Effect of temperature on biased random walks in disordered media

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We study diffusion on an energetically disordered lattice, where each bond between sites is characterized as a random energy barrier. In such a model it had previously been observed that the mean square displacement is sublinear with time at early times, but eventually reaches the classical linear behavior at long times, as a strong function of the temperature. In the current work we add the effect of directional bias in the random walk motion, in which along one axis only, motion in one direction is assigned a higher probability while along the opposite direction a reduced probability. We observe that for low temperatures a ballistic character dominates, as shown by a slope of 2 in the R^2 vs time plot, while at high temperatures the slope reverts to 1, manifesting that the effect of the bias parameter is obliterated. Thus, we show that for a biased random walk diffusion may proceed faster at lower temperatures. The details of how this crossover takes place, and the scaling law of the crossover temperature as a function of the bias are also given. [S1063-651X(97)51207-4]

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Biased random walk is a prototype model for studies of particle diffusion in disorded solids [1,2] where kinetic problems are concerned, such as conduction, viscous flow, polymer dynamics, etc. The characteristic of the bias implies a preferential direction for the motion, as opposed to purely stochastic motion. The problem becomes much more complicated when the underlying space is not a simple lattice, but contains a certain degree of randomness itself, such as, for example, a rugged energy landscape model that we recently introduced [3–5]. Every lattice site has its own energy (usually chosen randomly, from a random number distribution). Thus, the problem is not directly amenable to exact analytical theories, except mean field arguments. In the present study we continue the investigation of such systems, with the inclusion now of the bias characteristics.

The model used here is the one used in our previous studies [3–5], in which we now incorporate an external field (bias). Briefly, a square lattice is generated. Each bond between any two sites is a barrier with a height that is randomly chosen from a given distribution. The height of the barriers depends on the mean value $\langle E\rangle$ and on the dispersion parameter σ of the E distribution in the following way:

$$E_{ij}=\langle E\rangle-\sigma(x-0.5)\,. \tag{1}$$

Here x is a random number between 0 and 1 from a uniform random number distribution. All barriers remain unchanged (frozen) during the entire process. Diffusion is simulated by placing particles at random positions on the lattice, which then perform random walks. The decisions on which jumps to make are taken on the basis of the local environment. The probabilities P_{ij} to jump from site i to site j are calculated by

$$P_{ij}=\frac{1}{z}\exp(-E_{ij}/kT)\,. \tag{2}$$

Here z is the coordination number of the lattice. Also, k is the Boltzmann constant, which for convenience we take equal to 1, $k=1$. Thus the temperature is dimensionless, and it is measured in terms of energy units. There is also a finite probability of remaining on the same site (no jump), which is given by

$$P_{ii}=1-\sum_{j\neq i}P_{ij}\,. \tag{3}$$

In the present work, in one of the directions, say in direction y, a bias is introduced in a way that it makes it somewhat easier (more probable) for the jump to take place along the bias direction, as opposed to along the other directions. This is done by lowering the energy for a forward jump by a fixed amount, while the energy for a backward jump increases by the same amount. Thus the energy barriers for a motion along the bias direction become

$$E_{ij}^{(y)}=\langle E\rangle_y-\sigma_y(x-0.5)\mp\frac{\epsilon}{2}\langle E\rangle_y\,. \tag{4}$$

The minus sign pertains to the motion along the direction of bias, while the plus sign pertains to the opposite direction. Since negative values of $E_{ij}^{(y)}$ are not permitted, $E_{ij}^{(y)}$ is set equal to zero ($E_{ij}^{(y)}=0$) in all cases when negative values are obtained according to Eq. (4). The direction that contains no bias is not affected at all, and thus, the forward and the backward jumps in the x direction (the direction perpendicular to the bias) have the same probability as before. In this way the barrier (bond) energies in the x direction are defined by an expression similar to Eq. (1):

$$E_{ij}^{(x)}=\langle E\rangle_x-\sigma_x(x-0.5)\,. \tag{5}$$

In the present paper both quantities $\langle E\rangle_x=\langle E\rangle_y=0.5$. This model has the flexibility to give each of the coordinates

