

Generalized model for dynamic percolation

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We study the dynamics of a carrier, which performs a biased motion under the influence of an external field \vec{E} , in an environment which is modeled by dynamic percolation and created by hard-core particles. The particles move randomly on a simple cubic lattice, constrained by hard-core exclusion, and they spontaneously annihilate and reappear at some prescribed rates. We determine the density profiles of the “environment” particles, as seen from the stationary moving carrier, and calculate its terminal velocity V_c as the function of the applied field and other system parameters. For sufficiently small driving forces the force exerted on the carrier by the “environment” particles shows a viscouslike behavior. An analog Stokes formula for such dynamic percolative environments and the corresponding friction coefficient are derived. We show that the density profile of the environment particles is strongly inhomogeneous: In front of the stationary moving carrier the density is higher than the average density ρ_s , while past the carrier the local density is lower than ρ_s .

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I. INTRODUCTION

The percolation concept has turned out to be very useful for understanding transport and conduction processes in a wide range of disordered media, as exemplified by ionic conduction in polymeric, amorphous, or glassy ceramic electrolytes, diffusion in biological tissues, and permeability of disordered membranes [1–3].

Most of the situations discussed in Refs. [1–3] pertain, however, to systems with “frozen” disorder; that is, the random environment in which a given transport process takes place does not change in time. This is certainly the case in many instances, but it is not true in general. As a matter of fact, there are many experimental systems in which the static percolation picture does not apply, since the structure of the host material undergoes essential structural reorganizations on a time scale comparable to that at which the transport itself occurs. A few stray examples of such systems include certain biomembranes [4], solid protonic conductors [5], oil-continuous microemulsions [6–9], and polymer electrolytes [10–12].

More specifically, ionic transport across a biomembrane, such as, e.g. gramicidin-A, occurs by the motion of ions through molecular channels along which they encounter potential barriers that fluctuate in time. The fluctuations of potential barriers may significantly hinder the transport, and constitute an important transport-controlling factor [4]. In the case of protonic conduction by the Grotthuss mechanism [5], site-to-site motion of carriers occurs only between those neighboring H_2O or NH_3 groups that have a favorable relative orientation; thermally activated rotation of these groups is the structural host-reorganization process interacting with the carrier motion. Similarly, within oil-continuous microemulsions, the charge transport proceeds by charge being transferred from one water globule to another, as globules approach each other in their Brownian motion [6–9]. Finally, in polymer electrolytes, such as, e.g., polyethylene oxide

complexed nonstoichiometrically with the ionic salt NaSCN, the Na^+ ions are largely tetrahedrally coordinated by polyether oxygens, but at the same time that Na^+ ions hop from one fourfold coordination site to another, the oxygens themselves, along with the polymeric backbone, undergo large-amplitude wagging and even diffusive motion [10–12].

Clearly, all the above mentioned examples involve two characteristic time scales; one which describes the typical time τ between two successive hops of the carrier, and another associated with a typical renewal time τ^* of the environment itself; the latter is the time needed for the host medium to reorganize itself and thereby provide a new set of available pathways for transport. Consequently, the static percolation picture applies only when the characteristic time τ^* becomes infinitely large. For a finite τ^* dynamic percolation has to be considered, and one encounters quite a different behavior when compared to the random environments with quenched disorder. As a result, one observes an Ohmic-type or Stokes-type linear velocity-force relation for the carrier’s terminal velocities as a function of the applied field, in contrast to the threshold behavior predicted by the static percolation theory. However, the prefactor in the linear velocity-force relation may depend in a nontrivial way on the system’s parameters, and this dependence constitutes the main challenge for the theoretical analysis here. On the other hand, we note that in the above mentioned examples of the dynamic percolative environments quite different physical processes are responsible for the time evolution of the host medium. Consequently, one expects that the prefactor in the Stokes-type velocity-force relation should also be dependent on the precise mechanism which underlies the temporal reorganization of the environment.

Theoretical modeling of dynamic percolative environments has followed several avenues, which differ mostly in how the time evolution of the disorder is constrained. Is it constrained (a) by conservation laws or (b) by spatial and temporal correlations in the renewal events? Early models of

dynamic percolation [13,14] described the random environment within the framework of a standard bond-percolation model, in which the strength of each bond fluctuates in time between zero and a finite value. The dynamics of the host medium in these models [13,14] was accounted for by a series of instantaneous renewal events. These events were assumed to occur at random times, chosen from a renewal time distribution. In the renewal process the positions of all unblocked bonds are reassigned, such that after each renewal event a carrier “sees” a newly defined network. This approach is thus characterized by a *global dynamical disorder* without global conservation laws and correlations, since the entire set of random hopping rates is simultaneously renewed independently of the previous history. Another model characterized by a *local dynamical disorder* was proposed in Refs. [15] and [16], and subsequently generalized to the non-Markovian case in Ref. [17]. This model appears to be similar to the previous one, except that here the hopping rates at different sites fluctuate *independently* of each other. That is, individual bonds, rather than the whole lattice change in the renewal events. To describe the dynamical behavior in the *local dynamical disorder* case, a dynamical mean-field theory was proposed [15,16], based on the effective medium approximation introduced for the analysis of random walks on lattices with static disorder [18], and generalized to include the possibility of multistate transformations of the *dynamically* random medium [19]. More recently, several exactly solvable one-dimensional models with *global* and *local* dynamical disorder were discussed [20].

In the second approach, which emerged within the context of the ionic conductivity in superionic solids, the dynamical percolative environment was considered as a multicomponent mixture of mobile species in which one or several neutral components block the carrier component [21]. In particular, such a situation can be observed in a superionic conductor β'' alumina, doped with two different ionic species (e.g., Na^+ and Ba^{2+}), where small Na^+ ions are rather mobile, while the larger Ba^{2+} ions move essentially slower and temporarily block the Na^+ ions. Contrary to the previous line of thought, the dynamics of such a percolative environment has essential correlations, generated by hard-core exclusion interactions between the species involved; moreover, it obeys the conservation law—the total number of the particles involved is conserved. In Ref. [21], the frequency-dependent ionic conductivity of the light species was analyzed combining a continuous time random walk approach for the dynamical problem with an effective medium approximation describing the frozen environment of slow species. Next, as an explanation of the sharp increase of electrical conductivity transition in water-in-oil microemulsions when the volume fraction of water is increased toward a certain threshold value, in Refs. [7] and [8] it was proposed that the charge carriers are not trapped in the finite water clusters, but rather a charge on a water globule can propagate by either hopping to a neighboring globule, when they approach each other, or via the diffusion of the host globule itself. This picture was interpreted in terms of a model similar to that employed in Ref. [21], with the only difference being that here the “blockers” of Ref. [21] play the role of the transient charge carriers. In the model of Refs. [7] and [8], in which the host dynamics is influenced by spatial cor-

relations and conservation of the number of the water globules involved, the conductivity depends, hence, on the rate of cluster rearrangement. Finally, a similar problem of carrier diffusion in an environment created by mobile hard-core lattice-gas particles was analyzed in Ref. [22] by using the developed dynamic bond percolation theory of Refs. [13] and [14].

In this paper we propose a generalized model of dynamic percolation which shares common features with bond-fluctuating models of Refs. [13–17,19,20] as well as models involving mobile blockers of Refs. [21,22]. The system we consider consists of a host lattice, which here is a regular cubic lattice whose sites support at most a single occupancy, hard-core “environment” particles, and a single hard-core carrier particle. The environment particles move on the lattice by performing a random hopping between the neighboring lattice sites, which is constrained by the hard-core interactions, and may disappear from and reappear (renewal processes) on the empty sites of the lattice with some prescribed rates.¹ In turn, the carrier particle is always present on the lattice, i.e., it cannot disappear spontaneously, and is subject to a constant external force \vec{E} . Hence the carrier performs a biased random walk, which is constrained by the hard-core interactions with the environment particles, and probes the response of the percolative environment to the internal perturbation or, in other words, the frictional properties of such a dynamical environment.

