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Paul Ernest Parris
Missouri University of Science and Technology, parris@mst.edu

B. D. Bookout

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Effective-medium theory for the electric-field dependence of the hopping conductivity of disordered solids

P. E. Parris and B. D. Bookout*
Department of Physics and the Electronic Materials Institute, University of Missouri-Rolla, Rolla, Missouri 65401
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We derive a general effective-medium theory for describing biased diffusion on a bond-disordered lattice in the presence of an external driving field. In our theory, the effective medium associated with a disordered d-dimensional lattice is characterized, for each value of the applied field, by $2d$ independent parameters describing, respectively, the net drift velocity v_ν and the diffusion constant $D_{\nu\nu}$ describing the spread of a carrier packet about its mean value, for each of the d crystal axes. The theory correctly predicts the velocity transition occurring in an exactly soluble model studied by Derrida and, in contrast to other recent theories, correctly reproduces the critical velocity at which this transition occurs.

I. INTRODUCTION

Recent observations of negative differential mobility,[1] as well as the general anomolous field dependence of the drift velocity[2] seen in the high-field migration of photexcited charge carriers in molecularly doped polymers, have revived interest in the theoretical problem of hopping transport in energetically and spatially disordered systems in the presence of a strong biasing field.[3] An important theoretical tool which has proved useful in understanding hopping transport in disordered systems at *low* fields has been the development of effective-medium theories, which attempt to self-consistently identify an ordered system having the same macroscopic transport properties (i.e., diffusion tensor) as the actual disordered system of interest.[4–6] Traditionally, such approximate theories have been used to obtain important qualitative information about the effects of disorder on the low-field transport properties of condensed phases, and have proved to be surprisingly accurate except in the immediate neighborhood of critical points of the type encountered in percolation problems.

More recently, the techniques of effective-medium theory have been combined with real-space renormalization group ideas to provide an accurate quantitative method for computing the low-field conductivity of a wide class of energetically and spatially disordered materials.[7,8] An important prerequisite to the extension of numerical procedures of this type to the high-field conductivity of disordered systems is a corresponding effective-medium theory for describing hopping conduction in the presence of a strong biasing field. A review of the literature reveals the development of at least three distinct kinds of effective-medium theory for biased systems. Böttger and Bryksin,[9] e.g., have developed a simple effective-medium theory in which it is implicitly assumed that the forward and backward effective-medium rates (as measured with respect to the driving field) are related to one another in the same way as the bare rates. As a result, their effective medium can be characterized by a single parameter, which can be taken to be the drift velocity of the carriers as a function of the biasing field. Stephen,[10] on the other hand, uses a field theoretical analysis to derive an effective-medium theory to study directed percolation, and uses that theory to study the phase diagram of that model. An important feature of effective-medium theories of this type is that they contain more parameters than that of Böttger and Bryksin, allowing the effective medium to describe both the drift velocity of the carriers and the rate at which a localized packet of carriers will spread about its (drifting) mean value. In this respect Stephen's theory is similar to a one-dimensional effective-medium theory of Bernasconi and Schneider,[11] who focused on an interesting class of models related to a problem studied by Sinai.[12] A recent perturbative approach by Izzo *et al.*[13] also has this feature although the specific dependence of effective-medium parameters on the underlying distribution of rates is different in the theory of Izzo *et al.*[13] than that of the previous authors. Interestingly, in an application of their approach to an exactly soluble one-dimensional model studied by Derrida,[14] the effective-medium theory of Izzo *et al.* was shown to qualitatively reproduce the velocity transition appearing in that model, although it was found to incorrectly predict the critical field at which the mean velocity becomes nonzero.[13]

In this paper we derive an effective-medium theory for uniformly biased systems with bond disorder, applicable to lattices of arbitrary dimension. Our approach is of sufficient generality to allow for independent parameters describing the net drift velocity and net diffusion constant for each axis of the effective medium, and allows for the situation in which a biasing field is applied field along an arbitrary direction in space. When the field is applied along one of the crystal axes, our theory allows for three independent parameters: one to describe the drift velocity in the field direction, and two rates to describe the transverse and parallel rates of spreading. Our expressions reduce for a one-dimensional lattice to those of Bernasconi and Schneider.[11] Also, as in the theory of Izzo *et al.*, our approach predicts a velocity transition for the exactly soluble one-dimensional model of Derrida. In contrast to the effective-medium theory of Izzo *et al.*, however, our theory reproduces the exact drift velocity for that model.[13,14] Finally, we discuss the relation of our theory to the simpler one of Böttger and Bryksin, concluding that their theory is, in a certain sense, a non-self-consistent approximation to the theory developed in this paper.

