Critical behavior of random walks

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We have studied numerically the trapping problem in a two-dimensional lattice where particles are continuously generated. We have introduced interaction between particles and directionality of their movement. This model presents a critical behavior with a rich phase structure similar to spin systems. We interpret a change in the asymptotic density of particles as a phase transition. For high directionality the change is abrupt, possibly of first order. For small directionality the phase transition is of higher order. We have computed the phase diagram, the volume dependence of the critical point, and the relaxation time of the system in the large volume limit.

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I. INTRODUCTION

One of the problems of a discrete-time lattice random walk is the trapping problem [1]. It concerns the temporal evolution of a system composed by N random walkers moving into a random distribution of traps. This system has been used to model diffusion processes [2,3], absorption of atoms by molecules, and magnetization decay in high-T_c superconductors where the particles are represented by vortices [4].

We introduce an interaction, a so-called nonoverlapping interaction, by forbidding occupation of a single site by more than one particle. We have also extended previous models by introducing directionality in the particle movement. Directionality is implemented by assigning a final position represented by a lattice site, uniformly distributed in the lattice, to every particle. Particles will move to their final points according to a probability distribution that is explained below. Due to directionality, the mean number of steps that a particle needs to reach its final point (at distance r) is not proportional to r^2, as in the free case [5], but is proportional to r^γ with $\gamma<2$. This holds for a system without interaction, where the particles can be at the same lattice site. The effect of interaction increases when particle density increases.

The conflict between directionality and density is resolved when the system relaxes. We distinguish two evolution possibilities: the system reaches saturation which prevents the particles from moving in any direction, or it reaches a dynamical equilibrium state. In the latter situation, each particle walks for some time, until it reaches its final point where it disappears. The density of particles is asymptotically stable.

We have studied the transition between the dilute system and the saturated system. More precisely, is this change abrupt or continuous? (Is there a phase transition between the two evolutionary possibilities, and what is the order of this transition?) A rich phase diagram appears where we distinguish two regions, one of them with a first order transition, and another one with a higher order transition, possibly second order. We have calculated the behavior of the system when $V\to\infty$.

The time taken to reach the asymptotic state, the relaxation time τ_r, strongly depends on the directionality and density. The behavior of τ_r is similar to the behavior of the correlation length close to a phase transition in a spin model and to the magnetization relaxation of a high-T_c superconductor [4].

II. MODEL

Consider a two-dimensional discrete-time lattice with a coordination number of 4. We impose periodic conditions in both directions. Particles are on lattice sites n that are characterized by (n_0,n_1). The model can be described with the two parameters β and p.

For every time step, we consider all lattice sites. If the considered site is free, we create a particle with creation probability p. If the particle is created, a final point for this particle is generated uniformly in the lattice. If the considered site is occupied, the particle is moved in the direction μ (μ takes the values $+0,-0,+1,-1$) according to the probability distribution

$$P(\pm\mu)=Ne^{\pm[\mathrm{sgn}(n_\mu^f-n_\mu)\beta]}, \tag{1}$$

where n_μ^f is the coordinate μ of the final point of the particle, n_μ is the coordinate μ of the particle, and $\mathrm{sgn}(x)$ is the signum function. N is chosen to normalize the probability:

$$\sum_{\pm\mu}P(\mu)=1\ . \tag{2}$$

When the chosen site is occupied, the particle does not move and it remains at the same lattice site until the next time step. If the site is free and it is precisely the final point, the particle disappears. A particle can at most move once in one time step. To implement this, we assign to every site a "spin" taking the value 1 if the site is

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occupied, or 0 if it is free.

We describe the evolution of the system through the mean number of particles. By analogy with spin systems, this number is called the magnetization of the system,

$$M=(1/V)\sum_{i=1}^{V}\sigma(i)\ , \tag{3}$$

where $\sigma(i)$ equals 1 if the site is occupied and 0 if the site is free. The magnetization is analogous to the density of particles in the system.

The choice of the parameters p and β is due to the fact that these parameters present limits easy to recognize. β can be regarded as the inverse of the temperature of the system. Movements of the particle are more random when the temperature is increased. We will return to this point below.

It is interesting, and very intuitive, to recognize what happens for limiting values of the parameters. When $\beta\rightarrow 0$, the probability takes the simple form $P(\mu)=\frac{1}{4}$ which corresponds to a random choice of the next site. In the absence of other particles this is like a Brownian movement of particles with a "high temperature." When $\beta\rightarrow\infty$, the particle can only move in the direction μ which brings it nearer to its final point. In this case there are no alterations from the minimum-length path that joins the particle with its final point. Thus the system is at "zero temperature."

