Effective-medium approximation with asymmetric transition rates

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(Received 8 August 2001; published 4 April 2002)

An effective-medium approximation considering asymmetric transition rates is presented for a D-dimensional anisotropic random walk. Our approach allows to obtain a set of 2D frequency-dependent effective transition rates in a self-consistent way. Even when these coupled equations could look unwielding, we have been able to work out some particular cases, i.e., using a separablelike ansatz the asymmetric effective-medium approximation is shown to be reduced, under a transformation of variables, to the study of the symmetric case. Within this basic formalism, a biased diffusion problem in an anisotropic two-dimensional percolation model is analyzed. The asymmetric effective-medium approximation is finally compared against Monte Carlo simulations, and a good agreement is found for small bias values.

DOI: 10.1103/PhysRevB.65.165205

PACS number(s): 66.30.-h, 02.50.Ey, 05.60.-k

I. INTRODUCTION

Transport properties of disordered systems is a field of continuous research. It has many applications in the area of natural science, e.g., physics, chemistry, and biology. Such applications include transport in porous and fractured media, diffusion in catalytic processes and hopping conduction in amorphous solids, among others. Most of the natural systems in which diffusion occurs are, in fact, disordered systems, and it is necessary to develop new ways to describe transport phenomena. In such systems, usual techniques include Monte Carlo or molecular-dynamic simulations, renormalization group, continuous-time random walks, and effectivemedium approximation (EMA). Moreover, each technique has several generalizations.

The effective-medium theory was first considered, in diffusion problems, by Kirkpatrick,¹ who applied it to the study of random-resistor networks, but it was only in the early 80's that the formulation got a generalization to the frequencydependent behavior.^{2–5}

The extension of EMA to anisotropic systems was first studied, in the context of Kirkpatrick's formalism, in the long-time regime on square lattices.⁶ Next, the theory was generalized to other lattices,⁷ and recently the frequency-dependent behavior was developed.⁸

The earlier extension of EMA to asymmetric transitions rates, between pairs of sites, includes the one-dimensional formalism,^{9,10} and asymmetric transitions induced by switching on a uniform electric field in an originally three-dimensional symmetric system.¹¹ More recently, long-time¹² and frequency behavior¹³ were studied, in the context of diffusion in random-energy landscapes. In these systems the asymmetric bond conductance was introduced by means of site disorder. There, the fundamental idea is the use of the detailed balance condition to transform the algebra of asymmetric transition rates into symmetric ones.

It is possible to understand EMA considering two basic steps. First, replacing the disordered medium by a system with unknown *effective* transition rates W^e , with the exception of just one impurity between sites **a** and **b**, for which the

transition rate takes the value ω with the probability distribution function (PDF) $\mathcal{P}(\omega)$. Second, EMA imposes that the impurity Green function, $\mathbf{G}^{i} = [u\mathbf{1} - \mathbf{H}^{i}]^{-1}$, averaged over the PDF $\mathcal{P}(\omega)$, must be equal to the ordered Green function corresponding to the effective medium, $\mathbf{G}^0 = [u\mathbf{1} - \mathbf{H}^0(W^e)]$, where $\mathbf{H}^{i} = \mathbf{H}^{0} + \mathbf{V}$. Here \mathbf{H}^{0} is the transition-rate matrix of the ordered medium with effective transition rates W^e , \mathbf{H}^i is the transition rate matrix of a system composed of one impurity embedded in an ordered medium, and V is an auxiliary transition-rate matrix that contains the information of the introduced impurity. This condition establishes that the average fluctuations of the probability flux, passing through the bond connecting sites $\mathbf{a}=\mathbf{0}$ and $\mathbf{b}=\hat{\mathbf{e}}$, must vanish with respect to the effective medium that contains it.¹ Then, working out the self-consistent condition, a simple expression may be derived,

$$\left\langle \frac{(W^e - \omega)}{1 + 2(W^e - \omega)(\mathbf{G}_1^0 - \mathbf{G}_0^0)} \right\rangle_{\mathcal{P}(\omega)} = 0, \tag{1}$$

where $\langle \cdots \rangle_{\mathcal{P}(\omega)}$ denotes average over the PDF $\mathcal{P}(\omega)$. Here, $\mathbf{G}_1^0 \equiv \mathbf{G}_{(0,\hat{\mathbf{e}})}^0$ and $\mathbf{G}_0^0 \equiv \mathbf{G}_{(0,0)}^0$ are related to the probabilities of moving from the origin to one of its nearest neighbors and the return probability, respectively. From this condition the effective transition rate W^e is obtained as a function of the Laplace variable *u* for a given disordered model, characterized by the PDF $\mathcal{P}(\omega)$. This is the general frequency-dependent EMA for isotropic symmetric disordered systems (Laplace variable and frequency are used in an equivalent form due to their proportionality relation $u = 2\pi f$.)

The aim of the present paper is to present a generalization of EMA to the case of asymmetric transition rates in an anisotropic *D*-dimensional system. Our approach allows to obtain a set of 2D frequency-dependent effective transition rates in a self-consistent way. We remark that this scheme is a general approach; the crucial point is to be able to solve this set of 2D coupled equations. In this paper we show that after making a simplifying assumption about the nature of the disorder, the mathematical problem is reduced considerably. Particularly this assumption is what we call the *separablelike* ansatz to be able to solve the set of 2D equations. In this context, in the present paper, two examples are explicitly worked out. The more complex situation when the separablelike ansatz cannot be used, as in the *drift/no-drift* transition,¹⁴ is in progress and will be reported in future communications.

The outline of the paper is as follows. In Sec. II the general formalism of the asymmetric EMA is presented. In Sec. III the case of biased diffusion on both anisotropic percolative systems and a 2-dimensional binary-mixture model are treated; next our results are compared to Monte Carlo simulations. Concluding remarks are presented in Sec. IV. The Appendixes are devoted to some mathematical features.