II. MODEL

A particle undergoing a nearest-neighbor random walk on a bond-disordered lattice in the presence of a uniform bias field can be described by a master equation

$$\frac{d\rho_n}{dt} = -\sum_\nu \left[(W_{n-\nu,n} + W_{n+\nu,n})\rho_n - W_{n,n-\nu}\rho_{n-\nu} - W_{n,n+\nu}\rho_{n+\nu}\right], \quad (1)$$

for the probabilities $\rho_n(t)$ of finding the particle at lattice site $n \in Z^d$ at time t. In this equation, the unit vectors ν point along the positive direction of the crystal axes of a d-dimensional cubic lattice, and the hopping rate from site n to its neighbor at $n \pm \nu$ is $W_{n\pm\nu,n}$. These rates are assumed to reflect the intrinsic disorder of the system as well as the uniform bias that shifts the energy of the sites relative to one another. The Laplace transform of this equation takes the form

$$\epsilon R_n(\epsilon) - \rho_n(0) = -\sum_\nu \left[(W_{n-\nu,n} + W_{n+\nu,n})R_n - W_{n,n-\nu}R_{n-\nu} - W_{n,n+\nu}R_{n+\nu}\right], \quad (2)$$

in which $R_n(\epsilon)$ is the Laplace transform at frequency ϵ of the probability $\rho_n(t)$.

After configuration averaging over the disorder, every site in the crystal will be the same, on average, as any other. Thus, as shown explicitly, e.g., by Klafter and Silbey,[15] the averaged probabilities $P_n(\epsilon) = \langle R_n(\epsilon)\rangle$ will obey a set of linear, translationally invariant equations of the form

$$\epsilon R_n(\epsilon) - \rho_n(0) = -\sum_m M_{m-n}(\epsilon) P_n, \quad (3)$$

which reflect the bias on the system. These equations of motion, if they could be obtained exactly, would serve to define the true effective medium associated with the average transport properties of the system. In particular, they would correctly describe the rates with which an initially localized probability distribution will drift and spread, on average, in response to the imposed field. The simplest equations of this form having a sufficient number of parameters to describe both the drift and the spread of the probability distribution is just a translationally invariant form of (2), which retains connections only to nearest neighbors. A correct description of higher moments of the probability distribution would require, presumably, connections to greater-than-nearest neighbors. Thus, in a standard approximation,[5] we will assume in what follows that the configurationally averaged probabilities obey, in the presence of the field, the Laplace-transformed equations of motion

$$\epsilon P_n - p_n(0) = -\sum_\nu \left[(W_\nu^- + W_\nu^+)P_n - W_\nu^+ P_{n-\nu} - W_\nu^- P_{n+\nu}\right] = -\sum_m \Gamma_{n-m} P_m, \quad (4)$$

where $P_n(\epsilon)$ is the Laplace transform at frequency ϵ of the average probability $p_n(t) = \langle \rho_n(t)\rangle$ of finding a particle at lattice vector n at time t; $W_\nu^+(\epsilon)$ and $W_\nu^-(\epsilon)$ are frequency-dependent effective-medium hopping rates associated with forward and backward hops (defined with respect to the corresponding components of the bias field) between nearest neighbors along crystal axis ν, and Γ is the associated transition matrix. The frequency dependence of the rates, in principle, allows a characterization of the time dependence of the transport process. In this analysis we focus on the long time properties of the system, which are described by the zero frequency value of the effective-medium rates $W_\nu^\pm = W_\nu^\pm(0)$. In keeping with this focus, we will in what follows suppress any ϵ dependence which would normally be associated with these quantities.

The important point is that the effective medium of interest is essentially defined by these dynamical equations and is completely characterized by the set of $2d$ parameters $\{W_\nu^\pm\}$. Taking Fourier-Laplace transforms of (4) and solving the resulting equations for a particle initially located at the origin we obtain the probability Green's function at wave vector $k \in Z^d$,

$$G_k = \frac{1}{\epsilon + \Sigma_\nu 2\{\bar{W}_\nu[1-\cos k_\nu] + i\,\delta W_\nu \sin k_\nu\}}, \quad (5)$$