In the limit $p\rightarrow 0$, the system has a very low particle density, and there is little interaction between the particles. The particles move from their origin to their destination with small fluctuations depending on β. When β approaches 0, we see a typical random walk of particles that are generated with probability p. The number of surviving particles after n steps is related to the expected number of distinct sites visited by an n step random walk [6–10]. The particles arrive at this final site, at distance r, after r^2 steps. With increasing p, the system becomes more dense. Due to the interaction between particles, the number of steps that a particle needs to reach its final point increases. Ultimately there is a situation in which the system saturates, when the density becomes high enough to prevent any movement. No particle can move through the lattice and the temporal evolution of the system will not change significantly. When we increase the value of β, so that directionality increases, the particle arrives faster at its final point. In this case the value of p that produces saturation should be larger.

We distinguish other regions in our model. When β is large enough, the directionality is so strong that particles always choose the minimum path to reach their final point. This phenomenon prevents overlap between the paths of particles with opposite final points. The system saturates for smaller p values.

About the transition, we would like to point out that, for small values of β, the system can reach large values of magnetization without system saturation because the interaction is of little importance, so that a particle can reach its final site through various ways. Before saturation, the density is large, and the transition between the two phases is not abrupt.

On the other hand, for large β (but not large enough to produce the no overlap between paths explained below) every particle moves to its final point quickly. For small values of p, the density is small. When p increases, particles increasingly interact, and the system creates obstacles that propagate quickly. The system saturates more abruptly than for small β.

III. NUMERICAL SIMULATION

We have run Monte Carlo simulations in order to study the full parameter space of the model, the possible phase transition, and the behavior in the $V\rightarrow\infty$ limit, and the relaxation time. The two-dimensional square lattice has a length L, with periodic boundary conditions. Simulation has been performed by using a custom machine with 64 transputers T805 [11].

We have mapped out the (β,p) parameter space globally for some L values to find strong changes in the temporal evolution of the system. Time (t) is expressed in the number of iterations of the Monte Carlo simulation, where the iteration is a tentative sequential update of all lattice sites. The updating procedure for a single site has the following steps.

(A) If the site is free, generation of a random number between 0 and 1 occurs. If the randomly generated number is less than p, a particle appears at this site. Otherwise, no particle is created. In order to implement the "occupation" of a site, we assign a "spin" of value 1 to the site if the site is occupied, and 0 if the site is not occupied. In this way, we can obtain the number of particles in he system by summing all "spins."

(B) If the site considered is occupied by a particle, this particle attempts to move in one of the four directions according to the following. Since we know the probability for all directions from Eq. (1), we divide the interval [0,1] into four parts proportional to the probability assigned to every spatial direction. Next, a random number between 0 and 1 is generated. This number is contained in one of the four intervals into which the interval [0,1] is divided. The particle will move in a direction corresponding to that interval. With this algorithm, we reproduce the probability distribution weighted by β.

(1) If the chosen site is not occupied, the particle moves to it, and when that site is the final point of the particle, it disappears at this same step.

(2) If the site is occupied, the particle remains at its original point, and the next site in the lattice is considered. The interaction between particles is implemented by preventing a particle from moving into an occupied site.

(C) Particles move at most once per update.

When the final point is at a distance larger than $L/2$, considering distance as $x_{\max}-x_{\min}$, because of the periodic boundary conditions the most favorable direction is such that the particle takes the shortest path.

The asymptotic value of M,

$$M_\infty=\lim_{t\rightarrow\infty}M(t)\ ,$$

is the parameter which labels the phases of the model.

The relevant quantity in order to study the state of the system is the magnetization as defined in (3). M depends on t (t is the number of Monte Carlo iterations) and if M approaches 1 for $t \to \infty$, the system is saturated, and the number of particles that reach their final point does not compensate the rate of creation. If $M < 1$ the system reaches a dynamic equilibrium between creation and annihilation of particles.

M_∞ is not a true order parameter from a statistical point of view, because it is always positive over all the phase diagram. However, as we will see in the next sections, this quantity presents a clear change of behavior as a function of p at each value of β, and it is therefore a good parameter in order to establish where the transition takes place. We call the value where this change in M_∞ appears p_c. In fact p_c is a function of β and L, the lattice size.

