Motion of a driven tracer particle in a one-dimensional symmetric lattice gas

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Consider the dynamics of a tracer particle subject to a constant driving force E in a one-dimensional lattice gas of hard-core particles whose transition rates are symmetric. We show that the mean displacement of the driven tracer $\overline{X_T(E,t)}$ grows in time t as $\overline{X_T(E,t)}=\sqrt{\alpha t}$, rather than the linear time dependence found for noninteracting (ghost) bath particles. The prefactor α is determined implicitly, as the solution of a transcendental equation, for an arbitrary magnitude of the driving force and an arbitrary concentration of the lattice-gas particles. In limiting cases the prefactor is obtained explicitly. Analytical predictions are seen to be in good agreement with the results of numerical simulations. [S1063-651X(96)01809-0]

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I. INTRODUCTION

Dynamic and equilibrium properties of lattice gases, i.e., systems involving randomly moving particles with hard-core interactions, have received much interest within the last several decades. A number of important theoretical results have been obtained for such systems revealing nontrivial, many-body behavior [1–12]. Lattice-gas models often serve as microscopic models of complex physical phenomena. To name a few we mention dynamics of motor proteins [13,14], growth of interfaces, [15–17] traffic jams, and queuing problems [18]. A lattice-gas approach has been used for the derivation of Euler-type hydrodynamic equations, e.g., the Burgers equation [19,20]. Another important example concerns the spreading of molecularly thin wetting films, where experimental studies [21–23] have evidenced surprising universal laws which recently have been explained in terms of a lattice-gas model [24–26]. We believe also that a robust microscopic, molecular approach to such physical phenomena as shear-induced ordering in colloidal suspensions [27] or stick-slip motion of mica planes separated by an ultrathin liquid layer [28–31] could also begin with a description based on a lattice-gas picture.

At the present time two models are well studied in the literature. In the first, the so-called asymmetric exclusion process, all particles in the system perform stochastic motion, constrained by hard-core interactions, in the field of a constant driving force [1–9,32–34]. Here the velocity, diffusion constant and equilibrium configurations have been calculated exactly for different types of boundary conditions [e.g., [2,7,8,34], and references therein]. In the second, no external force is present and all particles have symmetric transition rates. Remarkably, in such a situation, the motion of a labeled, tracer particle is nondiffusive in low dimensions. For example, the mean-square displacement $\overline{X_T^2(E=0,t)}$ of a tracer particle (identical except for its observability to all other particles) in a one-dimensional (1D) symmetric lattice gas shows a sublinear growth with time [35,36]

$$\overline{X_T^2(E=0,t)}=\frac{C_0}{1-C_0}\left(\frac{2t}{\pi}\right)^{1/2}, \quad (1)$$

where C_0, $0\leqslant C_0<1$, denotes the mean (constant) concentration of vacant sites and the argument $E=0$ signifies that the external force is absent and that all particles have symmetric transition rates. Hence, in 1D trajectories $X_T(E=0,t)$ of such a tracer particle are more compact than those of particles without the hard-core constraints. In 2D the mean-square displacement $\overline{X_T^2(E=0,t)}$ shows a linear dependence on time with additional logarithmic terms [11,37]; in 3D it grows linearly in time with the diffusion constant being a nontrivial function of the particle concentration.

In the present paper we focus on the less studied and less understood situation in which only one particle (the tracer) experiences the action of an external (constant) driving force E and thus has asymmetric transition rates, while all other particles (bath particles) are not subject to this force and have symmetric transition rates. The tracer behavior in such a system with a vanishingly small driving force has first been examined in [3] in which the question of the validity of the Einstein relation for the hard-core lattice gases has been addressed. (This point will be discussed in more detail in Sec. IV D.) Such a model has been used [38] in a numerical study of the gravity driven motion of a finite rigid rod in a ''sea'' of hard-core monomers. Another physical example corresponds to the situation in which a charged particle diffuses in a lattice gas of electrically neutral particles in the presence of a constant electric field E. The extreme case of infinitely strong electric fields ($E=\infty$), which means that the tracer particle may move only in one direction, has been studied in [39]. It has been shown, for example, that in 1D systems the mean displacement $\overline{X_T(E=\infty,t)}$ of a charged tracer particle grows sublinearly with time,

$$\overline{X_T(E=\infty,t)} \propto (\alpha_\infty t)^{1/2}, \tag{2}$$

where α_∞ is a constant [39]. Equation (2) indicates that hard-core interactions give rise to an effective friction. In the one-dimensional case this force is much stronger than the viscous friction for one particle and grows in proportion to the mean displacement of the tracer, i.e., as $\sqrt{t}$, as this is a measure of the size of the compressed region preceding the tracer which hinders the ballistic motion of the driven particle.