where $\bar{W}_\nu = (W_\nu^+ + W_\nu^-)/2$, and $\delta W_\nu = (W_\nu^+ - W_\nu^-)/2$. It is an arbitrary choice whether we characterize the effective medium in terms of the parameter set $\{W_\nu^+, W_\nu^-\}$ or the equivalent set $\{\bar{W}_\nu, \delta W_\nu\}$. It is convenient to introduce a scaling variable W (which is nonzero but otherwise arbitrary at this point) and write Eq. (5) in the form

$$G_k = \frac{1}{\epsilon + 2W\Sigma_\nu\{\eta_\nu[1-\cos k_\nu] + i\,\delta_\nu \sin k_\nu\}}, \quad (6)$$

which allows us now to characterize the effective medium by the parameter W and by a set of dimensionless effective medium parameters $\eta_\nu = \bar{W}_\nu/W$ and $\delta_\nu = \delta W_\nu/W$. The Laplace-transformed real-space propagators are obtained by Fourier inversion, i.e.,

$$G_n = G_{n,0} = (2\pi)^{-d}\int \frac{e^{ik\cdot n}\,d\Omega_k}{\epsilon + 2W\Sigma_\nu\{\eta_\nu[1-\cos k_\nu] + i\,\delta_\nu \sin k_\nu\}}, \quad (7)$$

where the integration is over all wave vectors k in the first Brillouin zone ($\pi \geq k_\nu > -\pi$) of the cubic lattice, with $d\Omega_k = \Pi_\nu dk_\nu$. The propagator G_n gives the Laplace transform of the probability to find the particle at site n at time t if it was located at the origin of the effective medium at time $t=0$. The general solution to Eq. (4) can be written in terms of these propagators in the form

$$P_n^0(\epsilon) = \sum_m G_{n-m}(\epsilon) p_m(0). \quad (8)$$

It is a straightforward excercise to show for the translationally invariant effective medium that the Cartesian components of the mean drift velocity of a particle are given through the expression

$$v_\nu = \lim_{t\to\infty} \frac{d}{dt} \sum_n n_\nu P_n(t) = 2\,\delta W_\nu = 2\,\delta_\nu W, \tag{9}$$

while the linear spread of the drifting probability distribution about its mean position is determined by the Cartesian components of the diagonal diffusion tensor

$$D_{\nu\nu} = \lim_{t\to\infty} \frac{1}{2} \frac{d}{dt} \left[\sum_n n_\nu^2 P_n(t) - v_\nu^2 t^2 \right] = \bar{W}_\nu = \eta_\nu W. \tag{10}$$

To *self-consistently* determine the parameters W, η_ν, and δ_ν, we now introduce a defect in the translationally invariant effective medium. Specifically, along the bond connecting the sites at l and $l+\nu$, we replace the effective-medium rates $W_\nu^\pm$ along that particular bond with rates $F_\nu^\pm$ drawn *as a pair* from the distribution $\rho_\nu(F^+,F^-)$ of forward and backward rates associated with the actual bonds lying along the νth direction of the crystal in the actual disordered system of interest. The new equations of motion in the presence of this defect can be written in the form

$$\epsilon P_n - p_n(0) = \sum_m \Gamma_{n-m} P_m - (V_\nu^+ P_l - V_\nu^- P_{l+\nu}) \times (\delta_{n,l} - \delta_{n,l+\nu}), \tag{11}$$

in which the transition matrix Γ reproduces the translationally invariant equations of motion (4) associated with the effective medium, and we have introduced the notation

$$V_\nu^\pm = F_\nu^\pm - W_\nu^\pm . \tag{12}$$

The solution to this new equation can be written in the form

$$P_n = P_n^0 - (G_{n-l} - G_{n-l-\nu})(V_\nu^+ P_l - V_\nu^- P_{l+\nu}), \tag{13}$$

where P_n^0 is the solution (8) that would obtain in the absence of the defect for the initial conditions of interest. To solve this, we write the corresponding equations for the two probabilities P_l and $P_{l+\nu}$ which appear bracketed on the right hand side of (13), obtaining two equations in two unknowns. Multiplying the first equation by V_ν^+, the second by V_ν^-, and taking the difference we find after some simplification that the bracketed term itself can be written

$$V_\nu^+ P_l - V_\nu^- P_{l+\nu} = \frac{(V_\nu^+ P_l^0 - V_\nu^- P_{l+\nu}^0)}{1 + V_\nu^+ (G_0 - G_{-\nu}) + V_\nu^- (G_0 - G_\nu)}. \tag{14}$$