An important aspect of our model, which makes it different from the previously proposed models of dynamic percolation, is that we include the hard-core interaction between environment particles and the carrier molecule, such that the latter may influence the dynamics of the environment. This results, as we proceed to show, in the emergence of complicated density profiles of the environment particles around the carrier. These profiles, as well as the terminal velocity V_c of the carrier, are determined here explicitly, in terms of an approximate approach of Ref. [23], which is based on the decoupling of the carrier-particle-particle correlation functions into the product of pairwise correlations. We show that the environment particles tend to accumulate in front of the driven carrier, creating a sort of “traffic jam,” which impedes its motion. Thus the density profiles around the carrier are highly asymmetric: the local density of the environment particles in front of the carrier is higher than the average, and approaches the average value as an exponential function of the distance from the carrier. The characteristic length and amplitude of the density relaxation function are calculated explicitly. On the other hand, past the carrier the local density is lower than the average: We show that, depending on whether the number of particles in the percolative environ-

¹We hasten to remark that diffusive processes, of course, also result in a certain renewal of the environment; however, diffusive processes, as compared to the spontaneous creation and annihilation of particles, have completely different underlying physics and influence the evolution of the system in a completely different fashion, as we proceed to show. Following the terminology of Refs. [13–17,19,20], we thus choose here to distinguish between diffusive and creation-annihilation processes, referring to the latter as the renewal processes.

ment is explicitly conserved or not, the local density past the carrier may tend to the average value either as an exponential or even as an *algebraic* function of the distance, revealing in the latter case especially strong memory effects and strong correlations between the particle distribution in the environment and the carrier position. Further on, we find that the terminal velocity of the carrier particle depends explicitly on the excess density in the “jammed” region in front of the carrier, as well as on the environment particle density past the carrier. Both, in turn, are dependent on the magnitude of the velocity, as well as on the rate of the renewal processes and the rate at which the environment particles can diffuse away from the carrier. The interplay between the jamming effect of the environment, produced by the carrier particle, and the rate of its homogenization due to diffusive smoothing and renewal processes, manifests itself as a medium-induced frictional force exerted on the carrier, whose magnitude depends on the carrier velocity. As a consequence of such a nonlinear coupling, in the general case, (i.e., for arbitrary rates of the renewal and diffusive processes), V_c can be found only implicitly, as the solution of a nonlinear equation relating V_c to the system parameters. This equation simplifies considerably in the limit of small applied external fields \vec{E} , and we find that the force-velocity relation to the field becomes linear. This implies that the frictional force exerted on the carrier particle by the environment is *viscous*. This linear force-velocity relation can be therefore interpreted as the analog of the Stokes formula for the dynamic percolative environment under study; in this case, the carrier velocity is calculated explicitly as well as the corresponding friction coefficient. In turn, this enables us to estimate the self-diffusion coefficient of the carrier in the absence of an external field; we show that when only a diffusive rearrangement of the percolative environment is allowed, while the renewal processes are suppressed, the general expression for the diffusion coefficient reduces to the one obtained previously in Refs. [24] and [25]. We note that the result of Refs. [24] and [25] is known to serve as a very good approximation for the self-diffusion coefficient in hard-core lattice gases [26].

We finally remark that a qualitatively similar physical effect was predicted recently for a different model system involving a charged particle moving at a constant speed a small distance above the surface of an incompressible, infinitely deep liquid. It was shown in Refs. [27,28] that the interactions between the moving particle and the fluid molecules induce an effective frictional force exerted on the particle, producing a local distortion of the liquid interface, a bump, which travels together with the particle and effectively increases its mass. The mass of the bump, which is analogous to the jammed region appearing in our model, itself depends on the particle’s velocity, resulting in a nonlinear coupling between the medium-induced frictional force exerted on the particle and its velocity [27,28].

The paper is structured as follows: In Sec. II we formulate the model and introduce basic notations. In Sec. III we write down the dynamical equations which govern the time evolution of the environment particles and of the carrier. Section IV is devoted to an analytical solution of these evolution equations in the limit $t \rightarrow \infty$; here we also present some general results on the shape of the density profiles around a stationary moving carrier, and on the carrier terminal velocity,

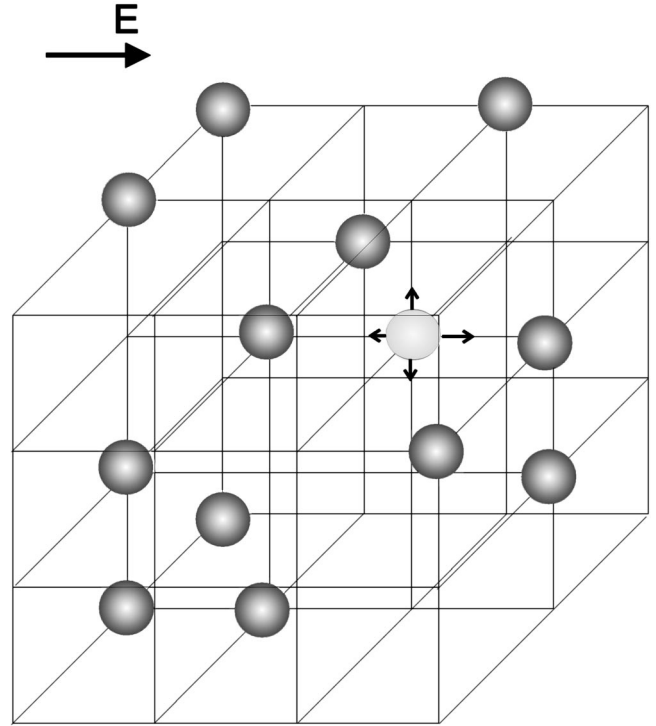


FIG. 1. A generalized model of dynamic percolation. Grey spheres denote the hard-core “environment” particles, which perform symmetric random hopping among the sites of a simple cubic lattice, and can be spontaneously annihilated and created. The lighter sphere is the carrier, which performs a biased random walk due to an external field \vec{E} , constrained by hard-core exclusion with the environment particles.

ity, which is given implicitly as the solution of a transcendental equation defining the general force-velocity relation for the dynamic percolative environment under study. In Sec. V we derive explicit asymptotic results for the carrier terminal velocity in the limit of small applied external fields \vec{E} and obtain the analog of the Stokes formula for such a percolative environment; here we also present explicit results for the friction coefficient of the host medium and for the self-diffusion coefficient of the carrier in the absence of an external field. The asymptotic behavior of the density profiles of the environment particles around the carrier is discussed in Sec. VI. Finally, we conclude in Sec. VII with a brief summary and discussion of our results.

II. MODEL

The model for dynamic percolation we study here consists of a three-dimensional simple cubic lattice of spacing σ , the sites of which are partially occupied by identical hard-core environment particles and a single, hard-core, carrier particle (see Fig. 1). For both types of particles the hard-core interactions prevent multiple occupancy of the lattice sites; that is, no two environment particles or a “carrier” particle and an environment particle can simultaneously occupy the same site, and particles cannot pass through each other.

The occupation of the lattice sites by the environment particles is characterized by the time-dependent occupation variable $\eta(\vec{r}, t)$, \vec{r} being the lattice vector of the site in ques-

tion. This variable assumes two values:

$$\eta(\vec{r}) = \begin{cases} 1 & \text{if the site } \vec{r} \text{ is occupied} \\ 0 & \text{if the site } \vec{r} \text{ is empty.} \end{cases} \quad (1)$$

Next we assume the following dynamics of the environment particles: The particles can spontaneously disappear from the lattice, and may reappear at random positions and random time moments, which is reminiscent of the host medium dynamics stipulated in Refs. [13–17,19,20]. We refer to these two processes generally as renewal processes. In addition, the environment particles move randomly within the lattice by performing nearest-neighbor random walks constrained by the hard-core interactions, which is the main feature of the approach in Refs. [21,22]. We stipulate that any of the environment particles waits a time $\delta\tau$, which has an exponential probability distribution with a mean τ^* , and then chooses from a few possibilities: (a) disappearing from the lattice at rate g , which is realized instantaneously, or (b) attempting to hop, at a rate $l/6$, onto one of six neighboring sites. The hop is actually fulfilled if the target site is not occupied at this time moment by any other particle; otherwise, the particle attempting to hop remains at its initial position, and (c) particles may reappear on any *vacant* lattice site with rate f .

Note that the number of particles is not explicitly conserved in such a dynamical model of the environment, which occurs because of the presence of the renewal processes; the particles diffusion, conversely, conserves the particles number. However, in the absence of attractive particle-particle interactions and external perturbances, the particle distribution on the lattice is uniform, and the average occupation $\overline{\rho(t) = \overline{\eta(\vec{r})}}$ of the lattice tends, as $t \rightarrow \infty$, to a constant value, $\rho_s = f/(f+g)$. This relation can be thought of as the Langmuir adsorption isotherm [29].

Hence the limit $\tau_{dif} \rightarrow \infty$ (or, $l \rightarrow 0$) corresponds to the ordinary site percolation model with immobile blocked sites. The limit $f, g \rightarrow 0$, ($\tau_{cr}, \tau_{an} \rightarrow \infty$), while keeping the ratio f/g fixed, $f/g = \rho_s/(1-\rho_s)$, corresponds to a typical hard-core lattice gas with the number of particles conserved.