II. ASYMMETRIC EMA

A. General formalism

In this section, we present the most general anisotropic asymmetric EMA formalism for diffusion on disordered lattices. This formalism is very general in the sense that it incorporates new features on the problem and contains previous EMA's with asymmetric transition rates.

Consider the master equation (ME) representing a random walk (RW) on a *D*-dimensional hypercubic lattice

$$\dot{\mathbf{P}} = \mathbf{H}\mathbf{P}.$$
 (2)

Here, **P** is the probability matrix whose elements are

$$\mathbf{P}_{\mathbf{r},\mathbf{r}'}(t) \equiv \langle \mathbf{r} | \mathbf{P}(t) | \mathbf{r}' \rangle = P(\mathbf{r},t | \mathbf{r}',0), \qquad (3)$$

with $P(\mathbf{r},t|\mathbf{r}',0)$ being the conditional probability of finding the particle at site \mathbf{r} at time *t*, given that it initially was at site \mathbf{r}' . The elements of the transition rate matrix \mathbf{H} are

$$\mathbf{H}_{\mathbf{r},\mathbf{r}'} \equiv \langle \mathbf{r} | \mathbf{H} | \mathbf{r}' \rangle = W_{\mathbf{r},\mathbf{r}'} - \delta_{\mathbf{r},\mathbf{r}'} \sum_{\mathbf{r}''} W_{\mathbf{r}'',\mathbf{r}}, \qquad (4)$$

where $W_{\mathbf{r},\mathbf{r}'}$ is the hopping transition rate from site \mathbf{r}' to site \mathbf{r} . In the following we only consider nearest-neighbor transition rates. For the symmetric ordered case $W_{\mathbf{r},\mathbf{r}'} = W$ and $\mathbf{H} = \mathbf{H}(W)$. The formal solution of the ME (2) in the Laplace representation (i.e., $t \rightarrow u$) is

$$\widetilde{\mathbf{P}}(u) = [u\mathbf{1} - \mathbf{H}]^{-1} \equiv \mathbf{G}(u).$$
(5)

Here, G(u) denotes the Green function of the RW operator **H**, and **1** is an identity matrix with the same dimension as **H**. We shall refer to the ordered case by using the "0" superscript, i.e., H^0 and $G^0(u)$.

An anisotropic asymmetric ordered system may be defined with the nearest-neighbor transition rates given by

$$W_{\mathbf{r}+\mathbf{s},\mathbf{r}} = \begin{cases} A_{\alpha} & \text{if } \mathbf{s} = \hat{\mathbf{e}}_{\alpha} \\ B_{\alpha} & \text{if } \mathbf{s} = -\hat{\mathbf{e}}_{\alpha} \\ 0, & \text{if } \mathbf{s} \neq \pm \hat{\mathbf{e}}_{\alpha}, \end{cases}$$
(6)

where $\hat{\mathbf{e}}_{\alpha}$ is a unit vector on the α axis ($\alpha = 1, 2, ..., D$). This means that, in each α axis, the transition rates in the positive and negative directions are A_{α} and B_{α} , respectively.

It is possible to write the Green functions $\mathbf{G}_{\mathbf{r},\mathbf{r}'}^{0}(u)$ corresponding to the asymmetric ordered case in terms of the Green function $\widetilde{\mathbf{Q}}_{\mathbf{r},\mathbf{r}'}^{0}(u)$ of the symmetric ordered case (see Appendix A),

$$\mathbf{G}_{\mathbf{r},\mathbf{r}'}^{0}(u) = \prod_{\alpha=1}^{D} \left(\frac{A_{\alpha}}{B_{\alpha}}\right)^{(\mathbf{r}_{\alpha}'-\mathbf{r}_{\alpha})/2} \widetilde{\mathbf{Q}}_{\mathbf{r},\mathbf{r}'}^{0} \left(u + \sum_{\alpha=1}^{D} s_{\alpha}\right), \quad (7)$$

where $s_{\alpha} = A_{\alpha} + B_{\alpha} - 2\sqrt{A_{\alpha}B_{\alpha}}$.

An anisotropic asymmetric disordered lattice is built up by associating each bond of the lattice with a pair of identically distributed random transition rates (ω_+, ω_-) . Now, let us consider an impurity on the α axis, embedded in an effective medium with 2D effective transition rates $\{W_{\pm\alpha}^e\}$ (two for each axis, one for each direction). The impurity transition rates are $(\omega_{+\alpha}, \omega_{-\alpha})$, characterized by a joint PDF $\mathcal{F}_{\alpha}(\omega_{+\alpha}, \omega_{-\alpha})$. The impurity transition matrix is now $\mathbf{H}^i = \mathbf{H}^0 + \mathbf{V}$, with

$$\mathbf{H}^{0} = \sum_{\mathbf{r},\alpha} |\mathbf{r}\rangle A_{\alpha} \langle \mathbf{r} - \hat{\mathbf{e}}_{\alpha} | + |\mathbf{r}\rangle B_{\alpha} \langle \mathbf{r} + \hat{\mathbf{e}}_{\alpha} | - |\mathbf{r}\rangle (A_{\alpha} + B_{\alpha}) \langle \mathbf{r} |,$$
(8)

and

$$\mathbf{V} = |\mathbf{a}\rangle \gamma_{1\alpha} \langle \mathbf{a}| + |\mathbf{a}\rangle \gamma_{2\alpha} \langle \mathbf{b}| + |\mathbf{b}\rangle \gamma_{3\alpha} \langle \mathbf{a}| + |\mathbf{b}\rangle \gamma_{4\alpha} \langle \mathbf{b}|.$$
(9)

Without loss of generality, we set $\mathbf{a} = \mathbf{0}$ and $\mathbf{b} = \hat{\mathbf{e}}_{\alpha}$. The coefficients $\gamma_{i\alpha}$ are defined by

$$\gamma_{1\alpha} = -\gamma_{3\alpha} = (A_{\alpha} - \omega_{+\alpha}),$$

$$\gamma_{4\alpha} = -\gamma_{2\alpha} = (B_{\alpha} - \omega_{-\alpha}).$$
 (10)