We now demand self-consistency by requiring that an average over the defect distribution associated with this one bond reproduce the solutions obtained for the same initial conditions in the fully averaged effective medium defined by Eq. (4). Assuming that the initial conditions [and thus the quantities $P_n^0(\epsilon)$] are independent of the averaging procedure, this requires that $\langle P_n(\epsilon)\rangle = P_n^0(\epsilon)$ for all n. Inspection of Eq. (13) reveals that this can be satisfied only if the average of the quantity,

$$\left\langle \frac{V_\nu^+}{1 + V_\nu^+ (G_0 - G_{-\nu}) + V_\nu^- (G_0 - G_\nu)} \right\rangle P_l^0 - \left\langle \frac{V_\nu^-}{1 + V_\nu^+ (G_0 - G_{-\nu}) + V_\nu^- (G_0 - G_\nu)} \right\rangle P_{l+\nu}^0, \tag{15}$$

appearing in Eq. (14) vanishes. Unlike the situation that occurs in the absence of a bias, Eq. (15) appears to depend upon the initial conditions through the functions $P_l^0(\epsilon)$ and $P_{l+\nu}^0(\epsilon)$. Clearly, in order that the characteristics of the effective medium be independent of these initial conditions we must require that the two averages appearing in this equation vanish independently, and, moreover, that these equations be *simultaneously* satisfied for each of the d crystal axes of the lattice. In this way we end up with $2d$ coupled equations

$$\left\langle \frac{V_\nu^\pm}{1 + V_\nu^+ (G_0 - G_{-\nu}) + V_\nu^- (G_0 - G_\nu)} \right\rangle = 0, \tag{16}$$

to determine the $2d$ parameters defining the effective medium. To make this expression useful we need to obtain and simplify expressions for the quantities

$$(G_0 - G_{\pm\nu}) = \frac{1}{(2\pi)^d} \int \frac{(1 - e^{\pm i k_\nu}) d\Omega_k}{\epsilon + 2W \Sigma_\mu \{ \eta_\mu [1 - \cos k_\mu] + i \delta_\nu \sin k_\mu \}}, \tag{17}$$

which appear in the denominator of (16). Separating this into real and imaginary parts, getting rid of some obviously odd integrals, and taking the zero-frequency limit, we find that $\lim_{\epsilon\to 0}(G_0 - G_{\pm\nu}) = (1/2W)\,[M_1^\nu \mp M_2^\nu]$, where

$$M_1^\nu = \frac{1}{(2\pi)^d} \int \frac{(1 - \cos k_\nu)(\Sigma_\mu \eta_\mu [1 - \cos k_\mu]) d\Omega_k}{(\Sigma_\mu \eta_\mu [1 - \cos k_\mu])^2 + (\Sigma_\mu \delta_\mu \sin k_\mu)^2} \tag{18}$$

and

$$M_2^\nu = \frac{1}{(2\pi)^d} \int \frac{\delta_\nu \sin^2 k_\nu \, d\Omega_k}{(\Sigma_\mu \eta_\mu [1 - \cos k_\mu])^2 + (\Sigma_\mu \delta_\mu \sin k_\mu)^2} \tag{19}$$

depend only upon the dimensionless constants $\{\eta_\nu, \delta_\nu\}$ which define the effective medium. These constants obey the easily proven sum rule

$$\sum_\nu (\eta_\nu M_1^\nu + \delta_\nu M_2^\nu) = 1. \tag{20}$$

Putting this back into the self-consistency condition and reinserting the definition (12) of $V_\nu^\pm$, we obtain

$$\left\langle \frac{F_\nu^\pm - W_\nu^\pm}{2W + [(F_\nu^+ + F_\nu^-) - (W_\nu^- + W_\nu^+)]M_1^\nu + [(F_\nu^+ - F_\nu^-) - (W_\nu^+ - W_\nu^-)]M_2^\nu} \right\rangle = 0. \tag{21}$$

Alternatively, by taking the sum and difference of the equations with positive and negative superscripts these can be put in the form

$$\left\langle \frac{\bar{F}_\nu - \bar{W}_\nu}{W + (\bar{F}_\nu - \bar{W}_\nu)M_1^\nu + (\delta F_\nu - \delta W_\nu)M_2^\nu} \right\rangle = 0,$$

$$\left\langle \frac{\delta F_\nu - \delta W_\nu}{W + (\bar{F}_\nu - \bar{W}_\nu)M_1^\nu + (\delta F_\nu - \delta W_\nu)M_2^\nu} \right\rangle = 0, \tag{22}$$

where $\bar{F}_\nu = (F_\nu^+ + F_\nu^-)/2$ and $\delta F_\nu = (F_\nu^+ - F_\nu^-)/2$ are the ''average sum'' and ''average difference'' of the forward and backward hopping rates across the defect.