At time $t=0$ we introduce at the origin of the lattice an extra particle, the carrier, whose role is to probe the response of the environment modeled by dynamic percolation to an external perturbation. We stipulate that only the carrier out of all participating particles cannot disappear from the system, and, moreover, that its motion is biased by some external constant force. As a physical realization, we envisage that the carrier is charged, while all other particles are neutral, and the system is exposed to constant external electric field \vec{E} . The dynamics of the carrier particle is defined as follows: We suppose that the waiting time between successive jumps of the carrier also has an exponential distribution with a mean value τ , which may in general be different from the corresponding waiting time of the environment particles. Attempting to hop, the carrier first chooses a hop direction with probabilities

$$p_\mu = \exp\left[\frac{\beta}{2}(\vec{E} \cdot \vec{e}_\mu)\right] / \sum_\nu \exp\left[\frac{\beta}{2}(\vec{E} \cdot \vec{e}_\nu)\right], \quad (2)$$

where β is the reciprocal temperature, \vec{e}_ν (or \vec{e}_μ) stand for six unit lattice vectors; $\nu, \mu = \{\pm 1, \pm 2, \pm 3\}$, connecting the carrier position with six neighboring lattice sites; and $(\vec{E} \cdot \vec{e}_\nu)$ denotes the scalar product. We adopt the convention that ± 1 corresponds to $\pm X$, ± 2 corresponds to $\pm Y$, and ± 3 corresponds to $\pm Z$. The jump is actually fulfilled when the target lattice site is vacant. Otherwise, as mentioned above, the carrier remains at its position. For simplicity we assume in what follows that the external field is oriented along the X axis in the positive direction, such that $\vec{E} = (E, 0, 0)$. Note also that for the choice of the transition probabilities as in Eq. (2), the detailed balance is naturally preserved.

III. EVOLUTION EQUATIONS

Let $P(\vec{R}_c, \eta; t)$ denote the joint probability that at a moment t the carrier occupies position \vec{R}_c and all environment particles are in configuration $\eta \equiv \{\eta(\vec{r})\}$. Next, let $\eta^{\nu, \mu}$ denote particle configurations obtained from η by exchanging the occupation variables of the sites \vec{r} and $\vec{r} + \vec{e}_\mu$, i.e. $\eta(\vec{r}) \leftrightarrow \eta(\vec{r} + \vec{e}_\mu)$, and $\hat{\eta}^{\vec{r}}$ be the configuration obtained from η by changing the occupation of the site \vec{r} as $\eta(\vec{r}) \leftrightarrow 1 - \eta(\vec{r})$. Clearly, the first type of process appears due to random hops of the environment particles, while the second one stems from the renewal processes, i.e. random creation and annihilation of the environment particles. Then, summing up all possible events which can result in the configuration (\vec{R}_c, η) or change this configuration for any other, we find that the temporal evolution of the system under study is governed by the following master equation:

$$\begin{aligned} \partial_t P(\vec{R}_c, \eta; t) = & \frac{l}{6\tau^*} \sum_\mu \sum_{\vec{r} \neq \vec{R}_c - \vec{e}_\mu, \vec{R}_c} \{P(\vec{R}_c, \eta^{\vec{r}, \mu}; t) \\ & - P(\vec{R}_c, \eta; t)\} + \frac{1}{\tau} \sum_\mu p_\mu \{(1 - \eta(\vec{R}_c)) \\ & \times P(\vec{R}_c - \vec{e}_\mu, \eta; t) - (1 - \eta(\vec{R}_c + \vec{e}_\mu)) \\ & \times P(\vec{R}_c, \eta; t)\} + \frac{g}{\tau^*} \sum_{\vec{r} \neq \vec{R}_c} \{(1 - \eta(\vec{r})) \\ & \times P(\vec{R}_c, \hat{\eta}^{\vec{r}}; t) - \eta(\vec{r})P(\vec{R}_c, \eta; t)\} \\ & + \frac{f}{\tau^*} \sum_{\vec{r} \neq \vec{R}_c} \{\eta(\vec{r})P(\vec{R}_c, \hat{\eta}^{\vec{r}}; t) \\ & - (1 - \eta(\vec{r}))P(\vec{R}_c, \eta; t)\}. \end{aligned} \quad (3)$$

Note that the terms in the first (second) line of Eq. (3) describe random hopping motion of the environment particles (biased motion of the carrier) in terms of the Kawasaki-type particle-vacancy exchanges, while the terms in the third and fourth lines account for the Glauber-type decay and creation of the environment particles.

A. Mean velocity of the carrier and correlation functions

From Eq. (3) we can readily compute the velocity of the carrier. Multiplying both sides of Eq. (3) by $(\vec{R}_c \cdot \vec{e}_1)$, and summing over all possible configurations (\vec{R}_c, η) , we find that the carrier's mean velocity $V_c(t)$, defined as

$$V_c(t) \equiv \frac{d}{dt} \overline{(\vec{R}_c \cdot \vec{e}_1)}, \quad (4)$$

obeys

$$V_c(t) = \frac{\sigma}{\tau} \{p_1(1 - k(\vec{e}_1; t)) - p_{-1}(1 - k(\vec{e}_{-1}; t))\}, \quad (5)$$

where $k(\vec{\lambda}; t)$ stands for the carrier-environment particle pair correlation function

$$k(\vec{\lambda}; t) \equiv \sum_{\vec{R}_c, \eta} \eta(\vec{R}_c + \vec{\lambda}) P(\vec{R}_c, \eta; t). \quad (6)$$

In other words, $k(\vec{\lambda}; t)$ can be thought of as the density distribution of the environment particles, as seen from a carrier which moves with velocity $V_c(t)$.

Hence $V_c(t)$ depends explicitly on the local density of the environment particles in the immediate vicinity of the carrier. Note that if the environment is perfectly homogeneous, i.e., if for any $\vec{\lambda}$ the density profile is constant, $k(\vec{\lambda}; t) = \rho_s$, which immediately implies a decoupling between $\eta(\vec{R}_c + \vec{\lambda})$ and $P(\vec{R}_c, \eta; t)$ in Eq. (6), then from Eq. (5) we obtain a trivial mean-field-type result

$$V_c^{(0)} = (p_1 - p_{-1})(1 - \rho_s) \frac{\sigma}{\tau}, \quad (7)$$

which states that the frequency of jumps of the carrier particles (τ^{-1}) is renormalized only by a factor $1 - \rho_s$, which gives the fraction of successful jumps.

The salient feature of our model is that there are essential backflow effects. The carrier effectively perturbs the spatial distribution of the environment particles, so that stationary density profiles emerge. This can be contrasted with the earlier dynamic percolation models [13–17, 19–22] in which the carrier had no impact on the embedding medium, and hence there was no rearrangement of the host medium around the carrier particle. As a consequence $k(\vec{\lambda}; t) \neq \rho_s$, and $k(\vec{\lambda}; t)$ approaches ρ_s only at infinite separations from the carrier, i.e., when $|\vec{\lambda}| \rightarrow \infty$. Therefore, we rewrite Eq. (5) in the form

$$V_c(t) = V_c^{(0)} - \frac{\sigma}{\tau} \{p_1(k(\vec{e}_1; t) - \rho_s) - p_{-1}(\rho_s - k(\vec{e}_{-1}; t))\}, \quad (8)$$

which explicitly shows the deviation of the mean velocity of the carrier from the mean-field-type result in Eq. (7) due to the formation of the density profiles.

B. Evolution equations of the pair correlation functions

From Eq. (5) it follows that in order to obtain $V_c(t)$, it suffices to compute $k(\vec{e}_{\pm 1}; t)$. Consequently, we have to

evaluate the equation governing the time evolution of the pair correlation functions. Multiplying both sides of Eq. (3) by $\eta(\vec{R}_c)$ and summing over all configurations (\vec{R}_c, η) , we find that $k(\vec{\lambda}; t)$ obeys

$$\begin{aligned} \partial_t k(\vec{\lambda}; t) = & \frac{l}{6\tau^*} \sum_{\mu} (\nabla_{\mu} - \delta_{\vec{\lambda}, \vec{e}_{\mu}} \nabla_{-\mu}) k(\vec{\lambda}; t) - \frac{(f+g)}{\tau^*} k(\vec{\lambda}; t) \\ & + \frac{f}{\tau^*} + \frac{1}{\tau} \sum_{\mu} \sum_{\vec{R}_c, \eta} p_{\mu} (1 - \eta(\vec{R}_c + \vec{e}_{\mu})) \\ & \times \nabla_{\mu} \eta(\vec{R}_c + \vec{\lambda}) P(\vec{R}_c, \eta; t), \end{aligned} \quad (9)$$

where ∇_{μ} denotes an ascending finite difference operator of the form

$$\nabla_{\mu} f(\vec{\lambda}) \equiv f(\vec{\lambda} + \vec{e}_{\mu}) - f(\vec{\lambda}), \quad (10)$$

and

$$\delta_{\vec{r}, \vec{r}'} = \begin{cases} 1, & \text{if the site } \vec{r} = \vec{r}' \\ 0, & \text{otherwise.} \end{cases} \quad (11)$$

The Kronecker δ term $\delta_{\vec{\lambda}, \vec{e}_{\mu}}$ signifies that the evolution of the pair correlations, Eq. (9), proceeds differently at large separations and at the immediate vicinity of the carrier. This stems from the asymmetric hopping rules of the carrier particle defined by Eq. (2).

