Diffusion in the dynamic Ising system: Simulation and scaling

C.-L. Chen a, Y. Shapir a, E.H. Chimowitz b,*

a Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627, USA
b Department of Chemical Engineering, University of Rochester, Rochester, NY 14627, USA

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Abstract

We investigate diffusion through dynamic network structures modeled by the Ising paradigm both at the infinite temperature condition – random dynamic percolation (RDP) limit – and at finite temperatures. In a 2d system the simulations yielded exponents for the diffusion coefficients that were consistent with other published theoretical results we are aware of at the RDP limit. These exponents showed very little change at the finite temperatures we investigated. This study suggests that the computational paradigm presented will be useful for theoretically investigating transport in systems exhibiting dynamic disorder, e.g. conductance behavior in supercritical microemulsion mixtures.

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1. Introduction

The analysis of diffusion through disordered structures is a problem of widespread interest to many areas of science and engineering [1]. Many of the most successful theories in this area have used percolation concepts, and applications have been made to a variety of problems. These have included analyzing ionic conduction in polymers [2–4], electron–hole recombination in amorphous semiconductors [5], polymer gelation [6], turbulent diffusion [7], and the efficacy of corrosion-resistant metal-organic coatings [8].

Theoretical studies in this area have usually adapted classical static percolation ideas whereby diffusion is studied through a ‘frozen’ (quenched) structure consisting of randomly distributed conducting-sites surrounded by non-conducting host material [9]. Computer simulations of the diffusion process have usually employed particles called random walkers (RWs) that diffuse throughout the system by ‘hopping’ from one conducting site to another. The rate of diffusion throughout the system depends upon the network structure’s fixed topological connectivity, as well as kinetic rules governing the RW hopping transition rates.

These types of theories have introduced many useful ideas to the field: exponents that govern the percolation transition, scaling concepts and the notion of critical thresholds that define the appearance of incipient spanning conducting clusters in a given lattice geometry [1]. In the case of classical percolation theory, however, the diffusion of the RWs is restricted to the conducting-site cluster in which the walker initially finds itself. This implies that below the static percolation threshold, the mean square displacement of a walker in the system approaches a finite value after some time, with the concomitant result that the conductivity becomes zero in the long-time limit. This is not the case, however, if the network structure is allowed to change its configuration over time [10–13]. This latter situation is often referred to as the dynamic or stirred percolation problem [14–18] and is the focus of the present Letter which was stimulated by our interest in analyzing conduction in dynamic supercritical microemulsion mixtures. Conductivity measurements in such systems have revealed the onset of sudden conductivity increases when increasing either the density of conducting microemulsion droplets, or the system temperature, above certain thresholds [18].

* Corresponding author.
E-mail address: chim@che.rochester.edu (E.H. Chimowitz).
There have been several studies of the intrinsic properties of dynamic network structures themselves. Seminal work by Binder and co-workers [10,19] used simulations to analyze the cluster size distribution in a phase-separating Ising model system [20] at finite temperatures. They argued that the time-dependent percolation transition belonged to the same universality class as that of uncorrelated random percolation [21]. Simulations have also been used to model the formation of porous structures by spinodal decomposition [22], and the problem of network growth in disordered media has received attention, often with the well-known diffusion-limited aggregation (DLA) model [23]. The DLA model was recently used to simulate electrical conductivity in 2d colloidal dispersions during aggregation and showed scaling exponent results above the percolation transition consistent with those of classical 2d random percolation [24].

However, the DLA model is very different to that studied here, where we present some results using a novel simulation approach to study diffusion in an Ising system at both finite temperatures and the random dynamic percolation (RDP) limit, i.e. in the limit that the system temperature is infinite.

2. Computational realization of the network structure

We developed dynamic network structures using kinetic Monte Carlo (KMC) simulations, consistent with Kawasaki dynamics, i.e. constant conducting-site density [20,25–27] on Ising lattice models [27–29]. At any point during the simulations conducting-site pathways (with density \( \phi \)) are taken to be given by the network of up spins using the Ising terminology, with the non-conducting sites represented by the down spins. The thermodynamic properties of this system are well established in terms of the reduced temperature \( T = \frac{k_B T}{\epsilon} \), where \( k_B \) is Boltzmann’s constant and \( T \) the spin (site)–spin (site) coupling parameter [20,30,31].

Given a lattice of size \( L \times L \) we pre-equilibrate the system by doing a number of Monte Carlo Steps (MCS), where a MCS consists of a complete sweep of spin exchanges, i.e. \( L^2 \) updates. After pre-equilibration we then commence the diffusion simulations. In addition to the ‘usual’ Ising parameters another important feature of our simulation model is the ability to update only a fraction of the conducting-sites during any step of the simulation. A (blind) RW is placed on a randomly selected conducting-site, and one of its neighboring sites is selected randomly. If this selected site is also a conducting-site, the RW moves to it. Otherwise, the RW remains fixed at its current position. We define the number of RW steps taken between consecutive system updates by the symbol \( n_R \), and the fraction of conducting-sites updated by \( q \). Thus, the number of conducting-sites updated each time is \( N_R = qL^2 \phi \). Furthermore, we define characteristic time scales for the RW and structure dynamics by the variables \( \tau_w \) and \( T_R \) – it is easy to show that \( T_R \sim q^{-1} \) and \( \tau_w \sim n_w^{-1} \). The ratio of \( \tau_w \) and \( T_R \) is an essential element in determining the system dynamics. In our simulations \( n_w \) is taken to be one, and thus \( T_R(q) \) is the only dynamic variable here. Both RW-site and RW–RW interactions could, in principle, be accommodated with this model, however, in this Letter we do not consider these since they would not be the salient feature in microemulsion mixtures.