Here we study the motion of a driven tracer particle in a symmetric lattice gas in the general case of fields of arbitrary strength and at arbitrary concentrations of the lattice-gas particles. Focusing on one-dimensional situations in which the hindering effect of the lattice-gas (bath) particles on the tracer motion is most pronounced, we devise a mean-field-type theory which allows simple calculation of the mean displacement of the tracer particle as a function of time and other pertinent parameters. We find that $\overline{X_T(E,t)}$ has the following dependence:

$$\overline{X_T(E,t)} = (\alpha t)^{1/2}, \tag{3}$$

where the parameter α is a time-independent constant, which is a complicated function of field strength E, which determines the transition probabilities p and q, and concentration of the bath particles C_p. This constant is determined here for arbitrary values of E and C_p. Our analytical findings are in excellent agreement with the results of the numerical simulations.

The paper is structured as follows: In Sec. II we describe the model. In Sec. III we present definitions and write down basic equations describing the motion of particles. In Sec. IV we determine explicitly the growth law for the mean displacement of the tracer particle Eq. (3) and evaluate a closed transcendental equation for the parameter α. In several limiting cases the dependence of α on the pertinent parameters is explicitly obtained. Section V presents results of numerical simulations and comparison of these with our analytical predictions. Finally, in Sec. VI we conclude with a summary of our results and a discussion.

II. THE MODEL

The model is defined in the following way. Consider a one-dimensional regular lattice of unit spacing, infinite in both directions, the sites $\{X\}$ of which are either singly occupied by identical particles or vacant. The particles are initially placed at random (constrained by the condition that double occupancy of sites is forbidden) with mean concentration $C_p = 1 - C_0$, where C_p is the mean site occupancy, C_0 being the mean site vacancy. The tracer particle is put initially at the origin, i.e., at $X=0$. A configuration of the system is characterized by an infinite set of (time-dependent) occupation variables $\{\tau_X\}$, where $\tau_X = 1$ if site X is occupied and $\tau_X = 0$ if site X is vacant. Consequently, the variable $\eta_X = 1 - \tau_X$ describes the probability that site X is vacant.

The dynamics of the bath particles is symmetric: each particle waits a (random) exponentially distributed time with mean 1 and then attempts to jump, with equal probability (1/2) to the right or left neighboring site. The jump actually occurs if the chosen site is empty. The tracer particle motion is asymmetric: the tracer waits a random exponentially distributed time with mean 1 and then randomly selects a jump direction. It chooses a right-hand (left-hand) adjacent site with probability p $(q = 1 - p)$. The jump occurs if the selected site is vacant. If the asymmetry in tracer jump probabilities is due to an external electric field E one has the relation $p/q = \exp(\beta E)$, where β is the inverse temperature. For simplicity we have set the tracer charge to unity. We also assume, without loss of generality, that E is oriented in the positive direction, i.e., $E > 0$, and thus $p > q$.

III. DEFINITIONS AND BASIC EQUATIONS

We start by writing the equations which describe dynamics of the tracer particle. Let $X_T(E,t)$ denote the position of the tracer at time t [by definition $X_T(0)=0$] and $P(X,t)$ be the probability that the tracer is at site X at time t. The mean displacement of the tracer particle, i.e., $\overline{X_T(E,t)}$, is then defined as

$$\overline{X_T(E)} = \sum_X X P(X,t). \tag{4a}$$

The time evolution of $P(X,t)$ is governed by the equation

$$\dot{P}(X,t) = -P(X,t)[p\,\eta_{X+1}(t) + q\,\eta_{X-1}(t)] + \eta_X(t)[pP(X-1,t) + qP(X+1,t)], \tag{4b}$$

where the dot denotes the time derivative. The first two terms on the right-hand side (rhs) of Eq. (4) describe, respectively, the change in $P(X,t)$ due to jumps of the tracer particle from the site X to sites $X \pm 1$, while the third and fourth terms account for jumps from the sites $X \pm 1$ to the site X. Multiplying both sides of Eq. (4) by X and summing over all lattice sites we arrive at the rate equation

$$\dot{\overline{X_T(E,t)}} = p f_1 - q f_{-1}, \tag{5}$$

where

$$f_\lambda = \sum_X P(X,t)\,\eta_{X+\lambda}(t) \tag{6}$$

is the pairwise tracer-vacancy correlation function, which can be thought of as the probability of finding at time t a vacancy at the distance λ from the tracer. The correlation function is defined in the frame of reference moving with the tracer and jumps of the tracer change the value of f_λ.