Note next that the contribution in the second line in Eq. (9), which is associated with the biased diffusion of the carrier, appears to be nonlinear with respect to the occupation numbers, such that the pair correlation function is effectively coupled to the evolution of the third-order correlations of the form

$$T(\vec{\lambda}, \vec{e}_{\nu}; t) \equiv \sum_{\vec{R}_c, \eta} \eta(\vec{R}_c + \vec{\lambda}) \eta(\vec{R}_c + \vec{e}_{\nu}) P(\vec{R}_c, \eta; t). \quad (12)$$

That is, Eq. (9) is not closed with respect to the pair correlations but rather represents a first equation in the infinite hierarchy of coupled equations for higher-order correlation functions. One faces, therefore, the problem of solving an infinite hierarchy of coupled differential equations, and needs to resort to an approximate closure scheme.

C. Decoupling approximation

Here we resort to the simplest nontrivial closure approximation, based on the decoupling of the third-order correlation functions into the product of pair correlations. More precisely, we assume that for $\vec{\lambda} \neq \vec{e}_{\nu}$, the third-order correlation fulfills

$$\begin{aligned} & \sum_{\vec{R}_c, \eta} \eta(\vec{R}_c + \vec{\lambda}) \eta(\vec{R}_c + \vec{e}_\nu) P(\vec{R}_c, \eta; t) \\ & \approx \left(\sum_{\vec{R}_c, \eta} \eta(\vec{R}_c + \vec{\lambda}) P(\vec{R}_c, \eta; t) \right) \\ & \quad \times \left(\sum_{\vec{R}_c, \eta} \eta(\vec{R}_c + \vec{e}_\nu) P(\vec{R}_c, \eta; t) \right), \end{aligned} \quad (13)$$

or, in other words,

$$\sum_{\vec{R}_c, \eta} \eta(\vec{R}_c + \vec{\lambda}) \eta(\vec{R}_c + \vec{e}_\nu) P(\vec{R}_c, \eta; t) \approx k(\vec{\lambda}; t) k(\vec{e}_\nu; t). \quad (14)$$

The approximate closure in Eq. (14) was already employed for studying related models of biased carrier diffusion in hard-core lattice gases, and was shown to provide quite an accurate description of both dynamical and stationary-state behaviors. The decoupling in Eq. (14) was first introduced in Ref. [23] to determine the properties of a driven carrier diffusion in a one-dimensional hard-core lattice gas with a conserved number of particles, i.e., without an exchange of particles with the reservoir. Extensive numerical simulations performed in Ref. [23] demonstrated that such a decoupling is quite a plausible approximation for the model under study. Moreover, a rigorous probabilistic analysis of Ref. [30] showed that for this model the results based on the decoupling scheme in Eq. (14) are exact. Furthermore, the same closure procedure was recently applied to study spreading of a hard-core lattice gas from a reservoir attached to one of the lattice sites [31]. Again, a very good agreement between the analytical results and the numerical data was found. Next, the decoupling in Eq. (14) was used in a recent analysis of a biased carrier dynamics in a one-dimensional model of an adsorbed monolayer in contact with a vapor phase [32], i.e., a one-dimensional version of the model to be studied here. Also in this case, excellent agreement was observed between the analytical predictions and the Monte Carlo simulations data [32]. We now show that the approximate closure of the hierarchy of the evolution equations in Eq. (14) allows us to reproduce, in the limit $f, g = 0$ and $f/g = \text{const}$, the results of Refs. [24] and [25], which are known (see, e.g., Ref. [26]) to provide a very good approximation for the carrier diffusion coefficient in three-dimensional hard-core lattice gases with an arbitrary particle density. We therefore expect that such a closure scheme will render a plausible description of the carrier dynamics in a three-dimensional generalized dynamic percolation model. We base our further analysis on this approximation.

Making use of Eq. (14), we find from Eq. (9) that the pair correlations obey the equation

$$\partial_t k(\vec{\lambda}; t) = \frac{l}{6\tau^*} \tilde{L} k(\vec{\lambda}; t) + \frac{f}{\tau^*}, \quad (15)$$

which holds for all lattice sites except for those at the immediate vicinity of the carrier, i.e., for all $\vec{\lambda}$ except for $\vec{\lambda} = \{\mathbf{0}, \vec{e}_{\pm 1}, \vec{e}_{\pm 2}, \vec{e}_{\pm 3}\}$, while at the sites adjacent to the carrier one has

$$\partial_t k(\vec{e}_\nu; t) = \frac{l}{6\tau^*} (\tilde{L} + A_\nu(t)) k(\vec{e}_\nu; t) + \frac{f}{\tau^*}, \quad (16)$$

where $\nu = \{\pm 1, \pm 2, \pm 3\}$. The operators \tilde{L} and coefficients $A_\nu(t)$ are given explicitly by

$$\tilde{L} \equiv \sum_{\mu} A_\mu(t) \nabla_\mu - \frac{6(f+g)}{l} \quad (17)$$

and

$$A_\mu(t) \equiv 1 + \frac{6\tau^*}{l\tau} p_\mu (1 - k(\vec{e}_\mu; t)), \quad (18)$$

where ∇_μ has been defined previously in Eq. (10): $\mu = \{\pm 1, \pm 2, \pm 3\}$. It is important to emphasize that all coefficients $A_\mu(t) = A_\mu(E, V_c; t)$, i.e., are functions of both the applied field and the carrier velocity.

Now several comments about Eqs. (15) and (16) are in order. First of all, let us note that Eq. (16) represents, from a mathematical point of view, the boundary conditions for the general evolution equation (15), imposed on the sites in the immediate vicinity of the carrier. Equations (15) and (16) have a different form, since in the immediate vicinity of the carrier its asymmetric hopping rules perturb essentially the environment particle dynamics. Equations (15) and (16) possess some intrinsic symmetries and hence the number of independent parameters can be reduced. That is, reversing the field, i.e. changing $E \rightarrow -E$, leads to the mere replacement of $k(\vec{e}_1; t)$ by $k(\vec{e}_{-1}; t)$ but does not affect $k(\vec{e}_\nu; t)$ with $\nu = \{\pm 2, \pm 3\}$, which implies that

$$k(\vec{e}_1; t)(-E) = k(\vec{e}_{-1}; t)(E) \quad \text{and}$$

$$k(\vec{e}_\nu; t)(-E) = k(\vec{e}_\nu; t)(E) \quad \text{for } \nu = \{\pm 2, \pm 3\}. \quad (19)$$

In addition, since the transition probabilities in Eq. (2) obey

$$p_2 = p_{-2} = p_3 = p_{-3}, \quad (20)$$

one evidently has that

$$k(\vec{e}_2; t) = k(\vec{e}_{-2}; t) = k(\vec{e}_3; t) = k(\vec{e}_{-3}; t), \quad (21)$$

and, by symmetry,

$$A_2(t) = A_{-2}(t) = A_3(t) = A_{-3}(t), \quad (22)$$

which somewhat simplifies Eqs. (15) and (16). Finally, we note that, despite the fact that by using the decoupling scheme in Eq. (14) we effectively close the system of equations on the level of the pair correlations, the solution of Eqs. (15) and (16) still poses serious technical difficulties. That is, these equations are strongly nonlinear with respect to the carrier velocity, which introduces a gradient term on the right hand side of the evolution equations for the pair correlation, and depends by itself on the values of the environment particle densities in the immediate vicinity of the carrier. Below we discuss a solution to this nonlinear problem, focusing on the limit $t \rightarrow \infty$.

IV. SOLUTION OF THE DECOUPLED EVOLUTION EQUATIONS IN THE STATIONARY STATE

Consider the limit $t \rightarrow \infty$, and suppose that the density profiles and the stationary velocity of the carrier have non-trivial stationary values

$$k(\vec{\lambda}) \equiv \lim_{t \rightarrow \infty} k(\vec{\lambda}; t), \quad V_c \equiv \lim_{t \rightarrow \infty} V_c(t), \quad \text{and} \quad A_\mu = \lim_{t \rightarrow \infty} A_\mu(t). \quad (23)$$

Next define the local deviations of $k(\vec{\lambda})$ from the unperturbed density as

$$h(\vec{\lambda}) \equiv k(\vec{\lambda}) - \rho_s. \quad (24)$$

Choosing $h(\mathbf{0}) = 0$, we obtain the fundamental system of equations

$$\tilde{L}h(\vec{\lambda}) = 0, \quad (25)$$

which holds for $\vec{\lambda} \neq \{\mathbf{0}, \vec{e}_{\pm 1}, \vec{e}_{\pm 2}, \vec{e}_{\pm 3}\}$, while for the special sites adjacent to the carrier, i.e. for $\vec{\lambda} = \{\mathbf{0}, \vec{e}_{\pm 1}, \vec{e}_{\pm 2}, \vec{e}_{\pm 3}\}$, one has

$$(\tilde{L} + A_\nu)h(\vec{e}_\nu) + \rho_s(A_\nu - A_{-\nu}) = 0. \quad (26)$$

Equations (25) and (26) determine the spatial distribution of the deviation from the unperturbed density ρ_s in the stationary state. Note also that in virtue of the symmetry relations in Eqs. (21) and (22), $h(\vec{e}_{\pm 2}) = h(\vec{e}_{\pm 3})$ and $A_2 = A_{-2} = A_3 = A_{-3}$.