As in the ordered case, there are two impurity Green's functions for the α axis, one for each direction. In terms of the ordered Green functions, we obtain for the transition $\mathbf{0} \rightarrow \hat{\mathbf{e}}_{\alpha}$

$$\mathbf{G}_{+\alpha}^{i}(u) = \frac{\mathbf{G}_{+\alpha}^{0} + (A_{\alpha} - \omega_{+\alpha}) [\mathbf{G}_{+\alpha}^{0} \mathbf{G}_{-\alpha}^{0} - (\mathbf{G}_{0}^{0})^{2}]}{1 + (B_{\alpha} - \omega_{-\alpha}) (\mathbf{G}_{+\alpha}^{0} - \mathbf{G}_{0}^{0}) + (A_{\alpha} - \omega_{+\alpha}) (\mathbf{G}_{-\alpha}^{0} - \mathbf{G}_{0}^{0})},$$
(11)

and for the transition $\hat{\mathbf{e}}_{\alpha} \rightarrow \mathbf{0}$

$$\mathbf{G}_{-\alpha}^{i}(u) = \frac{\mathbf{G}_{-\alpha}^{0} + (B_{\alpha} - \omega_{-\alpha}) [\mathbf{G}_{-\alpha}^{0} \mathbf{G}_{+\alpha}^{0} - (\mathbf{G}_{0}^{0})^{2}]}{1 + (A_{\alpha} - \omega_{+\alpha}) (\mathbf{G}_{-\alpha}^{0} - \mathbf{G}_{0}^{0}) + (B_{\alpha} - \omega_{-\alpha}) (\mathbf{G}_{+\alpha}^{0} - \mathbf{G}_{0}^{0})}.$$
(12)

 $\mathbf{G}^{0}_{+\alpha}(u)$ and $\mathbf{G}^{0}_{-\alpha}(u)$ refer to transitions from the origin to its nearest neighbors on either the positive or negative direction in the α axis, and $\mathbf{G}^{0}_{0}(u)$ is related to the return probability.

The situation considered above corresponds to just one impurity on the α axis. To take anisotropy into account, all possible axes where the impurity can be placed must be considered. Following the procedure in Ref. 8, the impurity Green functions for each axis must be averaged over the disorder, and equaled it to the ordered ones. Then, a set of 2D self-consistent conditions, i.e., two for each axis, are obtained, which have the form

$$\left(\frac{(W_{+\alpha}^{e} - \omega_{+\alpha})\mathbf{G}_{0}^{0} - (W_{-\alpha}^{e} - \omega_{-\alpha})\mathbf{G}_{+\alpha}^{0}}{1 + (W_{+\alpha}^{e} - \omega_{+\alpha})(\mathbf{G}_{-\alpha}^{0} - \mathbf{G}_{0}^{0}) + (W_{-\alpha}^{e} - \omega_{-\alpha})(\mathbf{G}_{+\alpha}^{0} - \mathbf{G}_{0}^{0})}\right)_{\mathcal{F}_{\alpha}(\omega_{+\alpha}, \omega_{-\alpha})} = 0,$$
(13)

$$\left\langle \frac{(W_{-\alpha}^{e} - \omega_{-\alpha})\mathbf{G}_{0}^{0} - (W_{+\alpha}^{e} - \omega_{+\alpha})\mathbf{G}_{-\alpha}^{0}}{1 + (W_{+\alpha}^{e} - \omega_{+\alpha})(\mathbf{G}_{-\alpha}^{0} - \mathbf{G}_{0}^{0}) + (W_{-\alpha}^{e} - \omega_{-\alpha})(\mathbf{G}_{+\alpha}^{0} - \mathbf{G}_{0}^{0})} \right\rangle_{\mathcal{F}_{\alpha}(\omega_{+\alpha}, \omega_{-\alpha})} = 0.$$
(14)

with $\alpha = 1, 2, \ldots, D$.

The model of disorder has to be specified by giving $\mathcal{F}_{\alpha}(\omega_{+\alpha}, \omega_{-\alpha})$, and then this set of 2D self-consistent conditions must be solved in order to obtain the frequency-dependent effective transition rates $\{W_{\pm\alpha}^e\}$.

If the transition rates of the model are symmetric in all directions, then $\omega_{+\alpha} = \omega_{-\alpha}$, $W^{e}_{+\alpha} = W^{e}_{-\alpha}$, and $\mathbf{G}^{0}_{+\alpha} = \mathbf{G}^{0}_{-\alpha}$. It is thus clear that the two conditions for each direction are equivalent and the anisotropic symmetric case is recovered.⁸ Obviously, there are cases where the transition rates are asymmetric on some axis, but symmetric in others. In such cases, the equations corresponding to the symmetric transition rates collapse and the number of total equations, as well as the effective transition rates to be determined, are reduced.

B. Separablelike model

As a special case a system may be considered in which the set of random variables, corresponding to asymmetric bonds, can be written as

$$\omega_{\pm\,\alpha} = \omega_{\alpha} a_{\alpha}^{\pm\,1} \,. \tag{15}$$

Here, the $a_{\alpha}^{\pm 1}$ factor is not necessarily an exponential function (Arrhenius's factor) of the external field, as when considering a Boltzmann factor due to the action of some electric field. Moreover, both ω_{α} and $a_{\alpha}^{\pm 1}$ may be functions of the parameters related to the asymmetry of the system. With these transformations, the asymmetric character of the system is preserved, but the self-consistent problem is substantially simplified.