IV. RESULTS AND PHASE DIAGRAM

A. General results about the phase diagrams

At each value of L, β, and p we run a Monte Carlo simulation. The starting configuration is obtained by creating a particle at each site with probability p. We start therefore with an initial magnetization of order pV.

We have studied several lattice sizes: $L = 20$, 40, 60, 80, and 100. We have run a different number of Monte Carlo (MC) iterations depending on the convergence of $M(t)$. At each value of the parameters, we have performed typically $(1-2)\times 10^5$ MC iterations. We have also made the simulation starting from different configurations, and we have allowed the system to evolve until 5×10^5 iterations, in order to compute the value of M_∞ accurately. We have computed the error in M_∞ and p_c by calculating the dispersion between the results obtained starting from different configurations.

At each MC iteration we measure the number of particles (3), obtaining $M(t)$ a function of the MC time t (see Fig. 1). Our order parameter, in order to determine the phase we are in, is the asymptotic value of this parameter M_∞. As can be seen in this figure, the time required to attain this asymptotic value depends strongly on p. At each β value in the small $p(p \ll p_c)$ region ("dilute system"), this behavior is reached after a small time, and also in the large $p(p \gg p_c)$ region. In the intermediate $p(p \approx p_c)$ region (where the system undergoes very large fluctuations), this time becomes enormous (see Sec. IV C).

We have carried out a careful study in order to assure that in every case further time evolution does not change $M(t)$, first from different starting configurations, to see if the final state depends on the initial one. We have found no evidence of this dependence. In Fig. 2, we show $M(t)$ for several starting configurations. Secondly, after $M(t)$ has reached an apparently asymptotic behavior, because the time evolution of $M(t)$ seems to be stable, we have completed up to four times more iterations (5×10^5 iterations); $M(t)$ continues stable.

In Fig. 3 we present the evolution of M_∞ as a function of p for two values of β and L fixed. As can be observed in this figure, the system presents two phases. There is a phase in which the system saturates, and another one in which asymptotic magnetization is less than 1.

First, for small values of p, there is no saturation. In this case, the density is small and the system never collapses. We go through the parameter space by increasing p. For $p > p_c$, the system changes from a value of M_∞ less than 1 to the saturation value.

However, the behavior of this quantity is different for large and small β. The system makes this change in a smooth way for small values of β, and the change is less smooth when β increases. For β close to 1, the change is abrupt; the density changes from a small value to 1 by making a jump.

For large β values the strong change at p_c tells us that M_∞ is discontinuous and we can speak of a behavior similar to a first order transition as in Z_2 spin gauge systems at high dimensions. As we will see, we can also find a quantity with a similar behavior to the correlation length in the spin systems, making this similarity stronger.

For smaller values of β also both phases are present, but now the change is smoother, and we can see that

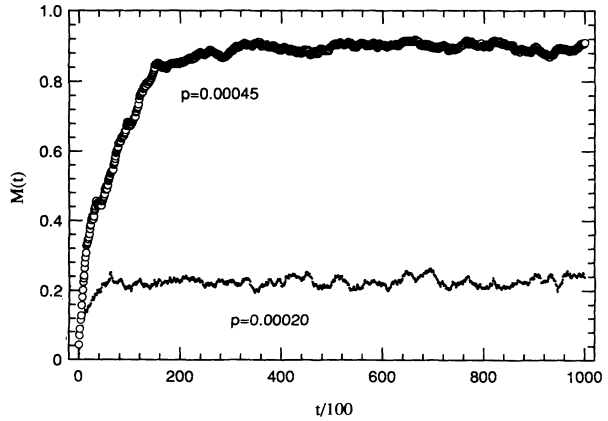

FIG. 1. Temporal evolution of magnetization for $p < p_c$ and $p > p_c$ performed for an $L = 40$ lattice with $\beta = 1.0$. p_c is 0.000 35.

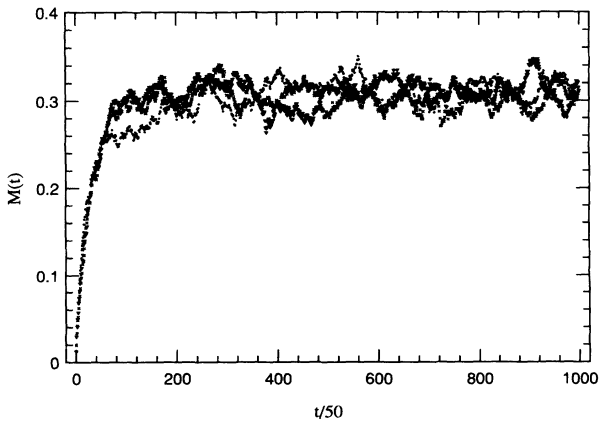

FIG. 2. Temporal evolution of M starting from three different configurations for $L = 40$, $\beta = 1.0$, and $p = 0.000\,25$.