The method for solving the coupled nonlinear equations (5), (25), and (26) is as follows: We first solve these equations, supposing that the carrier stationary velocity is a given parameter, or, in other words, assuming that A_ν entering Eqs. (25) and (26) are known. In doing so, we obtain $h(\vec{\lambda})$ in the parametrized form

$$h(\vec{\lambda}) = h(\vec{\lambda}; A_{\pm 1}, A_2). \quad (27)$$

Then, substituting particular values $\vec{\lambda} = \{\vec{e}_{\pm 1}, \vec{e}_{\pm 2}, \vec{e}_{\pm 3}\}$ into Eq. (27), and making use of the definition of A_μ in Eq. (18), we find a system of three linear equations with three unknowns of the form

$$A_\nu = 1 + \frac{6\tau^*}{l\tau} p_\nu (1 - \rho_s - h(\vec{e}_\nu; A_{\pm 1}, A_2)), \quad (28)$$

where $\nu = \{\pm 1, 2\}$, which will allow us to define all A_ν [and hence, all $h(\vec{e}_\nu)$] explicitly. Finally, substituting the results into Eq. (5), which can be written down in terms of A_ν as

$$V_c = \frac{l\sigma}{6\tau^*} (A_1 - A_{-1}), \quad (29)$$

we arrive at a closed-form equation determining the stationary velocity implicitly.

A. Formal expression for the density profiles in the dynamic percolative environment as seen from the stationary moving carrier

The general solution of Eqs. (25) and (26) can be most conveniently obtained by introducing the generating function

$$H(w_1, w_2, w_3) \equiv \sum_{n_1, n_2, n_3} h(\vec{\lambda}) w_1^{n_1} w_2^{n_2} w_3^{n_3}, \quad (30)$$

where n_1 , n_2 , and n_3 are the components of the vector $\vec{\lambda}$, $\vec{\lambda} = \vec{e}_1 n_1 + \vec{e}_2 n_2 + \vec{e}_3 n_3$. Multiplying both sides of Eqs. (25) and (26) by $w_1^{n_1} w_2^{n_2} w_3^{n_3}$ and performing summation, we then find that $H(w_1, w_2, w_3)$ is given explicitly by

$$H(w_1, w_2, w_3) = -l \frac{\sum_\nu (A_\nu (w_{|\nu|}^{|\nu|} - 1) h(\vec{e}_\nu) + \rho_s (A_\nu - A_{-\nu}) w_{|\nu|}^\nu)}{l \sum_\nu A_\nu (w_{|\nu|}^{-|\nu|} - 1) - 6(f+g)}, \quad (31)$$

an expression which allows us to determine the stationary density profiles as seen from the carrier which moves with a constant velocity V_c .

Inversion of the generating function defined by Eq. (31) then yields, after rather lengthy but straightforward calculations, the following explicit result for the local deviation from the unperturbed density:

$$h(\vec{\lambda}) = \alpha^{-1} \left\{ \sum_\nu A_\nu h(\vec{e}_\nu) \nabla_{-\nu} - \rho_s (A_1 - A_{-1}) \times (\nabla_1 - \nabla_{-1}) \right\} F(\vec{\lambda}), \quad (32)$$

where $F(\vec{\lambda})$ is given by

$$F(\vec{\lambda}) = \left(\frac{A_{-1}}{A_1} \right)^{n_1/2} \int_0^\infty e^{-x} I_{n_1} \left(2 \frac{\sqrt{A_1 A_{-1}}}{\alpha} x \right) \times I_{n_2} \left(2 \frac{A_2}{\alpha} x \right) I_{n_3} \left(2 \frac{A_2}{\alpha} x \right) dx \quad (33)$$

and

$$\alpha = \sum_\nu A_\nu + \frac{6(f+g)}{l} = A_1 + A_{-1} + 4A_2 + \frac{6(f+g)}{l}. \quad (34)$$

Consequently, the particle density distribution, as seen from the carrier moving with a constant velocity V_c , obeys

$$k(\vec{\lambda}) = \rho_s + \alpha^{-1} \left\{ \sum_\nu A_\nu h(\vec{e}_\nu) \nabla_{-\nu} - \rho_s (A_1 - A_{-1}) \times (\nabla_1 - \nabla_{-1}) \right\} F(\vec{\lambda}), \quad (35)$$

where we have to determine three yet unknown parameters A_1 , A_{-1} , and A_2 .

To determine these parameters, in Eq. (32) we set $\vec{\lambda} = \vec{e}_1$, $\vec{\lambda} = \vec{e}_{-1}$, and $\vec{\lambda} = \vec{e}_2$, which results in the system of three closed-form equations determining the unknown functions A_ν , $\nu = \{\pm 1, 2\}$,

$$A_\nu = 1 + \frac{6\tau^*}{l\tau} p_\nu \left\{ 1 - \rho_s - \rho_s(A_1 - A_{-1}) \frac{\det \tilde{C}_\nu}{\det \tilde{C}} \right\}, \quad (36)$$

where \tilde{C} is a square matrix of the third order defined as

$$\begin{pmatrix} A_1 \nabla_{-1} F(\vec{e}_1) - \alpha & A_{-1} \nabla_1 F(\vec{e}_1) & A_2 \nabla_{-2} F(\vec{e}_1) \\ A_1 \nabla_{-1} F(\vec{e}_{-1}) & A_{-1} \nabla_1 F(\vec{e}_{-1}) - \alpha & A_2 \nabla_{-2} F(\vec{e}_{-1}) \\ A_1 \nabla_{-1} F(\vec{e}_2) & A_{-1} \nabla_1 F(\vec{e}_2) & A_2 \nabla_{-2} F(\vec{e}_2) - \alpha \end{pmatrix}, \quad (37)$$

while \tilde{C}_ν stands for the matrix obtained from \tilde{C} by replacing the ν th column by a column vector $((\nabla_1 - \nabla_{-1})F(\vec{e}_\nu))_\nu$. Equation (35), together with the definition of the coefficients A_ν , constitutes the first general result of our analysis defining the density distribution in the percolative environment under study.

B. General force-velocity relation

Substituting Eqs. (32) and (37) into Eq. (29), we find that the stationary velocity of the carrier particle is defined

implicitly as the solution of equation

$$V_c = \frac{\sigma}{\tau} (p_1 - p_{-1}) (1 - \rho_s) \times \left\{ 1 + \rho_s \frac{6\tau^*}{l\tau} \frac{p_1 \det \tilde{C}_1 - p_{-1} \det \tilde{C}_{-1}}{\det \tilde{C}} \right\}^{-1}, \quad (38)$$

where \tilde{C}_1 and \tilde{C}_{-1} are the following square matrices of the third order:

$$\tilde{C}_1 = \begin{pmatrix} (\nabla_1 - \nabla_{-1})F(\vec{e}_1) & A_{-1} \nabla_1 F(\vec{e}_1) & A_2 \nabla_{-2} F(\vec{e}_1) \\ (\nabla_1 - \nabla_{-1})F(\vec{e}_{-1}) & A_{-1} \nabla_1 F(\vec{e}_{-1}) - \alpha & A_2 \nabla_{-2} F(\vec{e}_{-1}) \\ (\nabla_1 - \nabla_{-1})F(\vec{e}_2) & A_{-1} \nabla_1 F(\vec{e}_2) & A_2 \nabla_{-2} F(\vec{e}_2) - \alpha \end{pmatrix} \quad (39)$$

and

$$\tilde{C}_{-1} = \begin{pmatrix} A_1 \nabla_{-1} F(\vec{e}_1) - \alpha & (\nabla_1 - \nabla_{-1})F(\vec{e}_1) & A_2 \nabla_{-2} F(\vec{e}_1) \\ A_1 \nabla_{-1} F(\vec{e}_{-1}) & (\nabla_1 - \nabla_{-1})F(\vec{e}_{-1}) & A_2 \nabla_{-2} F(\vec{e}_{-1}) \\ A_1 \nabla_{-1} F(\vec{e}_2) & (\nabla_1 - \nabla_{-1})F(\vec{e}_2) & A_2 \nabla_{-2} F(\vec{e}_2) - \alpha \end{pmatrix}. \quad (40)$$

Equation (38) represents our second principal result defining the force-velocity relation in the dynamic percolative environment for an arbitrary field and arbitrary rates of the diffusive and renewal processes.