Then, it is necessary to transform the set of joint PDF's $\mathcal{F}_{\alpha}(\omega_{+\alpha}, \omega_{-\alpha})$ into a new set of PDF's $\mathcal{P}_{\alpha}(\omega_{\alpha})$ that describe the same asymmetric model via the transformation of variables (15). By considering the marginal distributions

$$f_{+\alpha}(\omega_{+\alpha}) = \int \mathcal{F}_{\alpha}(\omega_{+\alpha}, \omega_{-\alpha}) d\omega_{-\alpha},$$

$$f_{-\alpha}(\omega_{-\alpha}) = \int \mathcal{F}_{\alpha}(\omega_{+\alpha}, \omega_{-\alpha}) d\omega_{+\alpha}, \qquad (16)$$

the existence of $\mathcal{P}_{\alpha}(\omega_{\alpha})$ is ensured if the condition

$$f_{-\alpha}(\omega_{\alpha}a_{\alpha}^{-1}) = a_{\alpha}^{2}f_{+\alpha}(\omega_{\alpha}a_{\alpha})$$
(17)

holds. Then, we have

$$\mathcal{P}_{\alpha}(\omega_{\alpha}) = a_{\alpha} f_{+\alpha}(\omega_{\alpha} a_{\alpha}). \tag{18}$$

Considering Eq. (15) it may be assumed that the effective transition rates also undergo a similar transformation, i.e.,

$$W^e_{\pm\,\alpha} = W^e_{\,\alpha} a^{\pm\,1}_{\,\alpha} \,. \tag{19}$$

It seems natural, *a priori*, to take this transformation as correct. However since $W_{+\alpha}^e \neq W_{-\alpha}^e$, it would imply that the asymptotic mean velocity has a nonzero value for asymmetric models, this, in general, is not always the case (see Sec. III).

With these considerations and from Eqs. (13) and (14), we arrive at a set of D self-consistent equations for the $\{W_{\alpha}^{e}\}$ unknown rates, representing the anisotropic asymmetric system

$$\left\langle \frac{(W_{\alpha}^{e} - \omega_{\alpha})}{1 + (W_{\alpha}^{e} - \omega_{\alpha})\mathbf{M}_{\alpha}(u)} \right\rangle_{\mathcal{P}_{\alpha}(\omega_{\alpha})} = 0,$$
(20)

with

$$\mathbf{M}_{\alpha}(u) = a_{\alpha}^{-1} \mathbf{G}_{+\alpha}^{0} + a_{\alpha} \mathbf{G}_{-\alpha}^{0} - (a_{\alpha} + a_{\alpha}^{-1}) \mathbf{G}_{0}^{0}.$$
 (21)

Example. Let us now consider the isotropic 2-dimensional case in the limit u=0, where we get the property $a_{\alpha}=a$, i.e., independent of the axis direction. This property may physically be induced by an external field oriented along the main diagonal of a square lattice. In this case, the set of equations (20) reduce to only one self-consistent condition, i.e., one effective transition rate W^e . From Eqs. (7) and (A8), it can

be seen that in the limit $u=0, \mathbf{M}_{\alpha}(u=0)=(-2W^{e})^{-1}$. From this fact, the self-consistent condition reads

$$\left\langle \frac{W^e - \omega}{W^e + \omega} \right\rangle_{\mathcal{P}(\omega)} = 0.$$
 (22)

This coincides with the earlier result for the symmetric random-resistor network.¹ Thus, under condition (19), the effective transition rates W_{\pm}^{e} , in the long-time limit, can easily be obtained by solving the well-known symmetric condition (22) and multiplying the result by the factor $a^{\pm 1}$, which of course will depend on the specific asymmetric isotropic model.

Conjecture. At zero frequency and for the anisotropic 2-dimensional case we can still use the same ideas involved in getting Eq. (22); i.e., we solve the $W_{1(2)}^e$ as in the symmetric anisotropic EMA problem,^{6–8} then the solution of the asymmetric anisotropic problem is obtained as

$$W_{\pm 1}^{e} = W_{1}^{e} a_{1}^{\pm 1}, \qquad (23)$$
$$W_{\pm 2}^{e} = W_{2}^{e} a_{2}^{\pm 1},$$

where $W_{1(2)}^e$ are given by the solution of the set of selfconsistent conditions given in Ref. 8. By performing a series expansion for u=0 in the Green functions (A7) the set of equations is

$$\left\langle \frac{W_1^e - \omega_1}{1 - 2(W_1^e - \omega_1)(\pi W_1^e)^{-1} \arctan \sqrt{W_1^e(W_2^e)^{-1}}} \right\rangle_{\mathcal{P}_1(\omega_1)} = 0,$$
(24)

$$\left\langle \frac{W_2^e - \omega_2}{1 - 2(W_2^e - \omega_2)(\pi W_2^e)^{-1} \arctan \sqrt{W_2^e(W_1^e)^{-1}}} \right\rangle_{\mathcal{P}_2(\omega_2)} = 0.$$

Since in deriving the condition (22) the explicit functionality of the Green functions was used, it is not simple to derive this condition for more dimensions or in anisotropic conditions. That is why we made the previous conjecture in 2 dimension. In the following sections, this conjecture is tested.

Note that from the present formalism the 1-dimensional case worked out in Ref. 9 may be recovered. Also, the model for conductivity of a charged particle on a percolation system, under the action of an external uniform electric field, treated by Yu and Orbach in Ref. 11, may be recovered as an special case of the present asymmetric EMA. For details see Appendix B.

III. BIASED DIFFUSION ON DILUTED NETWORKS

A. Anisotropic percolation network

Let us consider the model introduced in Ref. 14 to describe biased diffusion on anisotropic percolation systems. The anisotropy is introduced by considering bond percolation on the square lattice with different occupation probabilities on each axis. Thus, in axis 1 the bond conductances Γ_1

(25)

take the value Σ_1 with probability p_1 , and zero otherwise (analogously for axis 2). This situation may be represented by a pair of distribution functions,

 $\mathcal{P}_1(\Gamma_1) = p_1 \,\delta(\Gamma_1 - \Sigma_1) + (1 - p_1) \,\delta(\Gamma_1),$

and

$$\mathcal{P}_2(\Gamma_2) = p_2 \,\delta(\Gamma_2 - \Sigma_2) + (1 - p_2) \,\delta(\Gamma_2). \tag{26}$$

The conductivity properties of such a system, in the case $p_2=1$, were studied with the anisotropic EMA in Ref. 8.