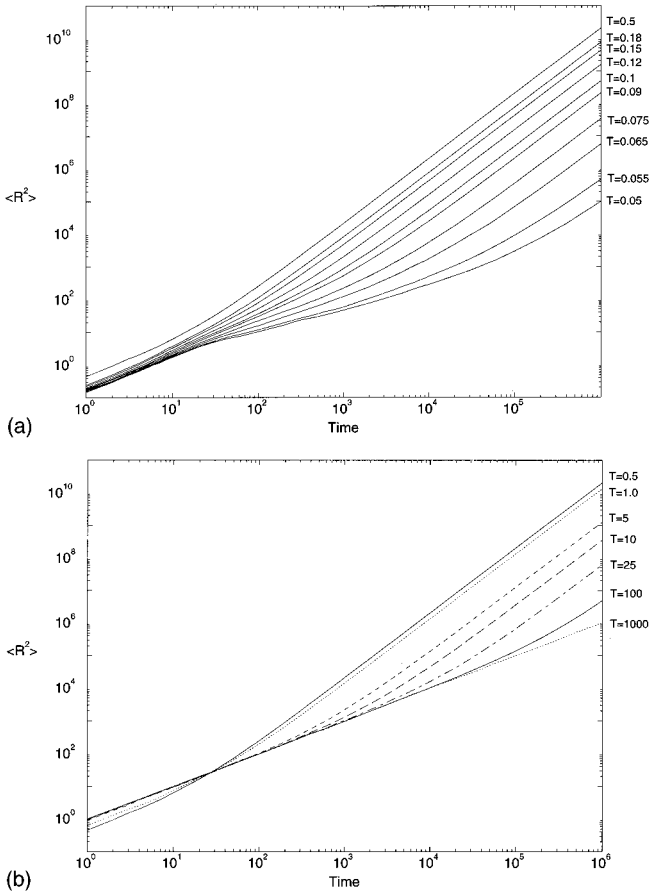

FIG. 1. Mean square displacement $\langle R^2 \rangle$ as a function of time (number of steps), for several different temperatures, $T=0.05$, 0.055, 0.065, 0.075, 0.09, 0.1, 0.12, 0.15, 0.18, 0.5 (a), and $T=0.5$, 1.0, 5, 10, 25, 100, 1000 (b), for a frozen 2D lattice of size 400×1000, in log-log form. The bias parameter $\epsilon=1.8$ and the dispersion $\sigma=1.0$. We used 1000 realizations.

of the two-dimensional lattice a different mean value of the energy barrier $\langle E \rangle_x$ and $\langle E \rangle_y$, and a different dispersion parameter σ_x and σ_y. This allows one to model the motion in more or less oriented systems, such as columnar liquid crystals or kinetics of electrophoresis. For instance, one-dimensional motion is obtained for $\langle E \rangle_x \gg \langle E \rangle_y$ and $\sigma_x=0$. Therefore, the algorithm permits one to have an asymmetric motion in two dimensions not only due to the bias but also when $\langle E \rangle_x \neq \langle E \rangle_y$, or $\sigma_x \neq \sigma_y$.

Our results are exhibited in the following three figures. In Fig. 1 we plot the mean square displacement, $\langle R^2 \rangle$, as a function of time for a value of the bias parameter $\epsilon=1.8$, and several different temperatures. We include a wide T range, from $T=0.05$ to $T=1000$. Because of the different regimes encountered we present this figure in two parts, (a) (low T) and (b) (high T). We observe in Fig. 1(a) that in the long time limit all slopes reach a limiting value of 2, which is the expected result, since this model represents a form of ballistic motion, whereby in the presence of external field (bias) the particle drifts with a constant velocity along the field so that $\langle R^2 \rangle \propto t^2$. But the time it takes to reach this limiting value is a strong function of temperature. The lower the temperature (0.05) the longer it takes. At early times a strongly sublinear behavior is exhibited. The origin of this sublinear

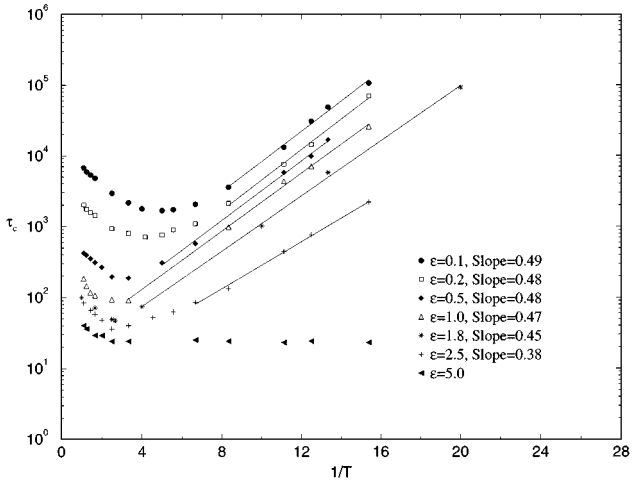

FIG. 2. Crossover time τ_c (the time after which $\langle R^2 \rangle$ becomes linear), as a function of $1/T$ for the same data as in Fig. 1 ($\epsilon=1.8$), with several more ϵ values, as shown.

section is the same as that observed for the simple case of no bias reported earlier by us [3–5]. The diffusing particle must overcome some effective activation energy, which is given by the barrier heights that are present. At low temperatures the particles are easily ''trapped'' in deep valleys, and spend a considerable amount of time on the same sites, before making a successful jump over a high barrier to a neighboring site. Since the temperature is low it takes considerable time to overcome these high barriers. But the important point is that eventually, at long t, the limiting slope is always attained, and the system is again in an ''equilibrium'' state. This limiting slope of 2 is reached for any value of $\epsilon \neq 0$. But the smaller the ϵ value, the longer it takes for this to happen. We thus choose a relatively large value ($\epsilon=1.8$) to speed up this effect.