V. CARRIER VELOCITY IN THE LIMIT OF SMALL APPLIED FIELD E , FRICTION COEFFICIENT AND CARRIER DIFFUSIVITY IN DYNAMIC PERCOLATIVE ENVIRONMENT

We now consider the case when the applied external field E is small. Expanding the transition probabilities p_1 and p_{-1} in the Taylor series up to the first order in powers of the external field, i.e.,

$$p_{\pm 1} = \frac{1}{6} \pm \frac{\sigma \beta E}{12} + O(E^2), \quad (41)$$

we find that V_c , defined by Eq. (29), follows

$$V_c \sim \frac{\sigma}{6\tau} \{ \sigma \beta E (1 - \rho_s) - (h(\vec{e}_1) - h(\vec{e}_{-1})) \}. \quad (42)$$

On the other hand, Eq. (32) entails that

$$h(\vec{e}_1) - h(\vec{e}_{-1}) = \frac{2\sigma\rho_s(1-\rho_s)\tau^*}{l\tau(\alpha_0\mathcal{L}(2A_0/\alpha_0) - A_0) + 2\rho_s\tau} \beta E + O(E^2), \quad (43)$$

where

$$A_0 = \lim_{E \rightarrow 0} A_\nu = 1 + \frac{\tau^*}{l\tau} (1 - \rho_s) \quad (44)$$

and

$$\alpha_0 = \lim_{E \rightarrow 0} \alpha = 6 \left(1 + \frac{\tau^* (1 - \rho_s)}{l\tau} + \frac{f+g}{l} \right), \quad (45)$$

while

$$\begin{aligned} \mathcal{L}(x) &\equiv \left\{ \int_0^\infty e^{-t} I_0^2(xt) (I_0(xt) - I_2(xt)) dt \right\}^{-1} \\ &= \{P(\mathbf{0}; 3x) - P(2\vec{e}_1; 3x)\}^{-1}, \end{aligned} \quad (46)$$

$P(\vec{r}; \xi)$ being the generating function,

$$P(\vec{r}; \xi) \equiv \sum_{j=0}^{+\infty} P_j(\vec{r}) \xi^j, \quad (47)$$

of the probability $P_j(\vec{r})$ that a walker starting at the origin and performing a Polya random walk on the sites of a three-dimensional cubic lattice will arrive on the j th step to the site with the lattice vector \vec{r} [3].

Consequently, we find that in the limit of a small applied field E the force-velocity relation in Eq. (38) attains the physically meaningful form of the Stokes formula $E = \zeta V_c$, which signifies that the frictional force exerted on the carrier by the environment particles is *viscous*. The effective friction coefficient ζ is the sum of two terms,

$$\zeta = \zeta_0 + \zeta_{coop}, \quad (48)$$

where the first term represents a mean-field-type result $\zeta_0 = 6\tau/\beta\sigma^2(1-\rho_s)$ [see Eq. (7)], and the second one ζ_{coop} obeys

$$\zeta_{coop} = \frac{12\rho_s\tau^*}{\beta\sigma^2 l(1-\rho_s)(\alpha_0\mathcal{L}(2A_0/\alpha_0) - A_0)}. \quad (49)$$

The second contribution has a more complicated origin, and is associated with the cooperative behavior—formation of an inhomogeneous stationary particle distribution around the carrier moving with constant velocity V_c . Needless to say, such an effect cannot be observed within the framework of previous models of dynamic percolation, since there the carrier does not influence the host medium dynamics [13–17, 19–22].

Let us now compare the relative importance of two contributions, i.e., ζ_0 and ζ_{coop} , to the overall friction. In Fig. 2 we plot the ratio ζ/ζ_0 versus the creation rate f for three different values of the density ρ_s , $\rho_s = 0.9, 0.7,$ and 0.5 , while the annihilation rate is prescribed by the relation $g = f(1-\rho_s)/\rho_s$. This figure shows that the cooperative behavior clearly dominates at small and moderate f (which also entails small values of g), while for larger f , when ζ/ζ_0 tends to 1, the mean-field behavior becomes most important. The cooperative behavior also appears to be more pronounced at larger densities ρ_s .

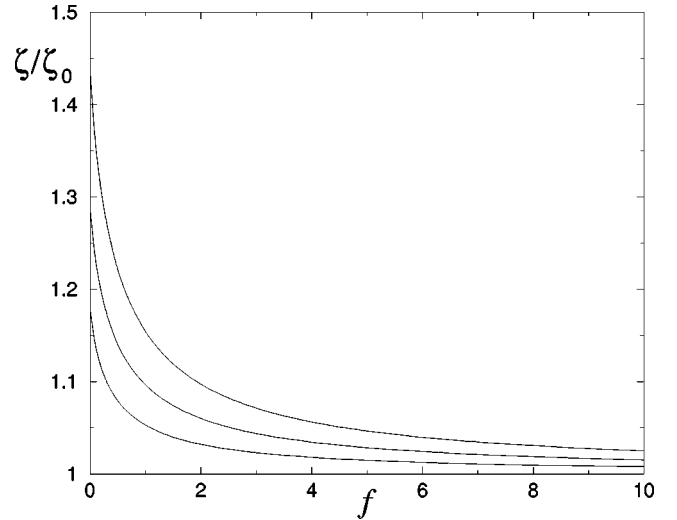


FIG. 2. The ratio of the overall friction coefficient and the mean-field friction vs the creation rate for three different values of the mean density ρ_s . The upper curve corresponds to $\rho_s = 0.9$, the intermediate curve to $\rho_s = 0.7$, and the lower curve to $\rho_s = 0.5$. The diffusion times of the carrier and of the “environment” particles are taken equal to each other, $\tau = \tau^*$, and the lattice spacing l is set equal to unity.

Next consider some analytical estimates. We start with the situation in which diffusion of the environment particles is suppressed, i.e. when $l = 0$. In this case, we obtain

$$\frac{\zeta_{coop}}{\zeta_0} = \frac{2\rho_s}{(1-\rho_s) \left(\frac{2}{y} \mathcal{L}(y) - 1 \right)}, \quad (50)$$

where

$$y = \frac{1}{3} \left(1 + \frac{\tau}{\tau^*} \frac{(f+g)}{(1-\rho_s)} \right)^{-1}. \quad (51)$$

Suppose first that ρ_s is small, $\rho_s \ll 1$. Then $y \approx 1/3(1 + \tau/\tau^*(f+g))$, and we can distinguish between two situations: when $\tau \ll (f+g)/\tau^*$, i.e. when the carrier moves faster than the environment reorganizes itself; and the opposite limit $\tau \gg (f+g)/\tau^*$, when the environment changes very rapidly compared to the motion of the carrier. In the former case we find that $y \approx 1/3$, which yields $\zeta_{coop}/\zeta_0 \approx 2\rho_s/(6\mathcal{L}(1/3) - 1)$, $\mathcal{L}(1/3) \approx 0.7942$, while in the latter case we have $y \approx \tau^*/3\tau(f+g)$ and $\zeta_{coop}/\zeta_0 \approx \rho_s\tau^*/3\tau(f+g)$. Note that in both cases the ratio ζ_{coop}/ζ_0 appears to be small, which signifies that at small densities ρ_s the mean-field friction dominates. Such a result is consistent with the behavior depicted in Fig. 2 and is not counterintuitive, of course, since in the absence of particle diffusion, which effectively couples the density evolution at different lattice sites, no significant cooperative behavior can emerge at small densities. On the other hand, at relatively high densities $\rho_s \sim 1$ and $\tau/(1-\rho_s) \gg \tau^*/(f+g) \gg \tau$, when the carrier moves at a much faster rate than that at which the host medium reorganizes itself, we find that $\zeta_{coop}/\zeta_0 \approx \tau^*/3\tau(f+g) \gg 1$. This result stems from the circumstance that in sufficiently dense environments modeled by dynamic percolation, a

highly inhomogeneous density profile emerges even in the absence of particle diffusion. Here, on the one hand, the carrier significantly perturbs the particle density in its immediate vicinity. On the other hand, the density perturbation created by the carrier does not shift the global balance between creation and annihilation events, i.e., the mean particle density is still equal to ρ_s , as we set out to show in what follows. The latter constraint then induces the appearance of essential correlations in particle distribution, and hence, the appearance of cooperative behavior.

Let us consider the opposite case when the renewal processes are not allowed, which means that the particle number is conserved and local density in the percolative environment evolves only due to particle diffusion. In this case we find

$$\frac{\zeta_{coop}}{\zeta_0} = \frac{2\tau^*\rho_s}{(l\tau + \tau^*(1-\rho_s))(6\mathcal{L}(1/3) - 1)}. \quad (52)$$

Here the ratio ζ_{coop}/ζ_0 can be large, and the ‘‘cooperative’’ friction dominates the mean-field one when $l\tau \ll \tau^*(3\rho_s - 1)$, which occurs at sufficiently high densities and in the limit when the carrier moves at a much faster rate than that at which the environment reorganizes itself. Otherwise, the mean-field friction prevails.

