rangle \, dt = O[(\ln m) \, m^{-C_5}]$$

We can now complete the proof of Eq. (9) by the method of Lemma 2.

3. SIMULATION RESULTS

The theoretical results summarized in Theorems 1 and 2 relate to the asymptotic distribution of t_m. However, the proofs are poorly suited to indicate the values of m required to ensure that the asymptotic results give useful approximations to the true ones. In particular, one wants to check the reliability of the expression in Eq. (4) for $\langle t_m \rangle$, since this parameter is required for the solution of the polymer problem. For these purposes we ran simulations on a variety of cases in from one to six dimensions.

Although the proofs in Section 2 are for Brownian motion in a continuum, they can be modified to make similar predictions for random walks on a lattice, the system easiest to simulate. We carried out a number of simulations for such systems, for both cases of zero-mean and biased random walks. In each case the initial configuration consisted of an equal number of random walkers placed on each site in the hypercube $[0, 1]^D$, where D is the dimension. The program was set to run until the first step at which the hypercube was empty of random walkers. Each run of the simulation program consisted of 1000 replications and the results were then averaged. In the case of zero-mean random walks we concentrated mainly on three or more dimensions, since, because of the recurrence properties of random walks in a lower number of dimensions, the simulations would have been too prohibitive to run.

Figure 1a shows data from our simulation program fitted to the equation

$$\langle t_m \rangle = a(m/\ln m)^b \tag{23}$$

for values of m from 160 to 1600. The parameters a and b were found by the nonlinear curve-fitting program MLAB available at the National Institutes of Health. The estimates of a and b are

$$\begin{aligned} a &= 3.551 \pm 0.0605 \\ b &= 0.659 \pm 0.0034 \end{aligned} \tag{24}$$

where the error terms are the standard errors calculated on the assumption that they have a Gaussian distribution. It is evident that the result for the exponent b is in the right ballpark with respect to the theoretically predicted value $b = 2/3$. However, if we plot

$$\langle t_m \rangle/(m/\ln m)^{2/3}$$

as a function of m, as in Fig. 1b, there is evidence of a trend which suggests that one is not yet in the asymptotic regime at $m = 1600$ walkers. We also