Now a bias field *B* is switched on, with $0 \le B \le 1$. The direction of the bias is selected along the main-diagonal direction, exploring the symmetry properties of the model.¹⁴ This bias acts on the system in such way that the transition rates increase by a factor (1+B) in the direction of the bias, and decrease by a factor (1-B) in the opposite direction. Then, each bond is characterized by two random conductances, represented by a set of joint PDF's,

$$\mathcal{F}_{1}(\omega_{+1},\omega_{-1}) = p_{1}\delta(\omega_{+1}-\sigma_{+1})\delta(\omega_{-1}-\sigma_{-1}) + (1-p_{1})\delta(\omega_{+1})\delta(\omega_{-1}), \quad (27)$$

and

$$\mathcal{F}_{2}(\omega_{+2},\omega_{-2}) = p_{2}\delta(\omega_{+2}-\sigma_{+2})\delta(\omega_{-2}-\sigma_{-2}) + (1-p_{2})\delta(\omega_{+2})\delta(\omega_{-2}), \quad (28)$$

with $\sigma_{\pm 1(2)} = \Sigma_{1(2)}(1 \pm B)$.

For this biased anisotropic model, condition (17) is fulfilled by considering for all α

$$a_{\alpha} = a = \sqrt{\frac{1+B}{1-B}}.$$
(29)

Thus, we can use transformation (15) to reduce the problem. Then, the new set of PDF's, according to Eq. (18), is

$$\mathcal{P}_1(\boldsymbol{\omega}_1) = p_1 \,\delta(\boldsymbol{\omega}_1 - \boldsymbol{\sigma}_1) + (1 - p_1) \,\delta(\boldsymbol{\omega}_1), \qquad (30)$$

and

$$\mathcal{P}_{2}(\omega_{2}) = p_{2}\delta(\omega_{2} - \sigma_{2}) + (1 - p_{2})\delta(\omega_{2}), \qquad (31)$$

with $\sigma_{1(2)} = \sum_{1(2)} \sqrt{1 - B^2}$.

We shall also assume the related transformation for effective transition rates (19) with the use of Eq. (29). Based on the conjecture of the preceding section we can use these ideas to work out the present asymmetric anisotropic percolation model. The first step is to solve the symmetric anisotropic case, i.e., to find $W_{1(2)}^e$. Then, the solution for the asymmetric problem is obtained by multiplying it by the factor $a_{1(2)}^{\pm 1}$, as in Eq. (23).

By using the PDF's (30) and (31) in the self-consistent conditions, Eq. (24), we get the following set of equations for the effective transition rates $W_{1(2)}^{e}$:

$$p_1\sigma_1 - W_1^e = \frac{2}{\pi}(\sigma_1 - W_1^e) \arctan\left(\sqrt{\frac{W_1^e}{W_2^e}}\right), \qquad (32)$$



FIG. 1. Velocity against the external field for the anisotropic bond percolation model in a two-dimensional lattice. The isotropic case $p_1=p_2=0.9$ and the anisotropic case $p_1=0.95, p_2=0.85$ are shown. The velocity is measured in units of the lattice constant per unit of time (diffusion attempts). *B* is a dimensionless bias parameter. Each curve has been rescaled in order to highlight the difference between them.

$$p_2\sigma_2 - W_2^e = \frac{2}{\pi}(\sigma_2 - W_2^e) \arctan\left(\sqrt{\frac{W_2^e}{W_1^e}}\right).$$

Now, by setting $\Sigma_1 = \Sigma_2 = \frac{1}{4}$, and using effective velocities as the unknown variables, instead of effective transition rates, in the set of equations (32), i.e., $v_{1(2)}^e(t \rightarrow \infty) = W_{1(2)}^e(a - a^{-1})$, the self-consistent anisotropic conditions result in

$$p_{1}B - 2v_{1}^{e} = \frac{2}{\pi} (B - 2v_{1}^{e}) \arctan\left(\sqrt{\frac{v_{1}^{e}}{v_{2}^{e}}}\right), \quad (33)$$
$$p_{2}B - 2v_{2}^{e} = \frac{2}{\pi} (B - 2v_{2}^{e}) \arctan\left(\sqrt{\frac{v_{2}^{e}}{v_{1}^{e}}}\right).$$

Note that for the isotropic case, the self-consistent conditions (24) take the form (22), therefore, the solution for the asymmetric problem is reduced to

$$W^{e}_{\pm} = (2p-1)(1\pm B)\Sigma$$

In order to test our result (33) we performed Monte Carlo simulations. The details of these simulations were discussed in Ref. 14. Random walks were performed on a square lattice for several disorder parameters p_1 and p_2 . The mean velocity was averaged over 10 walks on 1000 lattices, each one of 300×300 sites. Figure 1 shows the asymptotic mean velocity against the applied bias *B*, for both the isotropic and anisotropic cases. The curves of mean velocity against bias field show nonmonotonic behavior. For small bias, the mean velocity shows a linear increase with increasing bias, as expected. The curves then reach a maximum value before decreasing to zero for a critical bias value $B_c < 1$ (*drift/no-drift* transition). This behavior can be interpreted as the result of competing effects between bias and dead ends generated by the disorder (see Refs. 14,15).

As can be seen in Fig. 1, the asymmetric EMA, restricted to separablelike models, is in good agreement with Monte Carlo simulations for small bias, where the effects of dead ends are negligible.

We remark that due to the assumption of transformation (19) we expect that this approximation does not describe the *drift/no-drift* transition, because a zero mean velocity is not allowed except in the unbiased limit B=0. However, we expect that by using the fundamental Eqs. (13) and (14), i.e., without using a separablelike ansatz, we could describe the *drift/no-drift* transition around the critical B_c point, in the EMA context.