To estimate the carrier particle diffusion coefficient D_c we assume the validity of the Einstein relation, i.e., $\beta D_c = \zeta^{-1}$. We find that, in the general case, the carrier diffusion coefficient D_c reads

$$D_c = \frac{\sigma^2(1-\rho_s)}{6\tau} \left\{ 1 - \frac{2\rho_s\tau^*}{l\tau} \left(\alpha_0\mathcal{L}(2A_0/\alpha_0) - 1 + \frac{\tau^*(3\rho_s - 1)}{l\tau} \right)^{-1} \right\}. \quad (53)$$

In the particular case of a conserved particle number, when $f, g \rightarrow 0$ but their ratio f/g is kept fixed, $f/g = \rho_s/(1-\rho_s)$, the latter equation reduces to the classical result

$$D_c^{NK} = \frac{\sigma^2(1-\rho_s)}{6\tau} \left\{ 1 - \frac{2\rho_s\tau^*}{l\tau} \left(6A_0\mathcal{L}(1/3) - 1 + \frac{\tau^*(3\rho_s - 1)}{l\tau} \right)^{-1} \right\}, \quad (54)$$

obtained earlier in Refs. [24] and [25] by different analytical techniques. The result in Eq. (54) is known to be exact in the limits $\rho_s \ll 1$ and $\rho_s \sim 1$, and serves as a very good approximation for the self-diffusion coefficient in hard-core lattice gases of arbitrary density [26].

It also seems interesting to analyze how the random annihilation and creation of particles can modify the self-diffusion coefficient compared to the situation when the particle number is conserved. In Fig. 3 we plot the ratio D_c^{NK}/D_c ($= \zeta/\zeta_{NK}$) versus the creation rate f for three different values of the density ρ_s , $\rho_s = 0.9, 0.7$ and 0.5 . Again, the value of the annihilation rate g is prescribed by the relation $g = f(1 - \rho_s)/\rho_s$. Figure 3 shows that renewal processes considerably affect the friction coefficient, and that the ratio ζ/ζ_{NK}

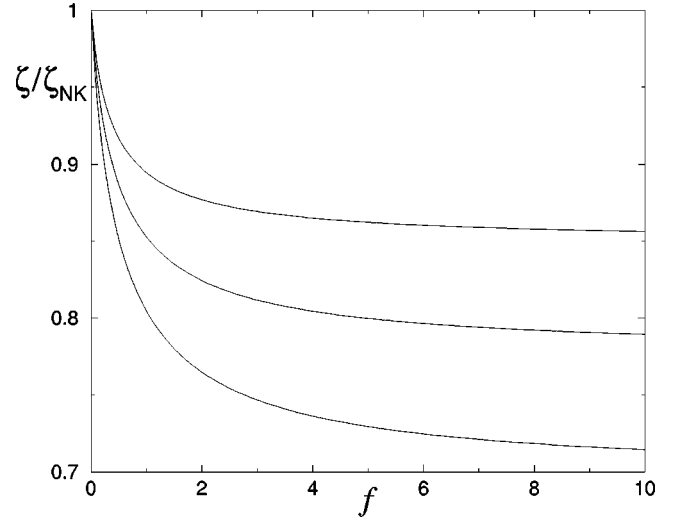


FIG. 3. The ratio of the overall friction coefficient and the friction coefficient in the conserved particle number case vs the creation rate for three different values of the mean density ρ_s . The upper curve corresponds to $\rho_s = 0.5$, the intermediate curve to $\rho_s = 0.7$, and the lower curve to $\rho_s = 0.9$. Diffusion times are $\tau = \tau^*$ and $l = 1$.

strongly deviates from the unity with the growth of the creation rate. The overall friction also falls off when the density increases.

Finally, in the absence of particle diffusion (fluctuating-site percolation), our result for the carrier particle diffusion coefficient reduces to

$$D_c^{per} = \frac{\sigma^2(1-\rho_s)}{6\tau} \left\{ 1 - 2\rho_s [4[(1-\rho_s) + (f+g)\tau/\tau^*]\mathcal{L}(y) + 3\rho_s - 1]^{-1} \right\}. \quad (55)$$

Note, however, that this result only applies when both f and g are larger than zero, such that the renewal processes take place. In fact, the underlying decoupling scheme is only plausible in this case. Similar to the approximate theories in Refs. [24] and [25], our approach predicts that in the absence of the renewal processes D_c^{per} vanishes only when $\rho_s \rightarrow 1$, which is an incorrect behavior.

VI. ASYMPTOTIC BEHAVIOR OF THE DENSITY PROFILES AT LARGE DISTANCES IN FRONT OF AND PAST THE CARRIER

The density profiles at large separations in front of and past the carrier can be readily deduced from the asymptotical behavior of the following generating function:

$$N(w_1) \equiv \sum_{n_1=-\infty}^{+\infty} h(n_1, n_2=0, n_3=0) w_1^{n_1}. \quad (56)$$

Inversion of Eq. (31), with respect to the symmetric coordinates n_2 and n_3 , then yields

$$\begin{aligned}
N(w_1) = & \frac{(A_1 h(\vec{e}_1) + \rho_s(A_1 - A_{-1}))(w_1 - 1) + (A_{-1} h(\vec{e}_{-1}) - \rho_s(A_1 - A_{-1}))(w_1^{-1} - 1)}{\alpha - A_1 w_1^{-1} - A_{-1} w_1} \\
& \times \int_0^\infty \exp[-x] I_0^2\left(\frac{2A_2}{\alpha - A_1 w_1^{-1} - A_{-1} w_1} x\right) dx + \frac{4A_2 h(\vec{e}_2)}{\alpha - A_1 w_1^{-1} - A_{-1} w_1} \int_0^\infty \exp[-x] I_0\left(\frac{2A_2}{\alpha - A_1 w_1^{-1} - A_{-1} w_1} x\right) \\
& \times \left(I_1\left(\frac{2A_2}{\alpha - A_1 w_1^{-1} - A_{-1} w_1} x\right) - I_0\left(\frac{2A_2}{\alpha - A_1 w_1^{-1} - A_{-1} w_1} x\right) \right) dx. \tag{57}
\end{aligned}$$

We note now that $N(w_1)$ is a holomorphic function in the region $\mathcal{W}_1 < w_1 < \mathcal{W}_2$, where

$$\mathcal{W}_1 = \frac{\alpha - 4A_2}{2A_{-1}} - \sqrt{\left(\frac{\alpha - 4A_2}{2A_{-1}}\right)^2 - \frac{A_1}{A_{-1}}} \tag{58}$$

and

$$\mathcal{W}_2 = \frac{\alpha - 4A_2}{2A_{-1}} + \sqrt{\left(\frac{\alpha - 4A_2}{2A_{-1}}\right)^2 - \frac{A_1}{A_{-1}}}. \tag{59}$$

As a consequence, the asymptotic behavior of $h(n_1, n_2 = 0, n_3 = 0)$ in the limit $n_1 \rightarrow \infty$ ($n_1 \rightarrow -\infty$) is controlled by the behavior of $N(w_1)$ in the vicinity of $w_1 = \mathcal{W}_2$ ($w_1 = \mathcal{W}_1$) (see, for example, the analysis of the generating function singularities developed in Ref. [33]).

A. Asymptotics of the density profiles at large separations in front of the carrier

Consider first the asymptotic behavior of the density distribution of the ‘‘environment’’ particles at large separations in front of the carrier. Using the fact that

$$\int_0^\infty \exp[-x] I_0(yx) (I_1(x) - I_0(x)) dx \tag{60}$$

is a regular function when $y \rightarrow 1/2$, while

$$\int_0^\infty \exp[-x] I_0^2(yx) dx \rightarrow \frac{1}{\pi} \ln\left(\frac{1}{1-2y}\right), \tag{61}$$

we find that

$$\begin{aligned}
N(w_1) \underset{w_1 \rightarrow \mathcal{W}_2^-}{\sim} & \left[\frac{(A_1 h(\vec{e}_1) + \rho_s(A_1 - A_{-1}))(\mathcal{W}_2 - 1)}{4\pi A_2} \right. \\
& \left. + \frac{(A_{-1} h(\vec{e}_{-1}) - \rho_s(A_1 - A_{-1}))(\mathcal{W}_2^{-1} - 1)}{4\pi A_2} \right] \\
& \times \ln(\mathcal{W}_2 - w_1). \tag{62}
\end{aligned}$$

Then, (cf. Ref. [33]) we obtain the asymptotical result

$$h(n_1, 0, 0) \underset{n_1 \rightarrow \infty}{\sim} \frac{K^+}{n_1} e^{-n_1/\lambda_+}, \tag{63}$$

where

$$\lambda_+ \equiv \ln^{-1}\left(\frac{\alpha/2 - 2A_2}{A_{-1}} + \sqrt{\left(\frac{\alpha/2 - 2A_2}{A_{-1}}\right)^2 - \frac{A_1}{A_{-1}}}\right) \tag{64}$$

and

$$\begin{aligned}
K^+ = & \left[\frac{(A_1 h(\vec{e}_1) + \rho_s(A_1 - A_{-1}))(\mathcal{W}_2 - 1)}{4\pi A_2} \right. \\
& \left. + \frac{(A_{-1} h(\vec{e}_{-1}) - \rho_s(A_1 - A_{-1}))(\mathcal{W}_2^{-1} - 1)}{4\pi A_2} \right] > 0, \tag{65}
\end{aligned}$$

which signifies that the density of the environment particles in front of the carrier is higher than the average value ρ_s and approaches ρ_s at large separations from the carrier as an exponential function of the distance.