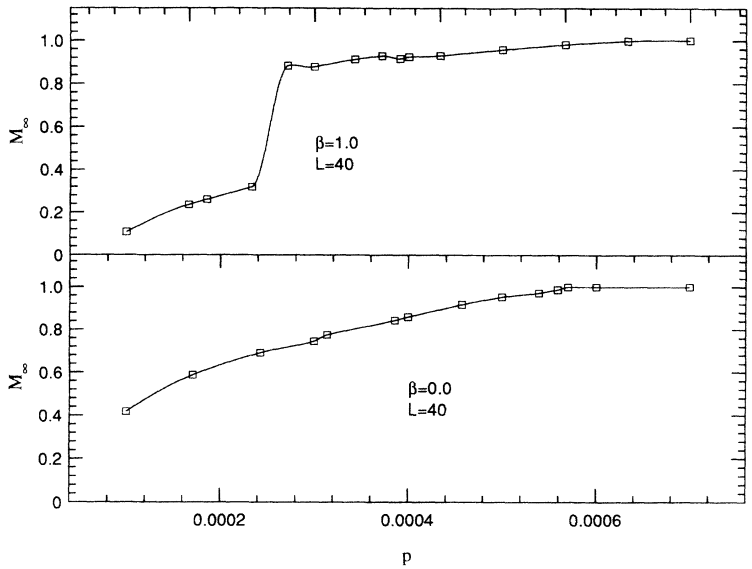

FIG. 3. Asymptotic magnetization for $p \approx p_c$, in an $L=40$ lattice with $\beta=0$ and for $\beta=1.0$. The discontinuity is abrupt for $\beta=1.4$ and smooth for $\beta=0.2$. The value of M_∞ is calculated after $(3-4)\times 10^5$ MC iterations.

there is no discontinuity in M_∞. However, for large p, $M_\infty = \text{const} = 1$, and for small p, $M_\infty \to 0$; therefore a discontinuity might occur for some $(\partial^n M/\partial^n p)$ at some intermediate value of p; this is similar to higher order phase transitions, where discontinuities at the nth derivative of operators are a signal of an $(n+1)$th order transition.

In the phase diagram on Fig. 4 we plot the values obtained for p_c for a wide range of β values. We can see how p_c increases until a maximum. After this maximum p_c decreases and for large β p_c decays slowly (Fig. 4).

We try to explain this behavior. At first, when β increases, particles arrive more quickly at their final point. Because of this the system supports larger p's without saturation. This fact occurs for the first region of β. When β has increased enough, particles cannot deviate from their shortest path to reach the final site. A particle cannot avoid other particles by going in the opposite sense. This produces a collapse that propagates quickly to the entire lattice. The value of p_c decreases for large β due to this phenomenon.

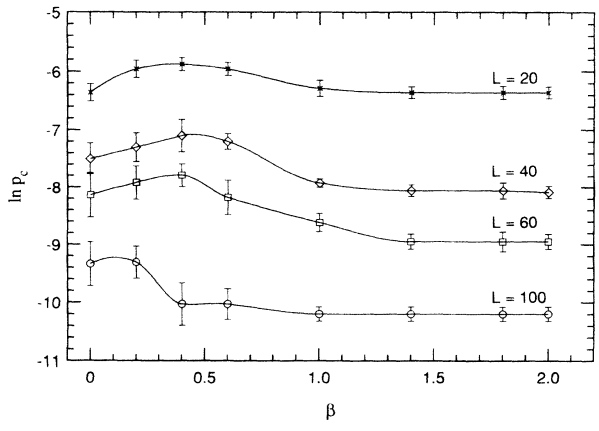

FIG. 4. Phase diagrams for $L=20$, 40, 60, and 100. We have used a logarithmic scale to represent p_c.

This behavior is related to the appearance of metastable states in diffusion-controlled processes [12]. The authors show that, in the case of equal initial concentrations of reactants, an extremely long-living metastable state is formed so that the whole system is split into areas or domains, each consisting of only one type of particle. The average size of such clusters grows slowly with time. In the system we are considering now, in the region of large β, the impossibility of particle crossing creates a wall which prevents particles from moving across it; two (or more) domains are formed and they grow and fill up the lattice.