Consider now evolution of f_λ, which completely determines the mean displacement of the tracer Eq. (5). The change in f_λ results from two different processes

$$\dot{f}_\lambda = \hat{L}_{bath}(f_\lambda) + \hat{L}_{trac}(f_\lambda), \tag{7}$$

where the operator $\hat{L}_{bath}$ accounts for the contribution coming from the motion of bath particles, whilst $\hat{L}_{trac}$ describes the contribution of the tracer motion itself. Explicitly, for $\hat{L}_{bath}(f_\lambda)$ we have (for $|\lambda| > 1$)

$$\hat{L}_{bath}(f_\lambda) = \tfrac{1}{2}(1-f_\lambda)(f_{\lambda-1}+f_{\lambda+1}) - \tfrac{1}{2}f_\lambda(1-f_{\lambda-1}+1-f_{\lambda+1}), \tag{8}$$

where the first term describes the ''birth'' of a vacancy at the occupied site $X+\lambda$ due to the jumps of a bath particle from $X+\lambda$ to vacant sites $X+\lambda\pm 1$; the second term describes the ''death'' of a vacancy at a vacant site $X+\lambda$ due to the jumps of a bath particle from sites $X+\lambda\pm 1$. One readily notices that the nonlinear terms in Eq. (8) cancel each other and $\hat{L}_{bath}$ is simply the second finite difference operator (for $|\lambda|>1$)

$$\hat{L}_{bath}(f_\lambda) = \tfrac{1}{2}(-2f_\lambda+f_{\lambda-1}+f_{\lambda+1}). \tag{9}$$

The ''diffusive'' free particlelike behavior in Eq. (9) is, of course, the consequence of the fact that all bath particles are identical, leading to the cancellation of the nonlinear terms in Eq. (8).

Consider now the contribution due to the motion of the tracer particle. In an explicit form we have (for $|\lambda|>1$)

$$\hat{L}_{trac}(f_\lambda) = qf_{-1}(1-f_\lambda)f_{\lambda-1} - qf_{-1}f_\lambda(1-f_{\lambda-1}) + pf_1(1-f_\lambda)f_{\lambda+1} - pf_1(1-f_{\lambda+1})f_\lambda, \tag{10}$$

where the terms on the rhs of Eq. (10) describe, respectively, the following events: (a) an *occupied* site at the distance λ from the tracer becomes *vacant* if the tracer jumps into the previously vacant left-hand adjacent site and the site at distance $\lambda-1$ is vacant; (b) a vacant site at distance λ from the tracer becomes occupied, if the tracer jumps into the previously vacant left-hand adjacent site and the site at distance $\lambda-1$ is occupied; (c) an occupied site at distance λ becomes vacant when the tracer jumps into the previously vacant right-hand site and the site at distance $\lambda+1$ is vacant; eventually, (d) a vacant site at distance λ becomes occupied when the tracer jumps into the previously vacant right-hand site and the site at distance $\lambda+1$ is occupied.

Next, similar reasoning gives the behavior of f_λ in the immediate neighborhood of a tracer, i.e., at sites with $\lambda=\pm 1$, which can be thought of as the boundary conditions for Eq. (7). Time evolution of $f_{\pm 1}$ again is due to both the motion of the bath particles and of the tracer, i.e., can be represented in the form of Eq. (7), but here the operators $\hat{L}_{bath}$ and $\hat{L}_{trac}$ are given as

$$\hat{L}_{bath}(f_{\pm 1}) = \tfrac{1}{2}f_{\pm 2}(1-f_{\pm 1}) - \tfrac{1}{2}f_{\pm 1}(1-f_{\pm 2}), \tag{11}$$

