

## Monte Carlo simulation of the two-dimensional random ( $\pm J$ ) Ising model

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A Monte Carlo simulation of the two-dimensional random ( $\pm J$ ) Ising model has characterized the equilibrium and dynamic behavior of the model. The spin-glass correlation length diverges algebraically with absolute temperature. The equilibration time obeys an Arrhenius law at low temperature. There is a “phase transition at zero temperature” and a glass transition at finite temperature. In the spin-glass frequency ( $f$ ) regime the noise power spectrum is proportional to  $1/f^{(1+\alpha)}$  with  $\alpha=0.28$ .

### I. INTRODUCTION

The two-dimensional random ( $\pm J$ ) Ising model<sup>1</sup> is studied by Monte Carlo simulation. This model has been studied previously by Monte Carlo<sup>2-5</sup> and transfer-matrix<sup>3,6-8</sup> methods. Excluding Ref. 5, previous Monte Carlo simulations have not been extensive enough to characterize the behavior of the model; the present extensive simulation is performed on the Monte Carlo computer at the University of Illinois at Urbana.

### II. MONTE CARLO METHOD

We study the two-dimensional random Ising model on a square lattice with nearest-neighbor interactions of magnitude  $J$  and of random sign. The model is simulated using the Monte Carlo method<sup>9</sup> with the “heat-bath” update algorithm.<sup>10</sup> The lattice is divided into two sublattices. The spins on the first sublattice are updated simultaneously, followed by the spins on the second. A single configuration of interactions for  $N=8124$  spins with periodic boundary conditions is studied. Averages are taken for  $10^6$  updates per spin after ignoring the first  $10^5$  updates. The Hamiltonian is

$$H = - \sum_{i,j} J_{ij} S_i S_j, \tag{1}$$

and we calculate the spin-glass correlation function

$$g_T(R) = \frac{1}{N} \sum_{i,j} \langle S_i S_j \rangle^2 \delta(R_{ij} - R), \tag{2}$$

which is a spatial average of  $\langle S_i S_j \rangle^2$  for fixed separation of the spins. Angular brackets  $\langle \ \rangle$  indicate a Monte Carlo time average which is equivalent to the thermodynamic average; for a large system the spatial average is equivalent to a configuration average over interactions. We define the Monte Carlo time  $t$  to be the number of updates per spin and calculate the relaxation function

$$q_T(t) = \frac{1}{N} \sum_i \langle S_i(t') S_i(t+t') \rangle, \tag{3}$$

in which a spin is correlated with itself at a later time.

### III. SPATIAL CORRELATIONS

The correlation function for several temperatures in the range  $0.86J \leq T \leq 3J$  is shown in Fig. 1. System equilibration is extremely slow at low temperatures and  $0.86J$  is the lowest temperature for which we obtain a reasonably accurate equilibrium average. We first test the scaling hypothesis<sup>11</sup> and write

$$g_T(R) = A_T G(R/\xi_T), \tag{4}$$

where  $\xi_T$  is the correlation length and  $G(x)$  is a universal scaling function. We further assume a parametrized form for  $\xi_T$ . We have

$$\xi_T = a(T - T_c)^{-\nu} + \xi_0. \tag{5}$$

We perform a least-squares fit of the data to (4) using the measured variances to weight the data points in the usual way. We represent  $\ln[G(x)]$  by a Taylor series in  $\ln(x)$ . The four parameters in (5) as well as  $A_T$  at each

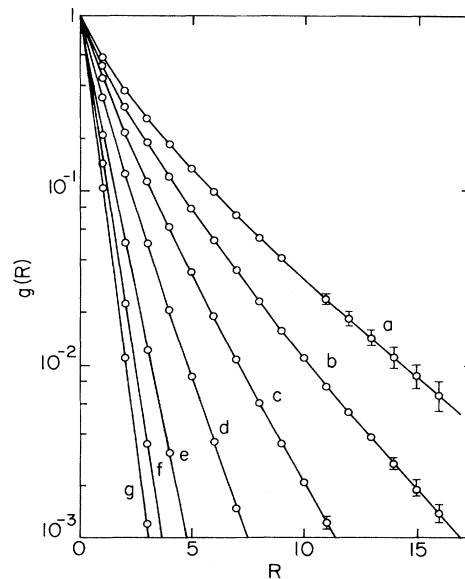


FIG. 1. Spin-glass correlation function vs distance for several temperatures: a,  $T=0.86J$ ; b,  $T=J$ ; c,  $T=1.2J$ ; d,  $T=1.5J$ ; e,  $T=2J$ ; f,  $T=2.5J$ ; and g,  $T=3J$ .

