Reaction-Controlled Diffusion: Monte Carlo Simulations

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Our primary focus in this study is anomalous diffusion, which can be characterized by the "walk dimension" d_w: $\langle \vec{x}^2(t) \rangle \sim t^{2/d_w}$ for $d_w \neq 2$. For ordinary diffusion exhibited by, for example, random walkers on a lattice of integer dimension, $d_w = 2$. Diffusion on a fractal, as well as other cases of anomalous diffusion, model a variety of phenomena, such as particle transport in random media with quenched disorder, percolation through porous or fractured media, and electron-hole recombination in amorphous semiconductors [1].

To probe this phenomenon further we investigate anomalous diffusion on a *dynamic* fractal. This coupled two-species non-equilibrium reaction- controlled diffusion model was introduced by Trimper et al. [2], and is different from the study of diffusion on a static fractal lattice in that the number of available paths is decreasing with time and that the available sites are mobile. Monte Carlo simulations were performed on one and two dimensional lattices containing two species of particles [3]. Particles of type A, whose diffusion we study here, may independently hop to an adjacent lattice site provided it is occupied by at least one B particle. B particles are subject to competing (diffusion-limited) annihilation and offspring reactions, which give rise to a dynamic fractal structure at the phase transition between an active and absorbing/inactive phase. These non-equilibrium continuous phase transitions are known to be described by either the Directed Percolation or Parity Conserving critical exponents. In an inactive, absorbing phase with exponentially decaying B density, the A particles become localized. In an active state with nonzero, largely homogeneous B particle saturation density, the A species displays ordinary diffusion. At the phase transition $\rho_B(t) \sim t^{-\alpha_B}$, and the A particles propagate subdiffusively with mean- square displacement $\langle \vec{x}(t)^2_A \rangle \sim t^{1-\alpha_A}$. Thus the B particle phase transition induces a localization transition in the A particle species. We shall present detailed measurements of A particle diffusion and B particle structures and densities in both the active and inactive phases, as well as at the phase transition. We find that within the accuracy of our simulation data, $\alpha_A \approx \alpha_B$ as predicted by a simple mean-field approach. This remains true even in the presence of strong spatio-temporal fluctuations of the B density. However, in contrast with the mean-field results, our data yield a distinctly non-Gaussian A particle displacement distribution $n_A(\vec{x}, t)$ that obeys dynamic scaling and looks remarkably similar for the different processes investigated here. Fluctuations of effective diffusion rates cause a marked enhancement of $n_A(\vec{x}, t)$ at low displacements $|\vec{x}|$, indicating a large fraction of practically localized A particles, as well as at large traversed distances. We also present a simple phenomenological model that captures the essential features of our results.

References

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