III. DISCUSSION

Equations (22) are our main results. They are similar to the equations obtained previously by Izzo *et al.*, except for a difference in denominators.[13] A close comparison shows that our denominator is ''more coupled'' than theirs. Their self-consistent condition, which was explicitly derived for a one-dimensional system would, in our notation, take the form[13]

$$\left\langle \frac{\bar{F} - \bar{W}}{W + (\bar{F} - \bar{W})M_1} \right\rangle = 0 = \left\langle \frac{\delta F - \delta W}{W + (\delta F - \delta W)M_2} \right\rangle. \tag{23}$$

For one-dimensional motion the integrals (18) and (19) can be done exactly by setting $\bar{W} = W$, for which $\eta = 1$. The integral

$$M_1 = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{(1-\cos k)^2 dk}{(1-\cos k)^2 + \delta^2 \sin^2 k} \tag{24}$$

can then be done by setting $z = e^{ik}$ and integrating around the unit circle to obtain $M_1 = (1+\delta)^{-1}$. From the sum rule (20) we also have the identity $M_1 + \delta M_2 = 1$, which leads to the result that

$$M_1 = M_2 = \frac{1}{1+\delta}. \tag{25}$$

Thus, in one dimension the self-consistent conditions (22) can be written

$$\left\langle \frac{\bar{F} - W}{\bar{F} + \delta F} \right\rangle = 0 = \left\langle \frac{\delta F - \delta W}{\bar{F} + \delta F} \right\rangle, \tag{26}$$

from which we deduce that the effective-medium diffusion constant is given by the expression

$$W = \left\langle \frac{\bar{F}}{\bar{F} + \delta F} \right\rangle \left\langle \frac{1}{\bar{F} + \delta F} \right\rangle^{-1} = \frac{1}{2} \left\langle 1 + \frac{F^-}{F^+} \right\rangle \left\langle \frac{1}{F^+} \right\rangle^{-1}, \tag{27}$$

while the drift velocity takes the form

$$v = 2\delta W = \left\langle \frac{2\delta F}{\bar{F} + \delta F} \right\rangle \left\langle \frac{1}{\bar{F} + \delta F} \right\rangle^{-1} = \left\langle 1 - \frac{F^-}{F^+} \right\rangle \left\langle \frac{1}{F^+} \right\rangle^{-1}. \tag{28}$$

These expressions are equivalent to the one-dimensional effective-medium results of Bernasconi and Schneider.[11] The expression for the velocity, moreover, has been shown by Derrida[14] to be the exact result for the one-dimensional random bias problem when $\langle F^-/F^+ \rangle < 1$ and $\langle \ln(F^-/F^+) \rangle < 0$. Thus, the effective-medium theory associated with Eqs. (22) correctly predicts the velocity transition, and indeed gives the exact velocity for the binary random bias model studied by Derrida.

In higher dimensions the integrals (18) and (19) cannot be performed analytically. They are easily computed numerically, however, and so it is a straightforward process to computationally implement the effective-medium theory defined by Eqs. (22) for arbitrary biasing fields. There are certain field directions, however, for which the self-consistent equations are more easily implemented. In what follows we investigate two such directions.

A. Field parallel to a crystal axis

The first case of interest is that in which the driving field is directed along a particular crystal axis, which we will denote by z, for which we will set $\eta_z = \eta$ and $\delta_z = \delta$. The set of effective-medium equations (22) is simplified for two reasons. First, for an isotropic system, all axes transverse to the field will be described by identical self-consistent equations. Second, there will be no macroscopic bias along directions perpendicular to the field axis. Thus, for these axes we can set $\bar{W}_\nu = W_\nu = W_\perp$ and $\delta W_\nu = 0 = \delta_\nu = M_2^\nu$. In addition, the scale factor W can be set to the value $W_\perp$, so that $\eta_\perp = 1$ for all tranverse directions. Thus, the equations for all transverse axes reduce to the same form, namely,

$$\left\langle \frac{\bar{F}_\perp - W}{\bar{F}_\perp + (d_\perp - 1)W} \right\rangle = 0, \tag{29}$$