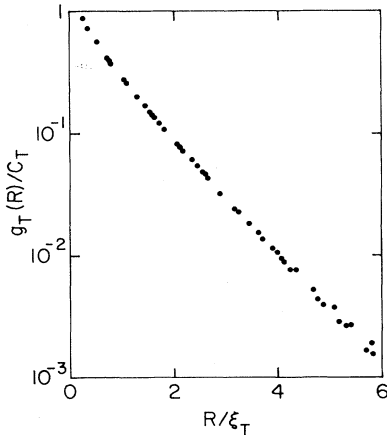


FIG. 2. Scaled spin-glass correlation function vs scaled distance.

temperature are treated as fitting parameters together with the coefficients of the Taylor series. The resulting weighted mean-square error is  $\chi$ -squared and we use the standard  $\chi$ -squared test to determine goodness of fit. For this procedure and  $0.86J \leq T \leq 3J$  we find a good fit with  $T_c = (0.10 \pm 0.25)J$ . The model has no small parameter and we expect  $T_c$  to be zero or of order  $J$ . We conclude that  $T_c$  is zero and use that value in subsequent analysis. With  $T_c = 0$  and  $0.86J \leq T \leq 3J$  we find a good fit for  $\nu = 2.42 \pm 0.10$ . The scaled data are shown in Fig. 2. We find that the scaling function

$$G(x) = \exp(-x)/x^\eta \tag{6}$$

provides as accurate a fit to the data as the Taylor series.

Note that (4) is in the proper scaling form only if  $A_T$  is proportional to  $\xi_T^{-\eta}$ : This is true only over the restricted

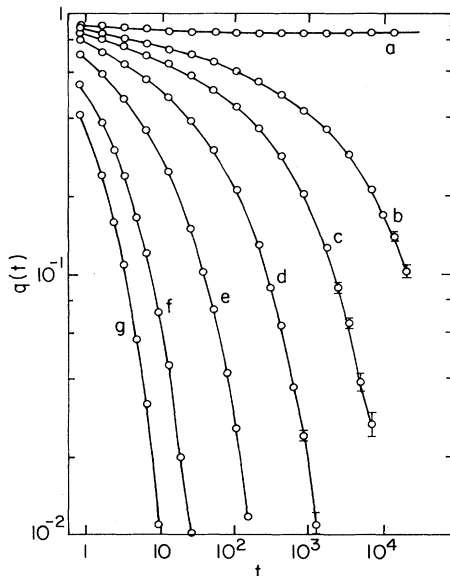


FIG. 3. Spin-glass relaxation function vs time for several temperatures: a,  $T=0$ ; b,  $T=0.86J$ ; c,  $T=J$ ; d,  $T=1.2J$ ; e,  $T=1.5J$ ; f,  $T=2J$ ; and g,  $T=2.5J$ .

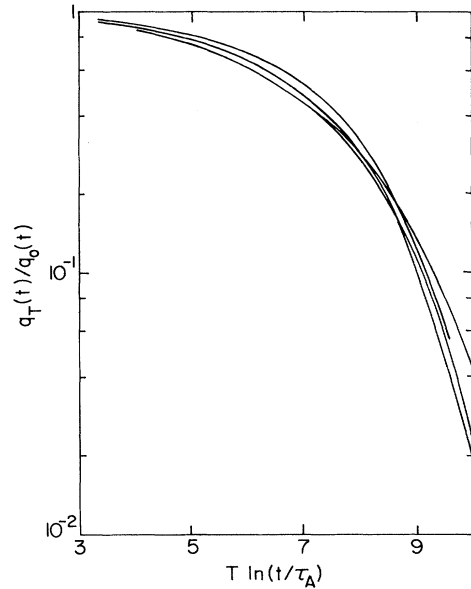


FIG. 4. Néel plot of the spin-glass relaxation function vs  $T \ln(t/\tau_N)$ .

temperature range  $0.86J \leq T \leq 1.5J$ . We incorporate this constraint by using

$$g_T(R) = B \exp(-R/\xi_T)/R^\eta, \tag{7}$$

with  $\xi_T$  given by (5) to fit the data and find a good fit for  $0.86J \leq T \leq 1.5J$ . The temperature range is not broad enough to determine  $T_c$  accurately and we must assume  $T_c = 0$ . We then find  $\nu = 2.64 \pm 0.23$  and  $\eta = 0.28 \pm 0.04$  using the  $\chi$ -squared test. The parameters in (5) are  $a = 2.34$  and  $\xi_0 = 0.442$ .