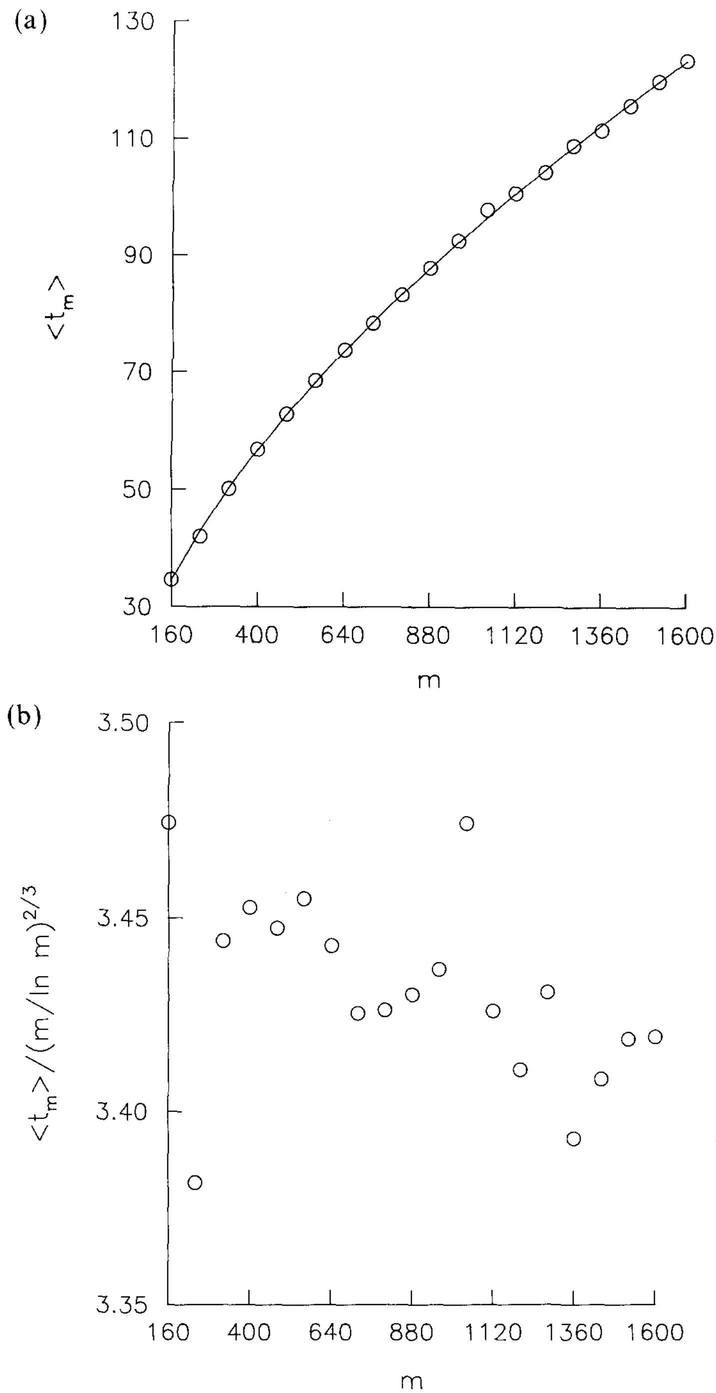

Fig. 1. (a) Simulation results for $\langle t_m \rangle$ for a zero-mean, three-dimensional random walk plotted as a function of m. The solid line is the result of fitting the data points to Eq. (23) with the parameters given in Eq. (24). (b) Calculated points for $\langle t_m \rangle/(m/\ln m)^{2/3}$ for the same data. There is some suggestion of a trend in the data.

fitted the second moment $\langle t_m^2 \rangle$ to the function given in Eq. (23), finding the parameter estimates

$$\begin{aligned} a_2 &= 14.313 \pm 0.650 \\ b_2 &= 1.302 \pm 0.0088 \end{aligned} \tag{25}$$

Again, the estimate of b_2 is very close to its theoretically predicted value of 4/3. However, a graph of $\langle t_m^2 \rangle/(m/\ln m)^{4/3}$, not shown here also shows evidence of drift as a function of m. Since the theoretically predicted probability densities of t_m are delta functions, one expects that $a_2 = a^2$. The estimated values of the a's given in Eqs. (24) and (25) do not quite obey this relation, since $a^2 = 12.61$, as opposed to $a_2 = 14.313$. This suggests that, although Eq. (23) gives a good approximation for the m dependence of $\langle t_m \rangle$, we are not yet in the asymptotic regime suggested by the results of Section 2.

To pursue this matter a bit further, we plotted the coefficient of variation

$$C(m) = \left(\frac{\langle t_m^2 \rangle}{\langle t_m \rangle^2} - 1 \right)^{1/2} \tag{26}$$

as a function of m. This is shown in Fig. 2 together with a fitted curve of the form

$$C(m) \approx 1.1629/(\ln m)^{0.9083} \tag{27}$$

Suppose that we characterize the asymptotic regime by $C(m) \approx 0.01$, the asymptotically predicted value being $C(\infty) = 0$. The fitted curve whose parameters are given in Eq. (27) then predicts that $m = 4 \times 10^{81}$. While this is perhaps an outrageous extrapolation, it does suggest that the regime in which the asymptotic theory is fully valid occurs for values of m that are at least many orders of magnitude greater than the maximum of 1600 used in our simulations.