where the quantity

$$\frac{1}{d_\perp}=M_1^\perp=\frac{1}{(2\pi)^d}\int d\Omega_k\frac{(1-\cos k_\nu)(\eta[1-\cos k_z]+\Sigma_{\mu\neq z}[1-\cos k_\mu])}{(\eta[1-\cos k_z]+\Sigma_{\mu\neq z}[1-\cos k_\mu])^2+\delta^2\sin^2 k_z} \tag{30}$$

defines an ''effective dimensionality'' for any crystal axis ν perpendicular to z. This dimensionality $d_\perp$ reduces to the Euclidean dimension d in the absence of an applied field. From the general sum rule (20) it also is straightforward to obtain for this limiting case the relation

$$(d-1)M_1^\perp+\eta M_1^z+\delta M_2^z=1, \tag{31}$$

which reduces the number of independent integrals in the effective-medium equations to 2.

It is also possible to point out the differences that arise in our effective-medium theory from that developed by Böttger and Bryksin.[9] To make contact with their approach, we consider a system in which the bias field alters the forward and backward rates between two sites by a multiplicative factor $F\rightarrow F^\pm=\gamma_\nu^\pm F$, where F is now a random variable associated with the strength of the specific bond connecting these sites and, e.g., $\gamma_\nu^\pm=\exp[\pm eE_\nu a/2kT]$, where $eE_\nu a$ is the field-induced potential energy drop across a lattice spacing a along axis ν, and kT is the mean thermal energy. Thus, rates associated with hops perpendicular to the field are not affected. In the theory of Böttger and Bryksin it is implicitly assumed that the rates $W^\pm$ which characterize the effective medium also have this multiplicative property, i.e., that $W_\nu\rightarrow W_\nu^\pm=W\gamma_\nu^\pm$, where W is a common (generally field-dependent) prefactor which is independent of the crystal axis. If we make this ansatz in our theory, and assume a field along the z axis as above, then the resulting effective medium will have a drift velocity

$$v_z=W(\gamma^+-\gamma^-),$$

where $\gamma^\pm=\gamma_z^\pm$, and the single parameter W must satisfy the associated self-consistent equations. For the axes transverse to the field these take the form

$$\left\langle\frac{F-W}{F+(d_\perp-1)W}\right\rangle=0, \tag{32}$$

with $d_\perp$ given by Eq. (30) in which $\eta=\frac{1}{2}(\gamma^++\gamma^-)$ and $\delta=\frac{1}{2}(\gamma^+-\gamma^-)$. Note that the ansatz allows for an *a priori* (but non-self-consistent) determination of the integrals, and therefore provides a unique field-dependent value $d_\perp$ which is independent of the single effective-medium parameter W. This allows W to be determined uniquely from Eq. (32). If the value of W obtained from this procedure also satisfies the two self-consistent conditions for motion along the z axis (i.e., parallel to the field direction), then the ansatz is verified and we arrive at a completely self-consistent solution. Unfortunately, analysis shows that, in general, this ansatz provides only an approximate solution to our full self-consistent equations. Indeed, by applying the sum rule (31) appropriate to this configuration it is straightforward to show that the ansatz of Böttger and Bryksin reduces both self-consistent equations (22) for the z axis to the single equation

$$\left\langle\frac{F-W}{F+(d_z-1)W}\right\rangle=0, \tag{33}$$

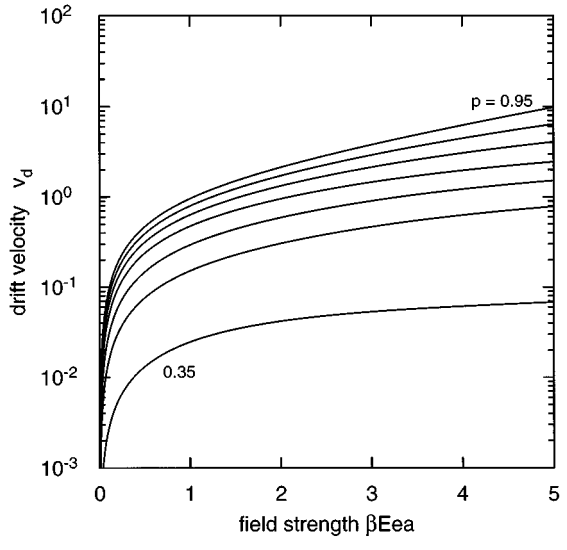

FIG. 1. Reduced drift velocity $v_d=v/F_0a$ for a bond percolating lattice versus the applied electric field, as predicted by the full self-consistent theory presented in this paper. From lower left to upper right, curves presented correspond to values of the unweakened bond fraction $p=0.35$, 0.45, 0.55, 0.65, 0.75, 0.85, and 0.95, respectively.