The Monte Carlo simulation is in good agreement with the transfer-matrix method<sup>8</sup> which found  $T_c = (0.02 \pm 0.11)J$  and  $\nu = 2.59 \pm 0.13$ . Previous estimates of the exponent by Binder<sup>12</sup> and Young<sup>5</sup> yielded  $\nu \approx 2$ . Static scaling of magnetic properties has been proposed by Kinzel and Binder.<sup>12,13</sup>

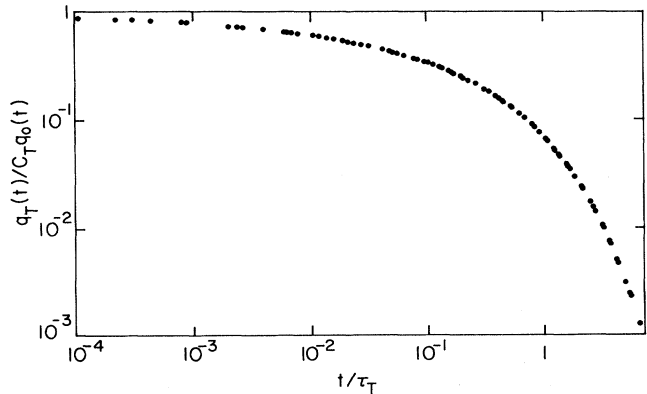


FIG. 5. Scaled spin-glass relaxation function vs scaled time.

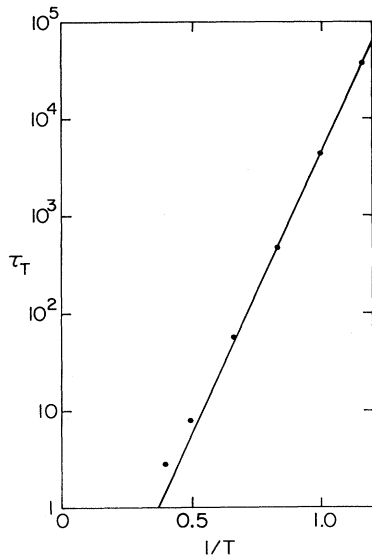


FIG. 6. Arrhenius plot of equilibration time vs inverse temperature.

#### IV. SPIN RELAXATION

The relaxation function  $q_T(t)$  for several temperatures in the range  $0.86J \leq T \leq 2.5J$  is shown in Fig. 3. The data for  $T=0$  shows that the system relaxes between degenerate ground states connected by single spin flips. We divide out this zero-temperature relaxation to remove the microscopic time scale and then test two models. We first test the Néel model<sup>14</sup> which considers relaxation over fixed energy barriers. We write

$$q_T(t)/q_0(t) = \int_0^\infty P(E) \exp(-t/\tau_E) dE, \quad (8)$$

with

$$\tau_E = \tau_N \exp(E/T). \quad (9)$$

For large  $t$  we find

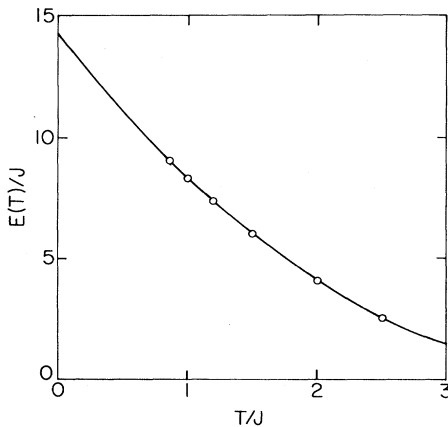


FIG. 7. Energy barrier determined from Eq. (14) vs temperature. Open circles are the data points and solid line is the Taylor-series fit discussed in the text.