B. Binary mixture

Let us now consider an isotropic binary-mixture model on a square lattice. In this model there exist two kinds of bonds \mathcal{A} and \mathcal{B} . The conductivities are $\Sigma_{\mathcal{A}}$ and $\Sigma_{\mathcal{B}}$, respectively, and they are distributed according to

$$\mathcal{P}(\Gamma) = p\,\delta(\Gamma - \Sigma_{\mathcal{A}}) + (1 - p)\,\delta(\Gamma - \Sigma_{\mathcal{B}}),\tag{34}$$

and we set $\Sigma_{\mathcal{A}} \ge \Sigma_{\mathcal{B}}$.

A bias field *B* is switched on, as in the anisotropic percolation model discussed in the preceding section, with $0 \le B$ <1. Again the bias is selected in the main-diagonal direction of the square lattice. Then, each bond is characterized by the joint PDF

$$\mathcal{F}(\omega_{+},\omega_{-}) = p \,\delta(\omega_{+} - \sigma_{\mathcal{A}+}) \,\delta(\omega_{-} - \sigma_{\mathcal{A}-}) \\ + (1 - p) \,\delta(\omega_{+} - \sigma_{\mathcal{B}+}) \,\delta(\omega_{-} - \sigma_{\mathcal{B}-}),$$
(35)

with $\sigma_{\mathcal{A}(\mathcal{B})\pm} = \Sigma_{\mathcal{A}(\mathcal{B})}(1\pm B)$.

Once again we use transformation (15), condition (17) is fulfilled by considering relation (29), and the new random variable ω is distributed according to

$$\mathcal{P}(\omega) = p\,\delta(\omega - \sigma_{\mathcal{A}}) + (1 - p)\,\delta(\omega - \sigma_{\mathcal{B}}),\tag{36}$$

with $\sigma_{\mathcal{A}(\mathcal{B})} = \sum_{\mathcal{A}(\mathcal{B})} \sqrt{1 - B^2}$.

Therefore, for the long-time limit, the solution of the symmetric EMA (Ref. 1) with the PDF (36) may be used to obtain the effective transition rate W^e . Then, the asymptotic mean velocity is obtained by multiplying this W^e by the factor $(a-a^{-1})$. The result is

$$v^{e} = 2B \left[(\Sigma_{\mathcal{A}} - \Sigma_{\mathcal{B}}) \left(p - \frac{1}{2} \right) + \sqrt{(\Sigma_{\mathcal{A}} - \Sigma_{\mathcal{B}})^{2} \left(p - \frac{1}{2} \right)^{2} + \Sigma_{\mathcal{A}} \Sigma_{\mathcal{B}}} \right].$$
(37)

Once again, the dependence on the bias *B* is linear, but the dependence on the disorder parameter *p* is not; except in the case $\Sigma_B = 0$ where the isotropic biased percolative model is recovered, i.e., $v^e = 2B(2p-1)\Sigma_A$.

In order to test our asymmetric EMA results, Monte Carlo simulations were performed. The details of these simulations are the same as in the percolative case.¹⁴ In Fig. 2 the dependence of the asymptotic mean velocity is plotted as a func-



FIG. 2. Velocity against the external field *B* for the binarymixture model. The bond concentration is fixed to (a) p=0.2, and (b) p=0.8. As indicated in each graphic, different values of $\Sigma_{\mathcal{B}}$ are presented for the same value $\Sigma_{\mathcal{A}}=0.25$. The units are the same as in Fig. 1.

tion of the bias B. In Fig. 3 we show the curves of the asymptotic mean velocity as a function of p.

It can be seen that the asymmetric EMA, with ansatz (19), is in good agreement with the Monte Carlo simulations ex-



FIG. 3. Velocity against the bond concentration *p* for the binary mixture model. The external bias field is fixed at (a) B = 0.2 and (b) B = 0.8. As indicated in each graphic, different values of $\Sigma_{\mathcal{B}}$ are presented for the same value $\Sigma_{\mathcal{A}} = 0.25$. The units are the same as in Fig. 1.

cept in the region of high disorder p and high bias B. This discrepancy increases as the strength of the conductances Σ_B decreases. In this case the Monte Carlo data of the mean velocity against the bias field curve shows nonmonotonic behavior, as in the percolation model, see Fig. 2(b). Even when Figs. 2 and 3 show good agreement with the numerical experiments; the unfortunate fact, shown in Fig. 3, is the discrepancy between Monte Carlo data and the asymmetric EMA for high bias B. Note that in the limit $p \rightarrow 1$ (the ordered case) the agreement is restored.

IV. CONCLUDING REMARKS

In this paper we have presented a general approach for tackling the problem of transport on asymmetric anisotropic disordered media. Particular emphasis has been done on separablelike solutions (including the Arrhenius models), therefore, by using a suitable transformation of random variables the asymmetric problem is reduced to the symmetric one. We have remarked that such models are not the most general possible, but still many interesting systems can be of this type. On the other hand we have shown that by assuming the ansatz of a separable effective rates solution, $W_{\pm\alpha}^e a_{\alpha}^{\pm 1}$, we can obtain a very good fit against Monte Carlo simulations, in the small bias limit. This fact restricts the utility of EMA to the small bias region of the drift phase.^{14,15}

We remark that our scheme of asymmetric anisotropic EMA is a general approach; the main difficulty is to solving the set of 2D self-consistent equations for the effective rates $W^{e}_{\pm\alpha}(u)$. By introducing the separablelike ansatz the mathematical problem is reduced considerably. In the present paper we have worked out two separable models of disorder (see Sec. III). From our general point of view, Eqs. (13) and (14), we hope that using a singular perturbation theory around the critical B_c point, our approach opens the possibility to study the more complex situation, as the *drift/no-drift* transition;¹⁴ work on this direction is currently under investigation.

ACKNOWLEDGMENTS

S.B. thanks a fellowship from Secretaría de Investigación de la Universidad Nacional del Comahue. This work has been partially supported by grants from CONICET (Grant No. 4948/96), and Secretaría de Investigación de la Universidad Nacional del Comahue. We also thank Professor V. Grünfeld for the English revision.