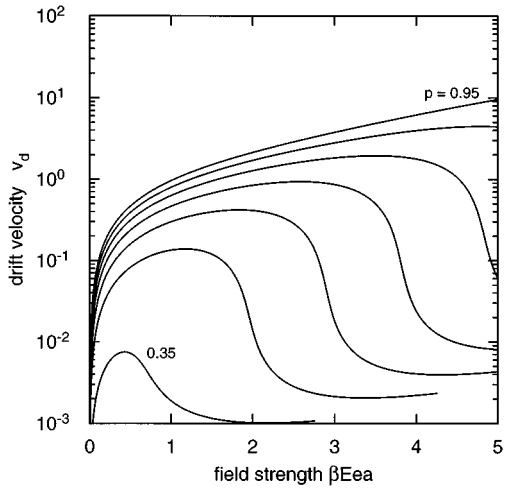

FIG. 2. Reduced drift velocity $v_d=v/F_0a$ for a bond percolating lattice versus the applied electric field, as predicted by the simple effective-medium theory of Böttger and Bryksin. From lower left to upper right, curves presented correspond to values of the unweakened bond fraction $p=0.35$, 0.45, 0.55, 0.65, 0.75, 0.85, and 0.95, respectively.

where $d_z = d_\perp/(d_\perp - d + 1)$. It is not hard to see that simultaneous solutions W to Eqs. (32) and (33) can be expected only if $d_z \to d_\perp$, which requires that $d_\perp \to d$. While this is a valid approximation for very low fields, the effective dimensionality $d_\perp$ and the Euclidean dimensionality d can deviate strongly at high fields. Thus, in a sense, the effective-medium theory of Böttger and Bryksin can be viewed as a low-field approximation to that of the current study.

B. Field along the body diagonal

Another situation in which the self-consistent equations simplify is that in which the applied field is along the "body diagonal" of the unit cell or the (1,1,1) direction of the crystal (we assume isotropy of the underlying lattice). By symmetry, the effective-medium equations for each axis will then have the same form, with $\delta_\nu = \delta$ and $\eta_\nu = \eta$, for all ν. In this limit there are just two independent coupled equations

$$\left\langle \frac{\bar{F} - W}{W + (\bar{F} - W)M_1 + (\delta F - \delta W)M_2} \right\rangle = 0 = \left\langle \frac{\delta F - \delta W}{W + (\bar{F} - W)M_1 + (\delta F - \delta W)M_2} \right\rangle, \tag{34}$$

where we have (without loss of generality) taken $\bar{W} = W$, so that $\eta = 1$. The symmetry of the problem in this limit also implies a simplification in the required integrals:

$$M_1 = \frac{1}{(2\pi)^d} \int d\Omega_k \, \frac{(1 - \cos k_\nu)(\Sigma_\mu [1 - \cos k_\mu])}{(\Sigma_\mu [1 - \cos k_\mu])^2 + \delta^2 (\Sigma_\mu \sin k_\mu)^2},$$

$$M_2 = \frac{1}{(2\pi)^d} \int d\Omega_k \, \frac{\delta \sin^2 k_\nu}{(\Sigma_\mu [1 - \cos k_\mu])^2 + \delta^2 (\Sigma_\mu \sin k_\mu)^2}. \tag{35}$$

The general sum rule (20) leads in this case to the relation

$$M_1 + \delta M_2 = \frac{1}{d}, \tag{36}$$

which allows us to express one of the constants in terms of the other. Thus, for example, we can write $M_1 = (1 - d\,\delta M_2)/d$, which reduces the self-consistency condition (22) to

$$\left\langle \frac{\bar{F} - W}{\bar{F} + (d-1)W + (\delta F - \delta \bar{F}) d M_2} \right\rangle = 0 = \left\langle \frac{\delta F - \delta W}{\bar{F} + (d-1)W + (\delta F - \delta \bar{F}) d M_2} \right\rangle. \tag{37}$$

It is interesting to note that in these circumstances the ansatz of Böttger and Bryksin, i.e.,

$$W_\nu \to W_\nu^\pm = w\,\gamma^\pm = \frac{2\gamma^\pm W}{\gamma^+ + \gamma^-}, \tag{38}$$

when applied to systems for which $F_\nu \to F_\nu^\pm = \gamma^\pm F$ (where the $\gamma_\nu^\pm$ are now independent of ν due to the symmetry of the applied field), does not lead to internal inconsistencies, as it did with the field along one axis. Indeed, in this situation the ansatz reduces both of these last two equations to

$$\left\langle \frac{F - w}{F + (d-1)w} \right\rangle = 0, \tag{39}$$

the solution to which is just the zero-field effective-medium rate associated with the distribution $\rho(F)$ of bond strengths associated with this type of system.