$$\hat{L}_{trac}(f_1) = -pf_1(1-f_2)+qf_{-1}(1-f_1), \tag{12}$$

and

$$\hat{L}_{trac}(f_{-1}) = pf_1(1-f_{-1})-qf_{-1}(1-f_{-2}). \tag{13}$$

Explicitly, we have for $f_{\pm 1}$ the following equations:

$$\dot{f}_1 = \tfrac{1}{2}f_2(1-f_1) - \tfrac{1}{2}f_1(1-f_2) - pf_1(1-f_2) + qf_{-1}(1-f_1), \tag{14}$$

$$\dot{f}_{-1} = \tfrac{1}{2}f_{-2}(1-f_{-1}) - \tfrac{1}{2}f_{-1}(1-f_{-2}) + pf_1(1-f_{-1}) - qf_{-1}(1-f_{-2}). \tag{15}$$

Another pair of boundary conditions for Eq. (10) can be obtained by assuming that correlations between $P(X,t)$ and $\eta_{X+\lambda}(t)$ vanish in the limit $\lambda\to\pm\infty$, which seems quite plausible on physical grounds, and which may be checked numerically. We have from Eq. (6)

$$f_{\lambda\to\pm\infty} = \eta_{\pm\infty}(t)\sum_X P(X,t) = C_0, \tag{16}$$

where we have used the normalization condition $\Sigma_X P(X,t)=1$ and also the assumption that at infinitely large separations from the tracer the mean concentration of vacancies is unperturbed and equal to its equilibrium value C_0.

Equations (5) and (7) to (13) constitute a closed system of equations for the derivation of $\overline{X_T(E,t)}$, within the framework outlined. Solutions to these equations will be discussed in the next section.

IV. SOLUTION OF DYNAMIC EQUATIONS AND ANALYTICAL RESULTS

We first turn to the continuous-space description and rewrite our equations in the limit of continuous λ. Then, for $\lambda\neq\pm 1$ we have for the operator

$$\hat{L}_{bath}(f_\lambda) \approx \frac{1}{2}\frac{\partial^2 f_\lambda}{\partial\lambda^2}, \tag{17}$$

and, at points $\lambda=\pm 1$, Eq. (11) yields

$$\hat{L}_{bath}(f_{\pm 1}) \approx \frac{1}{2}\frac{\partial f_\lambda}{\partial\lambda}\Big|_{\lambda=\pm 1}, \tag{18}$$

Next, expanding $f_{\lambda-1}\approx f_\lambda - \partial f_\lambda/\partial\lambda$ and $f_{\lambda+1}\approx f_\lambda + \partial f_\lambda/\partial\lambda$ we obtain for the operator $\hat{L}_{trac}$ Eq. (10) the following approximate expression:

$$\hat{L}_{trac}(f_\lambda) \approx -qf_{-1}\frac{\partial f_\lambda}{\partial\lambda} + pf_1\frac{\partial f_\lambda}{\partial\lambda} = \overline{\dot{X}_T(E,t)}\frac{\partial f_\lambda}{\partial\lambda}, \tag{19}$$

which holds for $\lambda\neq\pm 1$.

The approximation of Eq. (19), in which the coefficient before the gradient term is equal to the *mean* velocity of the tracer particle, is equivalent to the neglect of fluctuations in the tracer trajectory $X_T(E,t)$. In the following we show, however, that such a ''deterministic'' approximation is quite appropriate and leads to results which are in good agreement with simulation data. The reason this approximation works here is that in such a system the fluctuations of the tracer trajectories are essentially suppressed. This is due to the accumulation of the bath particles in front of the tracer which hinders fluctuations with $X_T(E,t)>\overline{X_T(E,t)}$. At the same time, the fluctuations with $X_T(E,t)<\overline{X_T(E,t)}$ are suppressed by the driving force. This leads to the mean-square deviation $\overline{\sigma^2(t)}=[\overline{X_T(E,t)}]^2-\overline{X_T^2(E,t)}$ growing only as $\sqrt{t}$ (see the numerical results in Fig. 2, where the $[\overline{\sigma^2(t)}]^{1/2}$ is plotted versus $\sqrt{t}$), in a striking contrast to the linear time depen-