APPENDIX A: THE GREEN FUNCTIONS

Consider the ME (2) and the ordered transition rates defined by Eq. (6). The ME explicitly reads

$$\partial_{t} \mathbf{P}_{\mathbf{r},\mathbf{r}'}(t) = \sum_{\alpha=1}^{D} \left[A_{\alpha} \mathbf{P}_{\mathbf{r}-\hat{\mathbf{e}}_{\alpha},\mathbf{r}'}(t) + B_{\alpha} \mathbf{P}_{\mathbf{r}+\hat{\mathbf{e}}_{\alpha},\mathbf{r}'}(t) \right] - \mathbf{P}_{\mathbf{r},\mathbf{r}'}(t) \sum_{\alpha=1}^{D} \left(A_{\alpha} + B_{\alpha} \right).$$
(A1)

Now use the following transformation $\mathbf{P}_{\mathbf{r},\mathbf{r}'}(t) \rightarrow \mathbf{Q}_{\mathbf{r},\mathbf{r}'}(t)$:

$$\mathbf{P}_{\mathbf{r},\mathbf{r}'}(t) = \mathbf{Q}_{\mathbf{r},\mathbf{r}'}(t) \exp\left[-\sum_{\alpha=1}^{D} \left(A_{\alpha} + B_{\alpha}\right) - 2\sqrt{A_{\alpha}B_{\alpha}}t\right] \prod_{\alpha=1}^{D} \left(\frac{A_{\alpha}}{B_{\alpha}}\right)^{\mathbf{r}_{\alpha}/2}, \quad (A2)$$

where \mathbf{r}_{α} is the α coordinate of the position \mathbf{r} . The Laplace transforms of the probabilities functions $\mathbf{P}_{\mathbf{r},\mathbf{r}'}(t)$ and $\mathbf{Q}_{\mathbf{r},\mathbf{r}'}(t)$ are related by

$$\mathbf{G}_{\mathbf{r},\mathbf{r}'}^{0}(u) \equiv \widetilde{\mathbf{P}}_{\mathbf{r},\mathbf{r}'}(u) = \prod_{\alpha=1}^{D} \left(\frac{A_{\alpha}}{B_{\alpha}}\right)^{(\mathbf{r}_{\alpha}-\mathbf{r}_{\alpha}')/2} \widetilde{\mathbf{Q}}_{\mathbf{r},\mathbf{r}'}^{0} \left(u + \sum_{\alpha=1}^{D} s_{\alpha}\right),$$
(A3)

with $s_{\alpha} = A_{\alpha} + B_{\alpha} - 2\sqrt{A_{\alpha}B_{\alpha}}$.

By introducing expression (A2) and its time derivative in Eq. (A1) we obtain a ME for the probability function $Q_{\mathbf{r},\mathbf{r}'}(t)$,

$$\partial_{t} \mathbf{Q}_{\mathbf{r},\mathbf{r}'}(t) = \sum_{\alpha=1}^{D} \left\{ \sqrt{A_{\alpha}B_{\alpha}} \left[\mathbf{Q}_{\mathbf{r}-\hat{\mathbf{e}}_{\alpha},\mathbf{r}'}(t) + \mathbf{Q}_{\mathbf{r}+\hat{\mathbf{e}}_{\alpha},\mathbf{r}'}(t) \right] \right\} - 2 \mathbf{Q}_{\mathbf{r},\mathbf{r}'}(t) \sum_{\alpha=1}^{D} \sqrt{A_{\alpha}B_{\alpha}}.$$
(A4)

In this way the asymmetric ME is transformed into a symmetric one.

The Green function for the ordered symmetric 1-dimensional case is given by

$$\widetilde{\mathbf{Q}}_{n,0}^{0}(u) = (2\sqrt{AB})^{|n|}(u^{2} + 4\sqrt{AB}u)^{-1/2}[u + 2\sqrt{AB} + (u^{2} + 4\sqrt{AB}u)^{1/2}]^{-|n|},$$
(A5)

where *n* is the site index. Introducing this function into expression (A3), the ordered asymmetric 1-dimensional Green functions is obtained. In the u=0 case we get

$$\mathbf{G}_{0}^{0}(u=0) = |A-B|^{-1},$$

$$\mathbf{G}_{+}^{0}(u=0) = 2A|A-B|^{-1}(A+B+|A-B|)^{-1}, \quad (A6)$$

$$\mathbf{G}_{-}^{0}(u=0) = 2B|A-B|^{-1}(A+B+|A-B|)^{-1}.$$

The elements $\widetilde{\mathbf{Q}}_0^0(u)$ and $\widetilde{\mathbf{Q}}_{+\alpha}^0(u)$, that we need from the 2-dimensional ordered anisotropic symmetric Green functions are⁸

$$\widetilde{\mathbf{Q}}_{0}^{0}(u) = \frac{\sqrt{\rho_{1}\rho_{2}}}{2\pi\sqrt{XY}}K(\sqrt{\rho_{1}\rho_{2}}),$$

$$\widetilde{\mathbf{Q}}_{+1}^{0}(u) = \frac{\sqrt{\rho_{1}\rho_{2}}}{\pi\sqrt{XY}} \left[\left(\frac{1}{2} + \frac{1}{\rho_{1}}\right)K(\sqrt{\rho_{1}\rho_{2}}) - \left(1 + \frac{1}{\rho_{1}}\right)\Pi(\rho_{1},\sqrt{\rho_{1}\rho_{2}}) \right],$$
(A7)

$$\widetilde{\mathbf{Q}}_{+2}^{0}(u) = \frac{\sqrt{\rho_1 \rho_2}}{\pi \sqrt{XY}} \left[\left(\frac{1}{2} + \frac{1}{\rho_2} \right) K(\sqrt{\rho_1 \rho_2}) - \left(1 + \frac{1}{\rho_2} \right) \Pi(\rho_2, \sqrt{\rho_1 \rho_2}) \right],$$