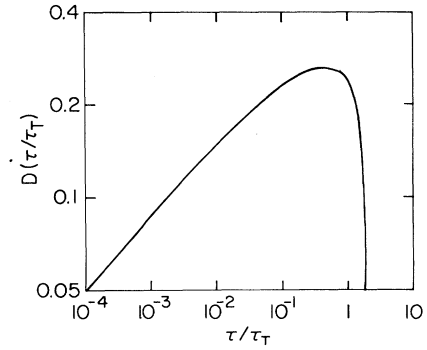


FIG. 8. Scaled relaxation-time distribution function vs scaled relaxation time.

$$q_T(t)/q_0(t) = I(T \ln(t/\tau_N)), \quad (10)$$

where

$$I(x) = \int_x^\infty P(E) dE. \quad (11)$$

The Néel model therefore predicts that the relaxation function is a universal function of  $T \ln(t/\tau_N)$ . In Fig. 4 we plot  $\log_{10}[q_T(t)/q_0(t)]$  vs  $T \ln(t/\tau_N)$  with  $\tau_N = 0.008\tau_\mu$ . Data for four temperatures  $0.86J \leq T \leq 1.5J$  are shown in the figure. The data should lie on a single universal curve if the Néel model were applicable; clearly, universal behavior is not observed even over this narrow temperature range. The plot is not improved by changing  $\tau_N$  or by introducing a vertical scale factor. We conclude that the Néel model is not applicable to the two-dimensional random Ising model.

We now test the dynamic scaling hypothesis<sup>15</sup>

$$q_T(t)/q_0(t) = C_T Q(t/\tau_T), \quad (12)$$

where  $\tau_T$  is the equilibration time and  $Q(x)$  is a universal scaling function. We fit the data assuming a parametrized form for  $Q(x)$  treating  $C_T$  and  $\tau_T$  at each temperature as free parameters. The data scale nicely for  $t \geq 2$  as shown in Fig. 5.

The equilibration time is normalized so that

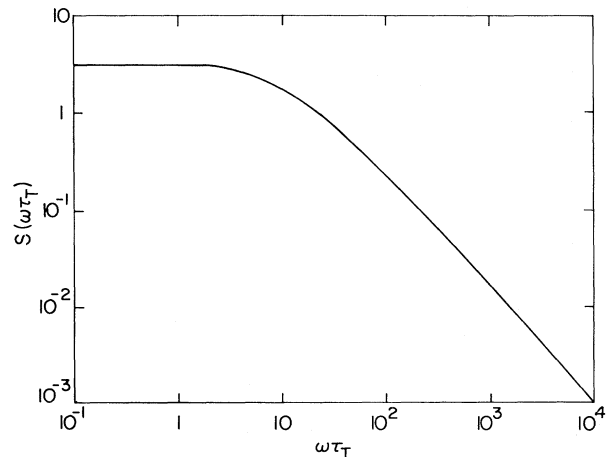


FIG. 9. Scaled power spectrum vs scaled angular frequency.

$$\tau_T = \frac{\int_0^\infty Q(t/\tau_T)t dt}{\int_0^\infty Q(t/\tau_T)dt} . \quad (13)$$

The plot of the logarithm of  $\tau_T$  vs  $1/T$  in Fig. 6 shows that the equilibration time exhibits Arrhenius behavior  $\tau_T = \tau_A \exp(E_0/T)$  at low temperature; the straight line drawn through the three low-temperature points has a slope  $E_0 = 13.2J$ . However, the coefficient of the exponential  $\tau_A$  is not the microscopic relaxation time  $\tau_\mu$  (equal to 1) but is of order  $0.008\tau_\mu$ . It is therefore physically incorrect to interpret this behavior as thermal activation over a fixed energy barrier. We can define an energy (or free-energy) barrier  $E(T)$  as follows

$$\tau_T = \tau_\mu \exp[E(T)/T] . \quad (14)$$

Arrhenius behavior is equivalent in the critical regime to a temperature-dependent energy barrier

$$E(T) = E_0 - T \ln(\tau_\mu/\tau_A) . \quad (15)$$

The scaling theory<sup>16</sup> also predicts linear behavior of  $E(T)$  at low temperatures. We fit  $E(T)$  from (14) using a Taylor expansion in  $T$  and find a good fit with  $E(T) = 14.16 - 6.59T + 0.785T^2$ . Figure 7 shows the fit to the energy-barrier data. The energy barrier increases with decreasing temperature as the correlation length increases. Young<sup>5</sup> finds an energy barrier linear in  $1/T$ ; this functional dependence is inconsistent with the present Monte Carlo data. From a transfer-matrix study of energy barriers, Morgenstern<sup>17</sup> estimates that a typical energy barrier in the  $\pm J$  model is  $(13 \pm 1)J$ .

