Brief Reports

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Diffusion in a disordered medium

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We have investigated the diffusion coefficient of a particle performing a random walk on a lattice with random jump rates. The mean-square displacement of the particle is a linear function of time for all times when the initial probability distribution corresponds to a stationary distribution. We discuss the implication of this result on the description of diffusion in disordered media by averaged equations.

In this Report we study a simple but nontrivial class of models for particle diffusion in a disordered medium. In the models considered, the particle performs a random walk on a periodic lattice; the jump rates associated with the sites of the lattice are random. We first complete the proof indicated in Ref. 1 that the mean-square displacement of the particle is a linear function of time for all times when stationary initial conditions are used. We then discuss the implications of this result for the description of diffusion in disordered media by averaged equations.

We consider a Bravais lattice in d-dimensions whose sites are indexed by a vector $\vec{n}$. The particle's evolution through the lattice is described by a master equation

$$\frac{d}{dt}P(\vec{n}t\,|\,\vec{m}t_0)=\sum_{\vec{n}'}[W_{\vec{n}',\vec{n}}P(\vec{n}'t\,|\,\vec{m}t_0)-W_{\vec{n},\vec{n}'}P(\vec{n}t\,|\,\vec{m}t_0)]\ . \tag{1}$$

$P(\vec{n}t\,|\,\vec{m}t_0)$ is the conditional probability; it is defined as the probability that the particle is at site $\vec{n}$ at time t given that the particle was at site $\vec{m}$ at t_0. $W_{\vec{n}',\vec{n}}$ is a transition rate from the site $\vec{n}'$ to site $\vec{n}$.

The transition rates of the models can be written as

$$W_{\vec{n}',\vec{n}}=q_{\vec{n}'}Q_{\vec{n}',\vec{n}}\ , \tag{2}$$

where $q_{\vec{n}'}$ denotes the jump rate assigned to site $\vec{n}'$ and $Q_{\vec{n}',\vec{n}}$ the spatial transition probability. The jump rate $q_{\vec{n}'}$ is a random function of the site variable $\vec{n}'$; however, all possible values must be larger than zero. The spatial transition probability is assumed to have the following symmetry property:

$$Q_{\vec{n},\vec{n}+\vec{l}}=Q_{\vec{n},\vec{n}-\vec{l}}\ . \tag{3}$$

The physical situation described by Eqs. (2) and (3) corresponds to a distribution of potential wells

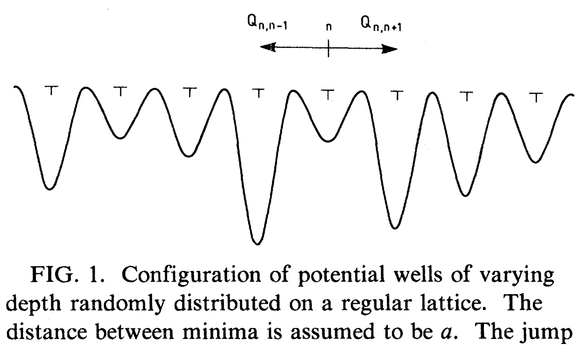

FIG. 1. Configuration of potential wells of varying depth randomly distributed on a regular lattice. The distance between minima is assumed to be a. The jump rates vary in value from site to site by the modulation of valley depths; the jump rates are smaller for valleys of increasing depth.

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whose depths are random, as suggested in Fig. 1. The symmetry property equation (3) requires equal transition probabilities to opposite neighbor sites; this is indicated in the figure by arrows of equal length.

The master equation (1) describes a Markovian continuous-time random-walk process,[2] and the associated waiting-time distributions are given by

$$\psi_{\vec{n}'}(t)=q_{\vec{n}'}\exp(-q_{\vec{n}'}t) \ . \tag{4}$$

In order to make the derivation more transparent, we restrict our discussion to nearest-neighbor transitions on a linear, square, simple cubic, etc., lattice. More complicated lattice structures and transitions to further sites are easily included.