IV. APPLICATION

To demonstrate the use (and abuse) of the approach that we have developed, we consider the biased percolation problem featured in the analysis of Böttger and Bryksin,[9] in which a region of field strengths and bond concentrations was found for which a negative differential drift velocity (NDDV) was predicted, i.e., a region for which the drift velocity decreases with increasing field strength. Thus, in keeping with the analysis of Ref. 9 we consider a three-dimensional bond percolating lattice with a field directed along the z axis. Hopping rates for this system are of the form $F_\nu^\pm = \gamma_\nu^\pm F$, in which $\gamma_z^\pm = \exp[\pm eEa/2kT]$ for $\nu = z$, and $\gamma_\nu^\pm = 1$ for all other axes. The bond strengths F are then drawn from the percolative binary distribution

$$\rho(F) = p\,\delta(F - F_0) + (1 - p)\,\delta(F - \xi F_0), \tag{40}$$

where ξ is a reduction factor associated with weak links in the system. In Fig. 1 we show the results of an implementation of the full set of self-consistent effective-medium equations for this problem with a reduction factor $\xi = 10^{-4}$. In this plot appear predicted values of the drift velocity as a function of field strength, for several different concentrations p of unweakened bonds. In Fig. 2 we show corresponding plots of the drift velocity as predicted by the earlier theory of Böttger and Bryksin,[9] which in our implementation corresponds to the solution of Eq. (33) (which, as we have pointed out, does not give an internally self-consistent solution to the full set of effective-medium equations). For large concentrations of weak bonds the differences are striking, with the simpler theory of Böttger and Bryksin showing a distinct

region of NDDV at high fields which is lacking in the fully self-consistent theory of this paper. Recent simulations by Gartstein and Conwell[3] have revealed that such a region of NDDV does, in fact, appear for this model, although the quantitative agreement of the simulation data with the Böttger-Bryksin theory was shown to be rather poor.

Nonetheless, this raises the question of how the apparently less self-consistent theory of Böttger and Bryksin[9] is able to qualitatively predict the general tendency observed in simulations, while the more fully self-consistent theory developed in this paper is not. Notwithstanding the adage that ''nothing succeeds like success'' we suggest that the apparent qualitative agreement of the Böttger-Bryksin theory is, to a certain extent, fortuitous, a judgement which we base on the following argument. The analysis of Gartstein and Conwell[3] convincingly shows that the negative differential drift velocity observed in the percolation problem can be identified as arising from ''field-induced traps.'' The latter are regions a particle can, at high fields, enter, but from which it cannot escape except by making a difficult hop against the field. The minimum ''defect'' which can be expected to act as a trap in this sense is, therefore, not a single bond, but a single strong bond leading along the field into a site out of which the only other bonds are weak. Viewed in this light it is rather hard to see how *any* effective-medium theory based upon the idea of embedding a single bond defect in an otherwise uniform system can be sensitive to the underlying physics associated with field-induced traps. Thus, in our view it is unreasonable to expect an effective-medium theory constructed at the bond level to reproduce the high-field properties of this particular model. We agree with the opinion expressed in Ref. 3 that high electric fields require a proper treatment of fluctuations at more extended length scales.

V. SUMMARY

We have presented a simple derivation of a general effective-medium theory suitable for studying problems involving hopping conduction on bond disordered d-dimensional lattices in the presence of biasing fields. The theory recovers exact results for the drift velocity of one-dimensional random bias models studied earlier, but fails to show the negative differential drift velocity associated with the bond percolation model due, we suggest, to the limited size of the defect used in the analysis. It seems reasonable to speculate that an effective-medium theory which incorporates an embedded defect of sufficiently large size, drawn at random from the disordered system of interest, would be sensitive to the fluctuations that are responsible for this kind of anomolous disorder-induced behavior. In a future publication we show how a combination of real-space renormalization group ideas and the basic effective-medium theory presented in this paper can be used to quantitatively reproduce the features observed in numerical simulations for the bond and site percolation model.[8]

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*Permanent address: East Central College, Union, Missouri.

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