where K(k) and $\Pi(\rho, k)$ are elliptic integrals of the first and third kind. Here, the following definitions were used: $\rho_1 = 4Y/(u+4X)$, $\rho_2 = 4X/(u+4Y)$, $X = \sqrt{A_1B_1}$, and $Y = \sqrt{A_2B_2}$. Taking $A_1 = A_2$ and $B_1 = B_2$, the isotropic case is recovered as X = Y; so the required elements of the Green functions, for the isotropic case, are given by:

$$\widetilde{\mathbf{Q}}_{0}^{0}(u) = \frac{2}{\pi(u+4X)} K \left(\frac{4X}{u+4X} \right),$$
(A8)
$$\widetilde{\mathbf{Q}}_{+}^{0}(u) = \frac{1}{2\pi X} K \left(\frac{4X}{u+4X} \right) - \frac{1}{4X},$$

where X must be taken as the ordered transition rate.

APPENDIX B: ASYMMETRIC TRANSITIONS RATES REVISITED

1. One-dimensional case

In this case the disorder is characterized by means of the joint PDF $\mathcal{F}(\omega_+, \omega_-)$ for the pair of identically distributed random variables $(W_{n+1,n}, W_{n,n+1})$, *n* being the site index. As expected, only two effective transition rates are found for the effective medium, one for each direction. Then, when considering one-dimensional systems, only one pair of equations is obtained.

In the zero frequency limit u=0 (long-time regime), the one-dimensional ordered Green functions depend on the modulus $|W_{+}^{e} - W_{-}^{e}|$ [see Eqs. (A6)]. As a consequence, the solution of the self-consistent conditions strongly depends on the relative values of the effective transition rates, i.e., if $W_{+}^{e} > W_{-}^{e}$ or $W_{+}^{e} < W_{-}^{e}$. By using Eqs. (A6) in Eqs. (13) and (14) with $\alpha = 1$, the solution may be expressed in terms of the asymptotic mean velocity $v^{e}(t \rightarrow \infty) = W_{+}^{e} - W_{-}^{e}$; and the final result is

$$v^{e}(t \rightarrow \infty) = \begin{cases} \left(1 - \left\langle \frac{\omega_{-}}{\omega_{+}} \right\rangle\right) \left\langle \frac{1}{\omega_{+}} \right\rangle^{-1} & \text{if } \left\langle \frac{\omega_{-}}{\omega_{+}} \right\rangle = \frac{W_{-}^{e}}{W_{+}^{e}} < 1 \\ - \left(1 - \left\langle \frac{\omega_{+}}{\omega_{-}} \right\rangle\right) \left\langle \frac{1}{\omega_{-}} \right\rangle^{-1} & \text{if } \left\langle \frac{\omega_{+}}{\omega_{-}} \right\rangle = \frac{W_{+}^{e}}{W_{-}^{e}} < 1. \end{cases}$$
(B1)

This one-dimensional zero-frequency result was originally presented by Bernasconi and Schneider.⁹ We remark that the asymmetric one-dimensional EMA does not predict any result for the case when $\langle \omega_-/\omega_+ \rangle > 1$ and $\langle \omega_+/\omega_- \rangle$ >1 (see Ref. 9).

2. Uniform electric field

Consider a *D*-dimensional isotropic symmetric system. It has independent and identically distributed random transition rates ω , with a PDF $\mathcal{P}(\omega)$. Consider a charged particle moving in this system. Now assume that an external uniform electric field \mathbf{E}_0 is switched on, such that the transition rates, corresponding to one bond, become $\omega_{\pm} = \omega a_{\alpha}^{\pm 1}$, with $a_{\alpha}^{\pm 1}$ $= \exp(\mp \hat{\mathbf{e}}_{\alpha} \cdot \mathbf{V}_0)$. Here $\mathbf{V}_0 = e\mathbf{E}_0/kT$ and $\alpha = 1, 2, \dots, D$. The term $a_{\alpha}^{\pm 1}$ takes into account all possible directions of the electric field \mathbf{E}_0 .

Under the condition (15), an equivalent system may be considered, characterized by the pairs of transition rates $(\omega_{+\alpha}, \omega_{-\alpha})$. These transition rates obey a joint PDF $\mathcal{F}_{\alpha}(\omega_{+\alpha}, \omega_{-\alpha})$, related to $\mathcal{P}(\omega)$ by

$$\mathcal{F}_{\alpha}(\omega_{+\alpha},\omega_{-\alpha}) = \langle \,\delta(\omega_{+}-\omega a_{\alpha})\,\delta(\omega_{-}-\omega a_{\alpha}^{-1}) \rangle_{\mathcal{P}(\omega)} \,. \tag{B2}$$

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In principle, the medium has 2*D* effective transition rates, due to the introduced asymmetry. Under the condition that the effective transition rates obey $W_{\pm\alpha}^e = W_{\alpha}^e a_{\alpha}^{\pm}$, the number of unknown rates is reduced to *D*. Then, from Eqs. (13) and (14), the following set of *D* self-consistent conditions is obtained:

$$\left\langle \frac{(W_{\alpha}^{e} - \omega)}{1 + (W_{\alpha}^{e} - \omega)\mathbf{M}_{\alpha}(u)} \right\rangle_{\mathcal{P}(\omega)} = 0,$$
(B3)

with $\mathbf{M}_{\alpha}(u)$ given by Eq. (21). This is the same result presented by Yu and Orbach in Ref. 11. Note that if the effective transition rates had not been supposed to fulfill the property $W^{e}_{\pm\alpha} = W^{e}_{\alpha} a^{\pm 1}_{\alpha}$, we would not have arrived at a set of *D* self-consistent equations. Indeed, this condition would imply the existence of a nonzero asymptotic mean velocity because $W^{e}_{\pm\alpha} \neq W^{e}_{-\alpha}$ for all α .

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