In addition to our analyses made of data from simulations in three dimensions, we also examined data from simulations from four- to six-dimensional random walks. As an example of the results found, in the case of six dimensions the fit of Eq. (23) to the data leads to parameter estimates

$$\begin{aligned} a_6 &= 4.444 \pm 0.064 \\ b_6 &= 0.384 \pm 0.003 \end{aligned} \tag{28}$$

The theoretical value of b is 0.333, which is quite far from the results found

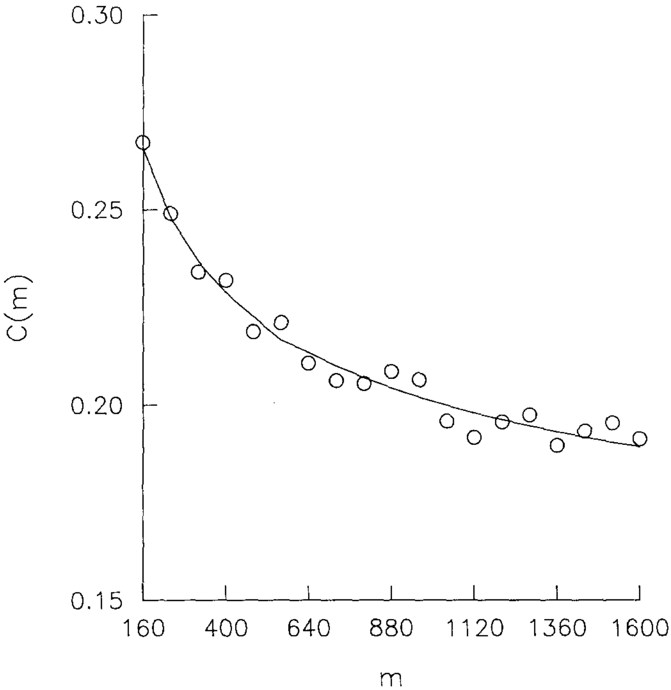

Fig. 2. Data points for the coefficient of variation $C(m) = (\langle t_m^2 \rangle / \langle t_m \rangle^2 - 1)^{1/2}$ as a function of m for a zero-mean, three-dimensional random walk. The solid line is the fitted curve specified in Eq. (27).

from our simulation, although the data are in good agreement with an equation of the form of Eq. (23), as can be seen from Fig. 3.

Finally, we also examined the case of a random walk in a field, in one dimension. The probability of stepping one lattice site to the right was chosen equal to 0.8 and that to the left equal to 0.2. In this case we examined the following form for $\langle t_m \rangle$:

$$\langle t_m \rangle = c(\ln m)^d \tag{29}$$

The significant bias in the transition probabilities allowed us to work with numbers of random walkers up to 4000, the quality of the fit being indicated by the curve plotted in Fig. 4. The fit is quite good, but the parameter estimates of c and d are

$$\begin{aligned} c &= 2.380 \pm 0.055 \\ d &= 1.183 \pm 0.011 \end{aligned} \tag{30}$$

