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Asymptotic diffusion coefficient of particles in a random medium

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Avramov, Milchev, and Argyrakis [Phys. Rev. E **47**, 2303 (1993)] have investigated the mean-square displacements of particles that perform random walks in two- and three-dimensional lattices with random barriers with uniform distributions of activation energies. They discussed the crossover between anomalous and normal diffusion, but they did not analyze the behavior of the mean-square displacements at long times where normal diffusion occurs. We point out that the asymptotic diffusion coefficients are well described by the effective-medium theory in the range of parameters investigated; they are in disagreement with the predictions of critical-path arguments in dimension $d = 3$.

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Recently, Avramov, Milchev, and Argyrakis [1] investigated the random-barrier model for particle diffusion in two and three dimensions by numerical simulations. They used uniform distributions of activation energies and the Arrhenius law to convert the activation energies into transition rates. By varying the ratio α between the temperature and the largest activation energy different ranges of the transition rates could be explored. The major point of the paper was the elucidation of the crossover from subdiffusive behavior at intermediate times to normal diffusion at long times. We agree fully with this analysis, which showed that the crossover is determined by percolation arguments. However, the authors did not analyze the diffusion coefficients that can be obtained from their simulations. In this Brief Report we will make such an analysis and we will point out that their asymptotic diffusion coefficients are well described by the effective-medium theory. For the parameter range that was investigated, their results are in disagreement with the predictions of (naive) critical-path arguments.

The effective-medium theory for hopping transport in the random-barrier model was formulated by several authors [2–4]. In the static limit the self-consistency condition for the effective hopping rates Γ_{eff} reduces to one that was already derived by Kirkpatrick for the random-resistor problem [5]

$$\left\{ \frac{\Gamma_{\text{eff}} - \Gamma}{(d-1)\Gamma_{\text{eff}} + \Gamma} \right\} = 0 \,. \tag{1}$$

The curly brackets indicate the average over the distribution of the transition rates Γ. This self-consistency condition was evaluated by Bernasconi [6] for a uniform distribution of activation energies between $E = 0$ and $E = E_c$. The result for $d \geq 2$ is

$$\Gamma_{\text{eff}} = \frac{\Gamma_0}{d-1} \, \frac{1 - \exp(\frac{1-d}{d\alpha})}{\exp(\frac{1}{d\alpha}) - 1} \,, \tag{2}$$

where $\alpha = k_B T / E_c$. Extensions of the result to other intervals of the energy are also possible. For fixed dimension d and small parameter α the expression reduces to

$$\Gamma_{\text{eff}} \underset{\alpha \to 0}{\longrightarrow} \frac{\Gamma_0}{d-1} \exp\left(-\frac{1}{d\alpha} \right) \,. \tag{3}$$

This expression should be compared with the result of the critical-path approach [7,6]

$$\Gamma_{\text{eff}} \approx \Gamma_0 \exp\left(-\frac{p_c}{\alpha} \right) \,, \tag{4}$$

where p_c is the threshold for bond percolation [8]. Both expressions agree in $d = 2$ where $p_c = 0.5$; in $d = 3$ there appears a difference since $p_c \approx 0.242$.

We generated our own Monte Carlo data on the mean-square displacements; they are in full agreement with the data of Avramov, Milchev, and Argyrakis [1]. Moreover, we also determined the mobility by applying small uniform bias fields in one lattice direction. Table I shows our results for the asymptotic diffusion coefficients, together with the predictions of the effective-medium theory (EMT) and the critical-path approach for $d = 3$. For these α values the data are well accounted for by the

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TABLE I. Comparison of diffusion coefficients and mobility obtained by different methods in $d = 3$. The quantities are given in units of $6\Gamma_0$.

α	EMT	Critical-path approach	Mean-square displacement	Mobility
1	0.1025	0.1308	0.103	0.1
0.5	0.06475	0.1027	0.0642	0.0629
0.2	0.01871	0.04970	0.0209	0.0166
0.1	0.003079	0.01482	0.00273	0.00143

effective-medium theory. As said above, in $d = 2$ the critical-path approach gives results identical to those of the EMT, which agree with the simulations, but in d=3 the data differ considerably from the critical-path expression. For smaller α values no reliable determination of the diffusion coefficient or the mobility was possible.

It is no surprise that the effective-medium theory is valid for α values down to about 0.1. Luck [9] studied the validity of the effective-medium theory by comparing it with exact perturbation expansions. He found that a difference appears in $d = 3$ in the fourth order of the perturbation theory, and the relevant parameter is a second moment μ_2, which is approximately $1/\alpha^2$ for small α. The difference is proportional to μ_2^2 in the fourth order and it is about 4.5% at $\alpha = 0.1$. The difference grows then $\sim \alpha^{-4}$ for smaller α values.

Corrections to the naive critical path prediction have been considered by Tyc and Halperin [10] and Le Doussal [11], which are of the form $(\alpha)^y$ with an exponent y that is not precisely known in $d = 3$. Using the two proposed exponents of Ref. [10] we find improvement of the predictions, but the agreement with our data is not as good as for the EMT. We point out that it is necessary to investigate much smaller values of the parameter α when the critical-path expression is put to a test. This would then also require the application of numerical methods that are appropriate for the static limit.

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