The mean-square displacement of the particle initially at site $\vec{m}$ is

$$\langle\,|\vec{n}-\vec{m}\,|^2\rangle_{\vec{m}}=\sum_{\vec{n}}|\vec{n}-\vec{m}\,|^2P(\vec{n}t\,|\,\vec{m}t_0) \ . \tag{5}$$

With the use of Eq. (1), the above discussed symmetry properties, and the equality

$$|\vec{n}-\vec{m}\,|^2=|\vec{n}-\vec{n}'\,|^2+2(\vec{n}-\vec{n}')\cdot(\vec{n}'-\vec{m}) + |\vec{n}'-\vec{m}\,|^2$$

a simple algebraic manipulation shows

$$\frac{d}{dt}\langle\,|\vec{n}-\vec{m}\,|^2\rangle_{\vec{m}}=\sum_{\vec{n}'}q_{\vec{n}'}P(\vec{n}'t\,|\,\vec{m}t_0) \ . \tag{6}$$

Since we have chosen nonzero jump rates, the transition matrix is irreducible, and the master equation (1) has one and only one stationary solution, which is

$$\rho_{\vec{n}}=\left[q_{\vec{n}}\sum_{\vec{m}}q_{\vec{m}}^{-1}\right]^{-1} \ . \tag{7}$$

Performing the average over the initial sites of Eq. (6), we obtain, in general,

$$\frac{d}{dt}\langle\,|\vec{n}-\vec{m}\,|^2\rangle=\sum_{\vec{n}'}q_{\vec{n}'}P(\vec{n}'t) \ , \tag{8}$$

or, if we choose the stationary distribution as initial condition,

$$\frac{d}{dt}\langle\,|\vec{n}-\vec{m}\,|^2\rangle=\sum_{\vec{n}'}q_{\vec{n}'}\rho_{\vec{n}'} = \left[\sum_{\vec{m}}q_{\vec{m}}^{-1}\right]^{-1}\sum_{\vec{n}'}1=A \ , \tag{9}$$

where the constant A is the harmonic mean of the jump rates. The right-hand site of Eq. (9) is independent of time; therefore the mean-square displacement is a linear function of time for all times.

The argument is independent of dimension and the distribution and variability of the jump rates. Other initial conditions, corresponding to a nonstationary distribution, will yield a mean-square displacement that is a nonlinear function of time. The constant in Eq. (9) is directly related to the diffusion coefficient, which is

$$D=\frac{a^2}{2d}A \ , \tag{10}$$

where a is the separation between nearest-neighbor lattice sites. A slight generalization of the derivation presented above yields results for different lattice topologies which may include anisotropic diffusion.

The second time derivative of the mean-square displacement is defined as a "velocity" autocorrelation function, whose time Fourier transform defines a frequency-dependent mobility. The "velocity" autocorrelation function for the models used in this note is a delta function at $t=t_0$ and thus, the corresponding mobility is frequency independent.

We have derived the mean square displacement of our class of models of disordered media directly from the master equation by performing the average over initial conditions chosen according to stationarity. It is the symmetry condition equation (3) that allowed the essential simplifications to be done. There are approximation schemes[3] that can be applied to our models as well as to more general classes of models that do not obey Eq. (3). These approaches[4] replace the inhomogeneous equations, after averaging over different configurations, by lattice-translational invariant equations. The equations appear in the form of generalized master equations or continuous-time random-walk theory. It has been claimed[3] that the correspondence between the inhomogeneous and the averaged equations can be made exact. Our result provides a stringent test on these formalisms. When such an approach is applied to our models, the resulting mean-square displacement must be linear in time for all times, when stationary initial conditions are used. For instance, systems with a random distribution of traps, corresponding to our models, have been described by continuous-time random-walk theory with waiting-time distributions $\psi(t)$ that do not depend on $\vec{n}-\vec{m}$ (decoupled approximation in the terminology of Ref. 3). For that approximation scheme, there has been a controversy whether the first jump of the particle after the arbitrarily chosen origin of time must be treated differently from all others or not.[5-7] When the first jump is treated differently such that stationary initial conditions are incorporated, the resulting mean-square displacement is in accordance with our result.[5,7] In the corresponding generalized master equation, an inhomogeneous term must be added which restores the time homogeneity for the derivation of the mean-square displacement.

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