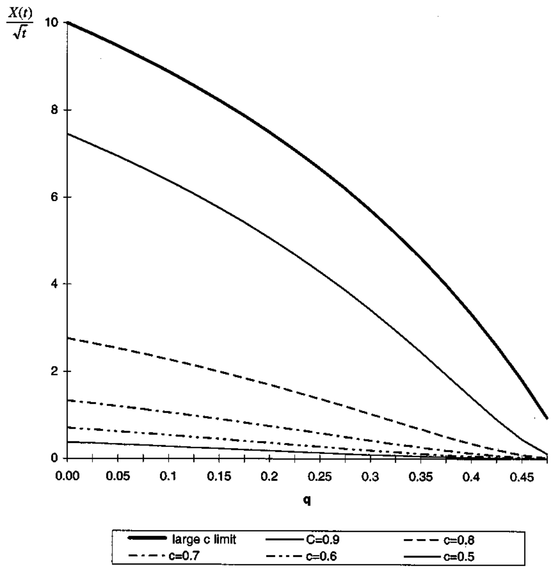

FIG. 1. Theoretical values of the prefactor in the dependence of the average tracer displacement $X(t)$ on $t^{1/2}$ vs the probability of the ''back step'' q.

dence for conventional driven diffusive motion. Finally, within the same ''deterministic'' picture we obtain

$$\hat{L}_{trac}(f_{\pm 1}) \approx \mp \overline{\dot{X}_T(E,t)}(1-f_{\pm 1}). \tag{20}$$

Combining Eqs. (17) to (20) we obtain the following continuous-space equation:

$$\dot{f}_\lambda = \frac{1}{2}\frac{\partial^2 f_\lambda}{\partial \lambda^2} + \overline{\dot{X}_T(E,t)}\frac{\partial f_\lambda}{\partial \lambda}, \tag{21}$$

which is to be solved subject to the boundary conditions

$$\dot{f}_{\lambda=\pm 1} = \pm\frac{1}{2}\frac{\partial f_\lambda}{\partial \lambda}\Big|_{\lambda=\pm 1} \mp \overline{\dot{X}_T(E,t)}(1-f_{\pm 1}) \tag{22}$$

and boundary conditions at $\lambda \to \pm\infty$, defined in Eq. (16).

A. Solutions for $\lambda \geqslant 1$

Let us consider first the behavior of f_λ for $\lambda \geqslant 1$. We introduce a scaled variable $\omega = (\lambda - 1)/\overline{X_T(E,t)}$, $(0 \leqslant \omega \leqslant \infty)$. In terms of ω Eq. (21) takes the following form:

$$\frac{d^2 f_\omega}{d\omega^2} + \alpha(\omega+1)\frac{d f_\omega}{d\omega} = 0, \tag{23}$$

in which we have set

$$\alpha = \frac{d}{dt}[\overline{X_T(E,t)}]^2, \tag{24}$$

and which is to be solved subject to the boundary conditions

$$f_{\omega=\infty} = C_0; \quad \frac{d f_\omega}{d\omega}\Big|_{\omega=0} = \alpha(1 - f_{\omega=0}). \tag{25}$$

We hasten to remark that such an approach presumes already that α is a time-independent constant and thus $\overline{X_T(E,t)}$ grows as $\sqrt{\alpha t}$. However, such an assumption will be seen to be self-consistent if it turns out to be possible (and we set out to show that this is actually the case) to find the solution of Eq. (23) satisfying the boundary conditions in Eqs. (25).

The appropriate solution to Eq. (23), which satisfies the boundary condition at infinity, reads

$$f_\omega = \frac{(C_0 - f_{\omega=0})}{I_+}\int_0^\omega d\omega\, \exp[-\alpha(\omega + \omega^2/2)] + f_{\omega=0}, \tag{26}$$

where

$$I_+(\alpha) \equiv I_+ = \int_0^\infty d\omega\, \exp[-\alpha(\omega+\omega^2/2)] = \left(\frac{\pi}{2\alpha}\right)^{1/2}\exp(\alpha/2)[1 - \mathrm{erf}(\sqrt{\alpha/2})], \tag{27}$$

erf(x) being the error function. The value of $f_{\omega=0}$, which is the probability of having the rhs adjacent to the tracer site vacant, is to be defined from the boundary condition at $\omega = 0$, Eq. (25), which gives

$$\frac{C_0 - f_{\omega=0}}{I_+} = \alpha(1 - f_{\omega=0}). \tag{28}$$

We note here that α is as yet unspecified parameter.