B. Volume dependence

We have performed the simulation for various lattice volumes. As can be observed in the figures, for fixed value of β, the value of p_c decreases when the lattice size increases. This behavior is expected because particles must walk larger distances when the lattice size increases. Therefore if the path if larger, a particle will find more particles in its way ("obstacles") to reach the final point. These two facts combine and p_c decreases. We can summarize this by saying that saturation is produced earlier when lattice size increases. The volume dependence of p_c for a given β value can be studied with accuracy for those values of β in which the transition is abrupt, because p_c is determined more precisely. We have studied this dependence for $\beta=1.4$ and $\beta=2.0$ The results can be observed in Fig. 5. We find that in both cases the dependence can be written in the form

$$p_c = AL^{-\alpha}, \tag{4}$$

where $\alpha=2.33\pm0.01$ for $\beta=1.4$, and $\alpha=2.36\pm0.01$ for $\beta=2.0$. We have checked that this power law is true for all values of $\beta > 1.0$.

The fact that $\alpha > 2$ in (4) is important in order to establish the $L \to \infty$ limit of the model in the particular case of

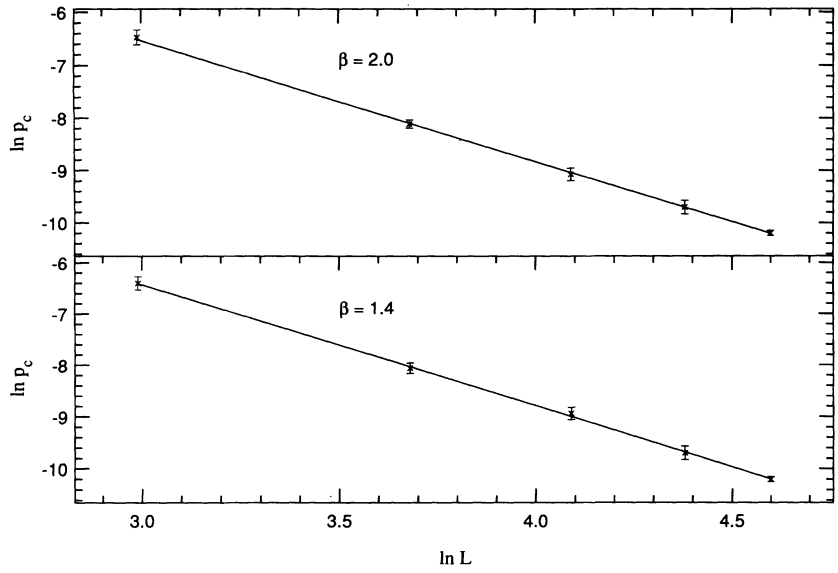

FIG. 5. Volume dependence of p_c for $\beta=1.4$ and 2. Points have been fitted to a straight line. The fit is good in general for $\beta>1.0$.

constant number of particles. That is to say, consider the special case where the same number of particles is created independently of L. To do that, we must fix p proportional to L^{-2}. At small t values, where the system is not saturated even in the $p>p_c$ region, the number of particles created at each time is of the order of

$$pL^2[1-M(t)]\propto pL^2 ,$$

valid if $M(t)\neq 1$. In the case of a constant rate of particle creation independently of L, the situation in the large L region is very different depending on α.

If $\alpha>2$, the system has only one saturated region in that limit, and if $\alpha<2$ only a dilute region is present. In the third case, $\alpha=2$, both phases coexist. In general, for any finite L two different phase are present in all cases.

For small β values, there is great difficulty in finding the critical point accurately. This is due to the fact that saturation is reached at high values of M. Thus we have not found a clear power law in this region.

C. Relaxation time

As we have pointed out, the system needs time to reach the asymptotic value of M. We have studied the evolution of this time with p, as a function of L and β. To be more definite we have measured, for every value of the parameter p, the time the system needs to reach a value of M equal to M_∞/e, called the relaxation time τ_r.

We expect small values of τ_r for values of p far from p_c. For p in the neighborhood of p_c, τ_r increases, and will reach its maximum value for $p=p_c$.

We have supposed that the temporal evolution follows an exponential law,

$$M_\infty - M(t) = Be^{(-1/\xi)t} . \tag{5}$$

With this definition, the relaxation time τ_r is given by ξ.