3. Results

In Fig. 1 we present a typical set of simulation results in this case at a temperature \( T = 2T_c \) where \( T_c \) is the lattice critical temperature. The general pattern of diffusion throughout the network shows three very distinctive modalities: short, intermediate and asymptotically long-time transport regimes. At short times we observe an increase in diffusion that quickly leads to a plateau region, during which time significant diffusion slow-down occurs since the RW is trapped in its initial cluster. At long times the system appears to approach a quasi-equilibrium state in which we find regular diffusion behavior.

The behavior seen in Fig. 1 is averaged over 500 different initial configurations and is suggestive of systems in which we might find scaling variables that collapse the data into an ‘universal’ curve [32] which led to the following analysis at fixed \( T \) and \( q \) with \( \phi \leq \phi_c \), for the most interesting case involving the slow network re-arrangement regime. The approach is similar to that suggested by Bunde and Havlin [32].

Below \( \phi_c \) the clusters are finite in size. We expect at short times the plateau height \( R \) to be the size of the largest clusters, times the probability of being in this cluster. Therefore,

\[
R^2 \sim (\phi_c - \phi)^{-\frac{\beta}{\nu}}
\]

where \( \nu \) is the scaling exponent for correlation length, and \( \beta \) is the the scaling exponent for the probability that a conducting-site belongs to an infinite cluster.

![Fig. 1. Simulation results for RW mean square displacement at \( T = 2T_c \) and various values of \( \phi \).](image-url)
We define \( t_x \), a crossover time, the time at which the onset of regular diffusion first occurs in the system, by a scaling relationship
\[
\begin{align*}
t_x & \sim (\phi_c - \phi)^{\theta_c},
\end{align*}
\]
with \( \theta_c \) being a new scaling exponent. Below the percolation threshold and above \( t_x \), we require the mean square displacement to follow the scaling form of
\[
\begin{align*}
r^2 & \sim (\phi_c - \phi)^{-s} t,
\end{align*}
\]
where \( s = 2\nu - \beta \). A scaling ansatz \([32]\) that includes these results is given by
\[
\begin{align*}
r^2 & \sim t(\phi_c - \phi)^{-s} F\left(\frac{t}{t_x}\right),
\end{align*}
\]
with the scaling function \( F(x) \) defined such that \( F(x) \sim x^{-1} \) when \( x \to 0 \) and \( F(x) \to \text{constant} \) when \( x \to 0 \). The long-time limit diffusion coefficient that follows from Eq. (4) is given by
\[
\begin{align*}
D & \sim (\phi_c - \phi)^{-s}.
\end{align*}
\]

From results like those shown in Fig. 1 we can calculate diffusion coefficients from the long-time limit. In Fig. 2 we show results for diffusion coefficients at various site densities and temperatures reasonably close to the static percolation point in a 2d network. Since the conducting-site density at finite temperatures at the dynamic percolation transition is temperature dependent it was first incumbent upon us to find this point for the Ising spin system described here. We did this following the finite-size scaling method described by Lironis et al. \([19]\) where \( P_{dc} \) in Fig. 3 is the probability of finding a spanning cluster. A set of results for \( T = 2T_c \) is shown in Fig. 3 where the intersection of the various ‘finite-size’ curves gives values for \( \phi_c \). In this case these were found to be \( \phi_c \approx 0.554 \) at \( 2T_c \) and \( \phi_c \approx 0.534 \) at \( 1.33T_c \), respectively.

While our results are for a 2d system, the qualitative data agreement between our simulation results and the appearance of actual experimental data in microemulsion solutions \([17]\) is striking.

Furthermore, results like those shown in Fig. 2 allowed us to evaluate the conductance exponent \( s \) for comparison with the only other published results on a variation of the RDP problem that we are familiar with. Our results are shown in Table 1 and the values for \( s \) should be compared with the range of values 2.3–2.9 given by Grest et al. \([33]\). Experimental data in 3d microemulsions \([16,17,34]\) have also been found to be consistent with the result where \( s \approx 2\nu - \beta \). In the 2d case \( s \approx 2.51 \).

### 4. Conclusions

In this Letter we provide some results for the problem of diffusion through dynamic pathways found by employing the Ising model paradigm to generate dynamic network structures. We studied diffusion both in uncorrelated systems (the RDP limit when \( T \to \infty \)) and in correlated systems at finite \( T \). Our simulation model shows a rich variety of diffusion behavior showing three very distinctive diffusion regions: short, intermediate and asymptotically long-time transport regimes.

In a 2d network our simulation results yielded exponents for the diffusion coefficient that were consistent with the only other published results we are aware of for the RDP limit. At finite temperatures these exponents were little changed.

This study suggests that the computer model presented here shows potential for being useful in studying basic transport phenomena in systems exhibiting dynamic, correlated disorder like that found in microemulsion mixtures, a problem we intend to address in the future.

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**Table 1**

<table>
<thead>
<tr>
<th>Exponents found from Fig. 2 results</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T )</td>
</tr>
<tr>
<td>( P_{dc} )</td>
</tr>
<tr>
<td>( s )</td>
</tr>
</tbody>
</table>

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**Fig. 2.** Diffusion coefficient scaling at various values of \( T \) and \( \phi \).
References