B. Solutions for $\lambda \leqslant -1$

Consider next the behavior of f_λ, Eq. (21), past the tracer particle, i.e., in the domain $\lambda \leqslant -1$. Now we choose the scaled variable $\theta = -(\lambda+1)/\overline{X_T(E,t)}$, $(0 \leqslant \theta \leqslant \infty)$. In terms of θ Eq. (21) takes the form

$$\frac{d^2 f_\theta}{d\theta^2} + \alpha(\theta - 1)\frac{d f_\theta}{d\theta} = 0, \tag{29}$$

with boundary conditions

$$f_{\theta=\infty} = C_0; \quad \frac{d f_\theta}{d\theta}\Big|_{\theta=0} = -\alpha(1 - f_{\theta=0}). \tag{30}$$

The solution of Eq. (29), which satisfies the boundary at $\theta = \infty$ reads

$$f_\theta = \frac{(C_0 - f_{\theta=0})}{I_-}\int_0^\theta d\theta\, \exp[\alpha(\theta - \theta^2/2)] + f_{\theta=0}, \tag{31}$$

where

$$I_-(\alpha) \equiv I_- = \int_0^\infty d\theta\, \exp[\alpha(\theta - \theta^2/2)] = \left(\frac{\pi}{2\alpha}\right)^{1/2}\exp(\alpha/2)[1 + \mathrm{erf}(\sqrt{\alpha/2})]. \tag{32}$$

The constant of integration $f_{\theta=0}$ (which defines the probability of having the left-hand side (lhs) adjacent to the tracer site vacant) is to be determined from the boundary condition at $\theta = 0$, which gives

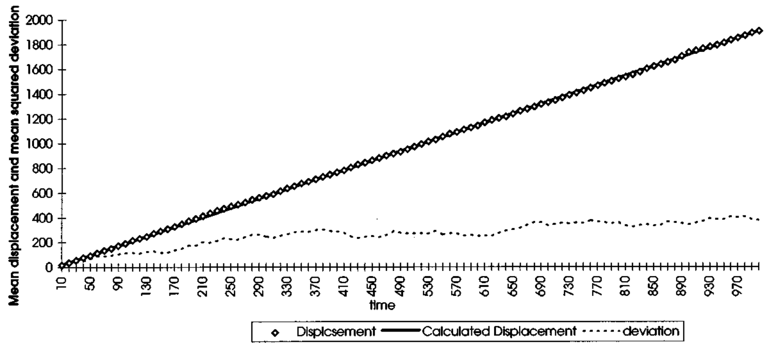

FIG. 2. Typical dependence of squared mean tracer displacement and mean-squared deviation on time.

$$\frac{C_0-f_{\theta=0}}{I_-}=-\alpha(1-f_{\theta=0}). \tag{33}$$

Now we have a system of equations (28),(33) and (5),(24), which determine the behavior of $\overline{X_T(E,t)}$, $f_{\omega=0}$ and $f_{\theta=0}$. In the following subsection we construct a closed-form transcendental equation for the parameter α.

C. Closed-form equation for α

We may formally rewrite Eq. (5) in terms of the parameters $f_{\omega=0}$ and $f_{\theta=0}$ as

$$\overline{\dot{X}_T(E,t)}=pf_{\omega=0}-qf_{\theta=0}. \tag{34}$$

Further, using Eqs. (34), (24), and (28) we have

$$\frac{(C_0-f_{\omega=0})}{2I_+\overline{X_T(E,t)}}=(pf_{\omega=0}-qf_{\theta=0})(1-f_{\omega=0}). \tag{35}$$

Let us note now that the rhs of Eq. (35) tends to zero as $\overline{X_T(E,t)}$ grows. This means that [except for the case $C_0=1$, when Eq. (35) has only a trivial solution $f_{\omega=0}=1$] the value $pf_{\omega=0}$ should tend to $qf_{\theta=0}$ as $t\to\infty$. Expressing $f_{\omega=0}$ as

$$f_{\omega=0}=\frac{qf_{\theta=0}}{p}+\phi, \tag{36}$$

where ϕ is a deviation from the equilibrium value $f_{\omega=0}$, and assuming that at sufficiently large times this deviation is small enough to allow linearization of the equation near the equilibrium, we have

$$\phi\approx\frac{pC_0-qf_{\theta=0}}{2pI_+(p-qf_{\theta=0})\overline{X_T(E,t)}}. \tag{37}$$