The following scaling function provides a good fit to the data:

$$Q(x) = \exp(-1.781x^{0.28} - 0.605x^{0.66} - 0.230x) . \quad (16)$$

The first exponent and the three coefficients were treated as free parameters in the least-squares-fitting procedure. We can interpret this universal relaxation function in terms of a scaled distribution of relaxation times  $D(\tau/\tau_T)$  where

$$Q(t/\tau_T) = \int_0^\infty D(\tau/\tau_T) \exp(-t/\tau) d\tau/\tau . \quad (17)$$

$D(x)$  is proportional to the number of relaxing modes per decade. We calculate  $D(\tau/\tau_T)$  by performing the inverse Laplace transform of (17) numerically; the result is shown in Fig. 8.  $D(\tau/\tau_T)$  is proportional to  $\tau_\alpha$  with  $\alpha = 0.28$  for  $\tau \ll \tau_T$  and the distribution cuts off at  $\tau \simeq \tau_T$ . At a particular temperature the scaling treatment is only valid for  $\tau \gg \tau_\mu$ .

We define the scaled power spectrum  $S(\omega\tau_T)$  in the usual way from the scaled relaxation function

$$S(\omega\tau_T) = 4 \int_0^\infty Q(t/\tau_T) \cos(\omega t) dt / \tau_T . \quad (18)$$

The scaled power spectrum is shown in Fig. 9; it is constant for  $\omega\tau_T \ll 1$  and falls off as  $1/\omega^{(1+\alpha)}$  for  $\omega\tau_T \gg 1$ . This scaled power spectrum is only valid for  $\omega \ll 1/\tau_\mu$ . The noise spectrum is similar to  $1/f$  noise ( $\omega = 2\pi f$ ).

The present model does not have a spin-glass phase transition at finite temperature. However it does exhibit glasslike behavior. If one makes a measurement on a time

scale  $\tau_m$  the system will appear to be paramagnetic and reversible for  $\tau_m \gg \tau_T$ . It will appear to be frozen and irreversible for  $\tau_m \ll \tau_T$ . It therefore undergoes a glass transition for  $\tau_m \simeq \tau_T$ . There is no spin-glass phase but there is a spin-glass regime of time scales  $t$  such that  $\tau_T \gg t \gg \tau_\mu$ . In the spin-glass regime the system is irreversible and exhibits  $1/f^{(1+\alpha)}$  noise. We reserve the term "glass transition" for systems whose equilibration time increases at least as rapidly as  $\exp(E/T)$  at low temperatures.

## V. CLUSTER PICTURE

We interpret the above Monte Carlo results using a simple cluster picture. The system behaves as though it were made up of independent clusters of spins with spins in a given cluster frozen together. A cluster picture of this sort has been used previously by Kinzel.<sup>4,18</sup> The radius of a typical cluster is the correlation length  $\xi_T$ . In order to reverse the direction of the spins within a cluster of Ising spins one must pass a domain wall across the cluster with all spins behind the domain wall reversed. There is an energy (or free-energy) barrier which is the maximum energy of the domain wall as it crosses the cluster. With increasing radius  $\xi_T$  this energy barrier should increase, explaining the qualitative behavior of the energy barrier in (15). Within the cluster picture this energy barrier exists only for Ising spins. For a cluster of planar or Heisenberg spins one can reverse the spin direction by simultaneously rotating all the spins. This costs no energy and there is no energy barrier to cluster rotation. This cluster picture is in qualitative agreement with my Monte Carlo<sup>19</sup> simulation of the two-dimensional random planar model where no activation energy to spin relaxation is found, and with several other simulations of random planar and Heisenberg models.<sup>20-24</sup> Random anisotropy fields or anisotropic interactions can convert a planar or Heisenberg model into an Ising model at low temperature and such models are expected to exhibit glasslike behavior.