B. Asymptotics of the density profiles at large separations past the carrier

We next consider the asymptotic behavior of the environment particle density profiles past the carrier particle, which turn out to be very different depending on whether the dynamics of the percolative environment obeys the strict conservation of the environment particle number or not (the renewal processes are suppressed or allowed). The sketch of this behavior is presented in Fig. 4.

(a) *Nonconserved particle number.* In the case when particles may disappear and reappear on the lattice, one has that the root $\mathcal{W}_1 < 1$. We then find, following essentially the same lines as in Sec. VIA that

$$\begin{aligned}
N(w_1) \underset{w_1 \rightarrow \mathcal{W}_1^-}{\sim} & \left[\frac{(A_1 h(\vec{e}_1) + \rho_s(A_1 - A_{-1}))(\mathcal{W}_1 - 1)}{4\pi A_2} \right. \\
& \left. + \frac{(A_{-1} h(\vec{e}_{-1}) - \rho_s(A_1 - A_{-1}))(\mathcal{W}_1^{-1} - 1)}{4\pi A_2} \right] \\
& \times \ln\left(\frac{1}{w_1 - \mathcal{W}_1}\right). \tag{66}
\end{aligned}$$

Hence, in the nonconserved case, the approach to the unperturbed value ρ_s is also exponential when $n_1 \rightarrow -\infty$, and follows

$$h_{n_1, 0, 0} \underset{n_1 \rightarrow -\infty}{\sim} \frac{K^-}{|n_1|} e^{-|n_1|/\lambda_-}, \tag{67}$$

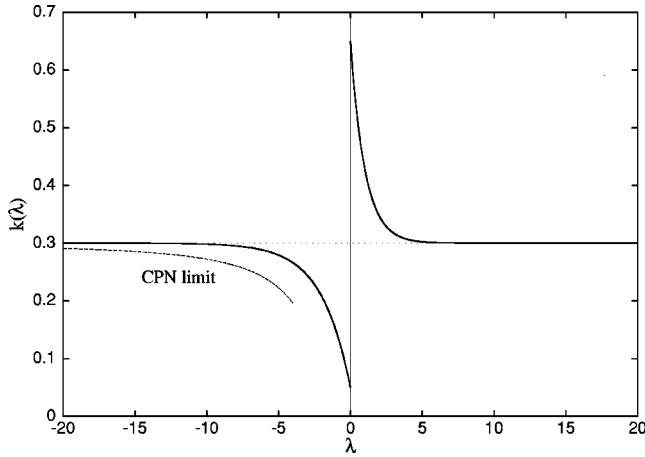


FIG. 4. A sketch of the asymptotic density profiles in front of and past the stationary moving carrier. The abbreviation CPN stands for the “conserved particle number.” The two solid lines in the $\lambda > 0$ and $\lambda < 0$ domains denote exponential profiles, Eqs. (63) and (67). The dashed line in the domain $\lambda < 0$ stands for the algebraic law [Eq. (72)].

where

$$\lambda_- \equiv \ln^{-1} \left(\frac{\alpha/2 - 2A_2}{A_{-1}} - \sqrt{\left(\frac{\alpha/2 - 2A_2}{A_{-1}} \right)^2 - \frac{A_1}{A_{-1}}} \right) \quad (68)$$

and

$$K^- = \left[\frac{(A_1 h(\vec{e}_1) + \rho_s(A_1 - A_{-1}))(\mathcal{W}_1 - 1)}{4\pi A_2} + \frac{(A_{-1} h(\vec{e}_{-1}) - \rho_s(A_1 - A_{-1}))(\mathcal{W}_1^{-1} - 1)}{4\pi A_2} \right] < 0, \quad (69)$$

which implies that the particle density past the carrier is lower than the average. Note that, in the general case, $\lambda_+ < \lambda_-$, which means that the depleted region past the carrier is more extended in space than the traffic-jam-like region in front of the carrier. The density profiles are therefore asymmetric with respect to the origin, $n_1 = 0$. Since creation of particles is favored (suppressed) in depleted (jammed) regions, while annihilation is suppressed (favored), one might expect that this will shift the overall density in the system, i.e. the average density of the environment particles will differ from ρ_s . Interestingly, the overall deviation, i.e. the sum of local deviations over the volume of the system, of the density of the environment particles from the average value ρ_s , appears to be equal exactly to zero,

$$H(w_1 = 1, w_2 = 1, w_3 = 1) \equiv 0, \quad (70)$$

and hence, the driven carrier does not perturb the global balance between creation and annihilation of the environment particles. This is not, however, an *a priori* evident result in view of the asymmetry of the density profiles.

(b) *Conserved particle number.* Finally, we turn to the analysis of the shape of the density profiles of the percolative environment past the carrier in the particular limit when the

host medium evolves only due to diffusion, while creation and annihilation of particles are completely suppressed. In this case, in which the particles number is explicitly conserved, one has that, for arbitrary values of the field and particle average density, the root $\mathcal{W}_1 \equiv 1$ and, consequently, the form of the generating function are qualitatively different from that in Eqs. (62) and (66),

$$N(w_1) \underset{w_1 \rightarrow 1^+}{\sim} \left[\frac{(A_1 h(\vec{e}_1) - A_{-1} h(\vec{e}_{-1}))}{4\pi A_2} + \frac{(2\rho_s(A_1 - A_{-1}))}{4\pi A_2} \right] \times (w_1 - 1) \ln \left(\frac{1}{w_1 - 1} \right). \quad (71)$$

Equation (71) implies that in the limit when the particle number is conserved, the large- n_1 asymptotic behavior of $h_{n_1,0,0}$ is described by an algebraic function of n_1 with a logarithmic correction; that is,

$$h_{n_1,0,0} \sim \frac{K_- \ln(|n_1|)}{n_1^2}, \quad (72)$$

where K_- is an n_1 -independent constant. Remarkably, the power-law decay of the correlations implies the existence of quasi-long-range order in the percolative environment past the carrier. In the conserved case the mixing of the three-dimensional percolative environment is not very efficient, and there are considerable memory effects—the host medium remembers the passage of the carrier on large space and time scales.

VII. CONCLUSIONS

To conclude, we analytically studied the dynamics of a carrier driven by an external field \vec{E} in a three-dimensional environment modeled by dynamic percolation on a cubic lattice partially filled with mobile, hard-core “environment” particles which can spontaneously disappear and reappear (renewal processes) in the system with some prescribed rates. Our analytical approach was based on the master equation, describing the time evolution of the system, which allowed us to evaluate a system of coupled dynamical equations for the carrier velocity and a hierarchy of correlation functions. We invoked an approximate closure scheme based on the decomposition of the third-order correlation functions, which was first introduced in Ref. [23] for a related model of a driven carrier dynamics in a one-dimensional lattice gas with conserved particle number. Within the framework of this approximation, we derived a system of coupled, discrete-space equations describing the evolution of the density profiles of the environment, as seen from the moving carrier, and its velocity V_c . We showed that V_c depends on the density of the environment particles in front of and past the carrier. Both densities depend on the magnitude of the velocity, as well as on the rate of the renewal and diffusive processes. As a consequence of such a nonlinear coupling, in the general case (i.e. for an arbitrary driving field and arbitrary rates of renewal and diffusive processes), V_c was found only implicitly, as the solution of a nonlinear equation relating its value to the system parameters. This equation, which

defines the force-velocity relation for the dynamic percolation under study, simplifies considerably in the limit of small applied field \vec{E} . We found that in this limit it attains the physically meaningful form of the Stokes formula, which implies, in particular, that the frictional force exerted on the carrier by the environment modeled by dynamic percolation is *viscous*. In this limit, the carrier velocity and the friction

coefficient were calculated explicitly. In addition, we determined the self-diffusion coefficient of the carrier in the absence of the field, and showed that it reduces to the well-known result of Refs. [24] and [25] in the limit when the particle number is conserved. Furthermore, we found that the density profile around the carrier becomes strongly inhomogeneous.

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