We found good agreement of our data with this formula. In Fig. 6 the result is plotted for a lattice size $L=40$ with $\beta=1.0$. We have shown in the inset the temporal

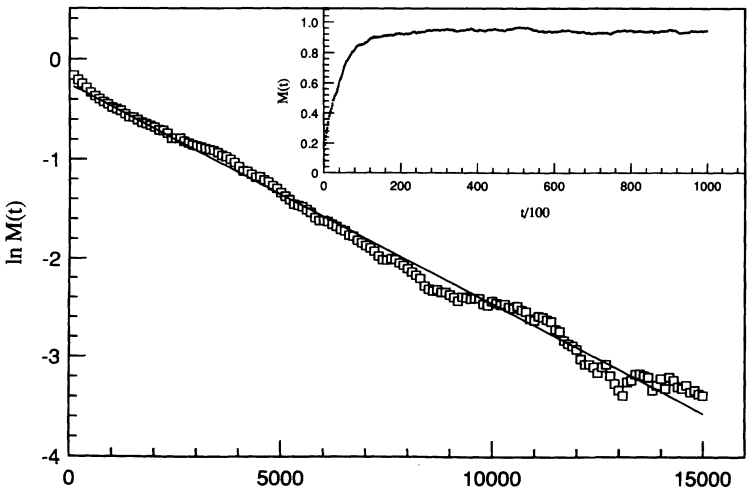

FIG. 6. $M_\infty - M(t)$ for $L=40$, $\beta=1.0$, $p=0.000\,45$. Points have been fitted to a straight line whose slope is τ_r.

evolution for a value of $p > p_c$. We have obtained the value of ξ by plotting $\ln[M - M(t)]$, fitting to a straight line whose slope is $1/\xi$:

$$\ln[M_\infty - M(t)] = A - (1/\xi)t \ . \quad (6)$$

The fit to a straight line is good for $p > p_c$, because the behavior of M is better defined. M does not fluctuate when the system reaches saturation. For small values of p, the system is less "determinate," M fluctuates around its mean value, and the fit is less accurate. Finally, we have represented the evolution of τ_r for various values of the parameter p, finding the expected behavior (see Fig. 7).

The correlation ξ has a behavior similar to that of the correlation length in a spin system around a phase transition. For large values of β, for p greater than p_c but close to it, there is little correlation. For p less than p_c, but close to it, the correlation is also small. This is due to the fact that in both cases the system reaches the asymptotic behavior in a short time. In fact, the transition is discontinuous and M_∞ is lower than 1 for $p < p_c$ and $M_\infty \approx 1$ for $p > p_c$ (Fig. 3). At p_c, M_∞ depending on the starting configuration, the system evolves to the saturation or to the dilute regime, in a similar way to a spin system at the critical temperature in a first order phase transition.

For β small, the determination of p_c has large statistical errors, and it has not been possible to measure τ_r accurately. With our partial results a possible scenario could be the following.

For small values of β, near p_c, M_∞ is continuous, approaching 1 for $p \to p_c$ (Fig. 3). For $p < p_c$, the system evolves in a finite time to M_∞, and τ_r is finite; also for $p > p_c$. At $p = p_c$ the system needs an infinite time to reach M_∞, and then τ_r diverges. This behavior is similar to a second order phase transition.

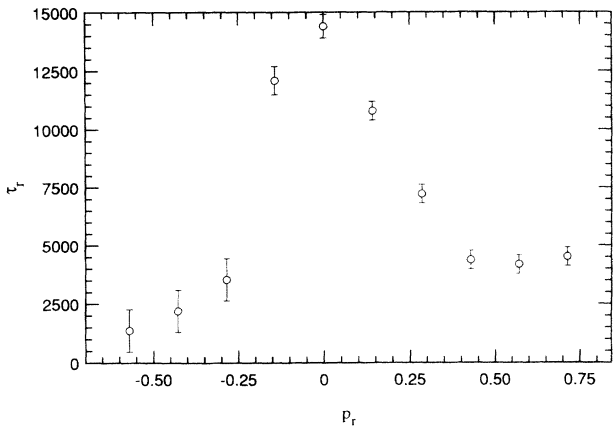

FIG. 7. Evolution of τ_r with p, for $\beta = 1.0$ in an $L = 40$ lattice. We have plotted τ_r as a function of $(p - p_c)/p_c$, called p_r. τ_r is maximal for $p_r = 0$, i.e., for $p = p_c$.

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