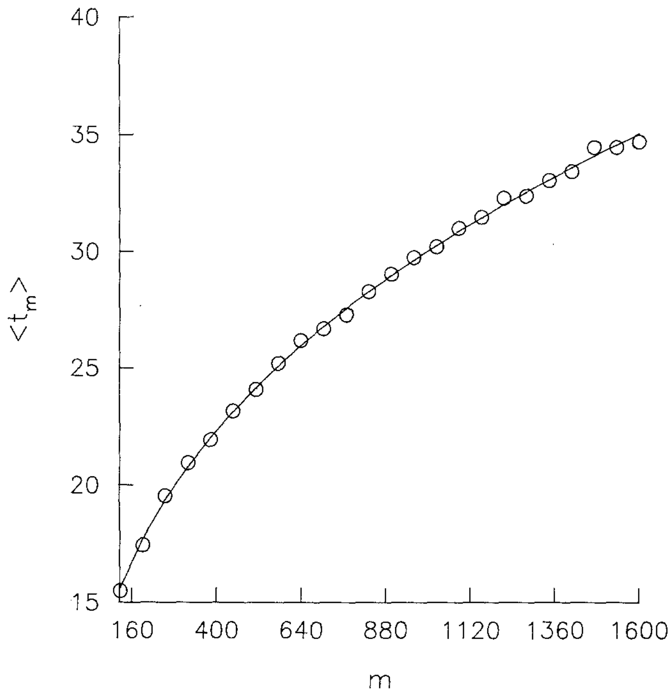

Fig. 3. Simulation results for $\langle t_m \rangle$ for a zero-mean, six-dimensional random walk plotted as a function of m and compared to the fitted curve whose form is given in Eq. (23). The parameters used are those in Eq. (28).

The theoretical value of d is 1, suggesting, as in the zero-mean case, that much larger values of m are needed to ensure the validity of the asymptotic theory, although the theoretical form for $\langle t_m \rangle$ seems to give a quite satisfactory fit to the data. We also plotted the coefficient of variation in this case as a function of m, fitting the data to

$$C(m) \approx 1.29/(\ln m)^{1.19} \tag{31}$$

The quality of the fit is the same as that in Fig. 2, and so is not shown here. Equation (31) suggests that the number of random walkers necessary to ensure that $C(m) = 0.01$ is 6×10^{25}, which, as before, is orders of magnitude larger than the numbers we were constrained to use.

A few remarks are in order about our results in the context of the original polymer problem that motivated the present research. Since the only parameter appearing in the theory of τ in Eq. (1) is $\langle t_m \rangle$, and since this parameter is well approximated by Eq. (23), we conclude that the

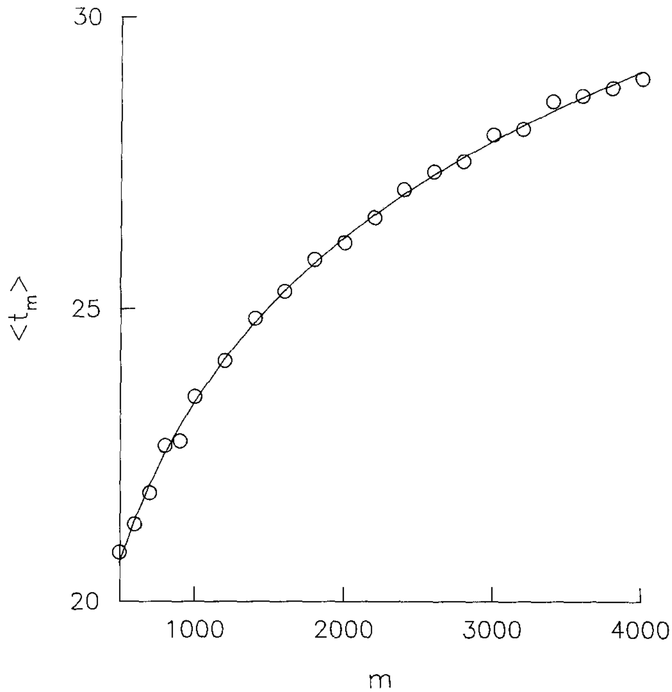

Fig. 4. Simulation results for $\langle t_m \rangle$ for a random walk in one dimension in which the probability of a single step transition to the right is 0.8 and that to the left is 0.2. The results are fitted to the function $\langle t_m \rangle = c(\ln m)^d$, where the parameters c and d are found in Eq. (30). Notice that the parameter d differs considerably from 1.

theory is in good accord with experiment. The exponent, as we have seen, is close to the predicted value of 2/3 for numbers of random walkers around 1000, which is a physically reasonable number for these kinds of polymer models. Thus, one finds that the parameter α in Eq. (1) is close to 1/3. It would be interesting to carry out measurements over a sufficiently large range in M to see whether the logarithmic term is indeed present in τ, which would increase one's confidence in the basic theory to a considerable degree.

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