## VI. CONCLUSIONS

The Monte Carlo simulation has characterized the behavior of the two-dimensional random ( $\pm J$ ) Ising model. The correlation function scales and we find a "phase transition at zero temperature" with the correlation length depending algebraically upon temperature [Eq. (5) with  $T_c = 0$ ]. This is qualitatively and quantitatively in agreement with the transfer-matrix results. The relaxation function also scales and we find that the equilibration time obeys an Arrhenius law at low temperatures. For a fixed measurement time there is therefore a "glass transition" at finite temperature  $T_g$  such that  $\tau_m = \tau_{T_g}$ . For  $T > T_g$  the system equilibrates and behaves as a paramagnet; for  $T < T_g$  the system does not equilibrate within the measurement time and appears frozen and irreversible. For fixed  $T$  there is a paramagnetic regime of time scales,  $t \gg \tau_T$ , and a spin-glass regime of time scales  $\tau_\mu \ll t \ll \tau_T$ . In the spin-glass regime the noise spectrum is proportional to  $1/f^{1+\alpha}$ .

The simple cluster picture enables one to understand the

behavior of the model at length scale  $\xi_T$ . The scaling model<sup>16</sup> encompasses a range of length and time scales; it predicts algebraic behavior of  $\xi_T$ , linear behavior of  $E(T)$ , and approximately  $1/f$  noise. The scaling model is in qualitative agreement with the present Monte Carlo simulation.

#### ACKNOWLEDGMENTS

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- <sup>1</sup>J. Vannimenus and G. Toulouse, *J. Phys. C* **10**, L537 (1977).  
<sup>2</sup>S. Kirkpatrick, *Phys. Rev. B* **16**, 4630 (1977).  
<sup>3</sup>I. Morgenstern and K. Binder, *Phys. Rev. B* **22**, 288 (1980).  
<sup>4</sup>Z. Kinzel, *Z. Phys. B* **46**, 59 (1982).  
<sup>5</sup>A. P. Young, *Phys. Rev. Lett.* **50**, 917 (1983).  
<sup>6</sup>I. Morgenstern and K. Binder, *Phys. Rev. Lett.* **43**, 1615 (1979).  
<sup>7</sup>I. Morgenstern, *Phys. Rev. B* **23**, 6071 (1982).  
<sup>8</sup>H.-F. Cheung and W. L. McMillan (unpublished).  
<sup>9</sup>N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *J. Chem. Phys.* **21**, 1087 (1953).  
<sup>10</sup>R. J. Glauber, *J. Math. Phys.* **4**, 294 (1963).  
<sup>11</sup>L. P. Kadanoff, *Physics (N.Y.)* **2**, 2631 (1966).  
<sup>12</sup>K. Binder, *Z. Phys. B* **48**, 319 (1982).  
<sup>13</sup>W. Kinzel and K. Binder, *Phys. Rev. Lett.* **50**, 1509 (1983).  
<sup>14</sup>L. Néel, *Adv. Phys.* **4**, 191 (1955).  
<sup>15</sup>B. I. Halperin and P. C. Hohenberg, *Phys. Rev. Lett.* **19**, 700 (1967); *Phys. Rev.* **177**, 952 (1969).  
<sup>16</sup>W. L. McMillan (unpublished).  
<sup>17</sup>I. Morgenstern, *Phys. Rev. B* **27**, 4522 (1983).  
<sup>18</sup>W. Kinzel, *Phys. Rev. B* **26**, 6303 (1982).  
<sup>19</sup>W. L. McMillan (unpublished).  
<sup>20</sup>K. Binder, *Z. Phys. B* **26**, 339 (1977).  
<sup>21</sup>D. Stauffer and K. Binder, *Z. Phys. B* **41**, 237 (1981).  
<sup>22</sup>L. R. Walker and R. E. Walstedt, *Phys. Rev. Lett.* **47**, 1624 (1981).  
<sup>23</sup>K. Binder and W. Kinzel, *J. Phys. Soc. Jpn.* **52**, Suppl. P, 209 (1983).  
<sup>24</sup>K. Levin, *Phys. Rev. Lett.* **50**, 80 (1983).