In Fig. 1(b) the temperature is progressively raised from $T=0.50$ to $T=1000$. We observe an opposite effect: the $\langle R^2 \rangle$ values now decrease as the temperature is increased. More importantly, the limiting slope of 2 progressively changes to a limiting value of 1, which is fully attained at the highest temperature $T=1000$. The reason for this behavior is the following: As the temperature is progressively increased there is enough thermal energy to overcome barriers of any height, so that the bias effect which results in simultaneous increase and decrease of two barriers along one direction is not that important anymore. At infinite temperature the slope of the R^2 line would be exactly equal to 1, as the effect of the bias would be completely lost. Additionally, in this plot this has a consequence that the slope=1 curve would necessarily cross with the slope=2 curves, as we can clearly see.

For all curves of Fig. 1 the time it takes to reach this limiting slope, τ_c, is a characteristic quantity. The question can immediately be raised about its dependence on the temperature. Our earlier result [3] for the case of no bias ($\epsilon=0$) had shown (from the τ_c vs $1/T$ plot) a regular Arrhenius behavior. However, the R^2 data were monotonic with temperature, while here this is not the case. If we still make this plot, we see in Fig. 2 that below a certain temperature ($T<0.20$) we get straight lines for all cases, i.e., we have Arrhenius behavior. Above $T>0.20$ we do not get

TABLE I. Slopes of the straight lines of the Arrhenius plots of the crossover times t_c, for several bias values investigated in Fig. 2.

ϵ	Slope of t_c
0	0.51
0.1	0.49
0.2	0.48
0.5	0.48
1.0	0.47
1.8	0.45
2.5	0.38

Arrhenius behavior due to the thermal effect discussed above. In this plot we have also included several additional ϵ values, $\epsilon=0.1$, 0.2, 0.5, 1.0, 2.5, and 5.0. In Table I we show the slopes of the straight lines, for all these cases. We observe that for $\epsilon=0$ we get a slope of approximately 0.5, which was explained in the past to conform with the percolation picture, as $p_c=0.50$ is the critical percolation threshold for bond percolation. Then, for different ϵ values we get slopes that are smaller than 0.5. The difference from 0.5 is proportional to ϵ, i.e., the larger the bias the more different is the crossover value.

The same interpretation as in the case of $\epsilon=0$ [3–5], is also valid here, but only for the section of low T. This suggests again an expression of the form

$$\tau_c=\exp\left(\frac{E_{eff}}{kT}\right), \tag{6}$$

leading to the semilog straight line sections of Fig. 2. The τ_c values that were used in this figure were derived as the cross-point of the two straight line segments (early time and late time) of each curve in Fig. 1. The best fits from linear least squares were used in each case. The first and last points to calculate the fit were chosen arbitrarily, by optically estimating the departure from linear behavior.

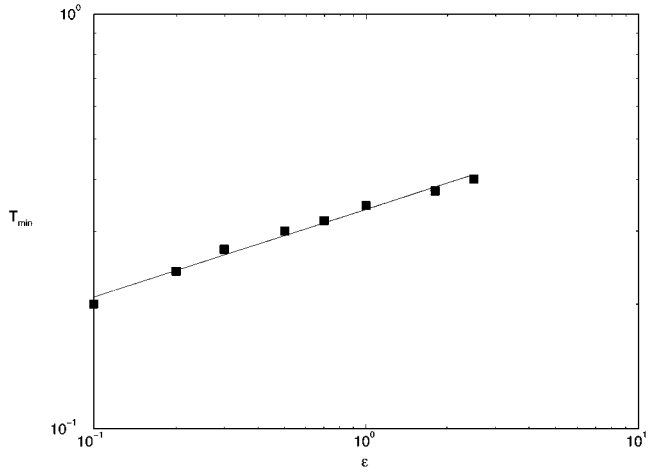

FIG. 3. Plot of T_{min} vs ϵ from the data of Fig. 2.

In Fig. 2 we also observe that each ϵ line goes through a τ_c minimum value, which corresponds to a characteristic temperature, T_{min}. In order to see how T_{min} behaves with the bias, we plot T_{min} vs ϵ in Fig. 3. We observe that in log-log axes we get a straight line with slope equal to 0.21 ± 0.01.

In conclusion, we presented a model of inhomogeneous diffusion with a directional bias. Transitions to nearest neighbors follow Boltzmann statistics. We observe a crossover from ballistic to classical diffusion with increasing temperature. This is because the increasing temperature progressively erases the effect of the bias in this model. This crossover transition obeys a scaling law with the bias of the walk.

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