Now, from Eq. (33) we express $f_{\theta=0}$ through the parameter α, which gives

$$f_{\theta=0}=\frac{C_0+\alpha I_-}{1+\alpha I_-}, \tag{38}$$

and substituting Eq. (38) into Eq. (37) we get

$$\phi\approx\frac{C_0(p-q)+\alpha I_-(pC_0-q)}{2pI_+(p-qC_0+(p-q)\alpha I_-)\overline{X_T(E,t)}}. \tag{39}$$

Finally, noticing that $\overline{\dot{X}_T(E,t)}=p\phi$, and using the definition of the parameter α Eq. (24) we obtain the following closed transcendental equation for α:

$$\alpha=\frac{C_0(p-q)+\alpha I_-(pC_0-q)}{I_+[p-qC_0+(p-q)\alpha I_-]}, \tag{40}$$

which, after some algebraic transformations, can be cast into a compact, symmetric form

$$\left(\alpha I_+(\alpha)+\frac{q-pC_0}{p-q}\right)\left(\alpha I_-(\alpha)+\frac{p-qC_0}{p-q}\right)=\frac{pq(1-C_0)^2}{(p-q)^2}, \tag{41}$$

where the α dependence of $I_\pm$ [Eqs. (27) and (32)] has been made explicit.

A simple analysis shows that Eq. (41) has positive bounded solutions $\alpha(p,C_0)$ for any values of p, $q=1-p$ and C_0 (except the trivial case $C_0=1$ when bath particles are absent). This means, in turn, that our approach to the solutions of coupled Eqs. (23), (25), (29), and (30) is self-consistent and $\overline{X_T(E,t)}$ actually grows in proportion to $\sqrt{t}$. In the trivial case when $C_0=1$ [when one expects, of course, the linear growth of $\overline{X_T(E,t)}$] Eq. (41) reduces to

$$(\alpha I_+-1)(\alpha I_-+1)=0 \tag{42}$$

whose root is given by

$$\alpha I_+=1, \tag{43}$$

which means that $\alpha=\infty$ and thus $\overline{X_T(E,t)}$ grows at a faster rate than $\sqrt{t}$.

Behavior of the prefactor α is presented in Fig. 1, in which we plot the numerical solution of Eq. (41) for different values of the transition probabilities and different concentrations C_0. In the next subsection we present analytical estimates of the behavior of α in several limiting situations.

D. Analytical estimates of limiting behaviors of the parameter α

We start by considering situations in which the parameter α can be expected to be small; namely, when p is close to q (in other words when p is only slightly above 1/2) or when the vacancy concentration is small $C_0 \ll 1$. In the limit of small α the leading terms in Eqs. (27) and (32) behave as

$$I_{\pm} \approx \left(\frac{\pi}{2\alpha}\right)^{1/2} \tag{44}$$

and Eq. (41) takes the form

$$\left[\left(\frac{\pi\alpha}{2}\right)^{1/2} + \frac{q-pC_0}{p-q}\right]\left[\left(\frac{\pi\alpha}{2}\right)^{1/2} + \frac{p-qC_0}{p-q}\right] = \frac{pq(1-C_0)^2}{(p-q)^2}, \tag{45}$$

and gives for small α, $\alpha \ll 1$,

$$\alpha \approx \frac{2}{\pi}\left(\frac{C_0(p-q)}{1-C_0}\right)^2. \tag{46}$$

Consequently, in this limit the explicit formula for the mean displacement will read

$$\overline{X_T(E,t)} \approx \frac{C_0(p-q)}{1-C_0}\left(\frac{2t}{\pi}\right)^{1/2} = \frac{C_0 \tanh(\beta E/2)}{1-C_0}\left(\frac{2t}{\pi}\right)^{1/2}. \tag{47}$$

At this point it might be instructive to recall the analysis in [3] which concerned the validity of the Einstein relation for one-dimensional hard-core lattice gases. Define the ''diffusion coefficient'' of the tracer particle in the symmetric case as $D = \lim_{t\to\infty} D(t)$, where $D(t) = \overline{X_T^2(E=0,t)}/(2t)$ and the ''mobility'' as $\mu = \lim_{E\to 0}[U(E)/E]$, where the stationary velocity is given by $U(E) = \lim_{t\to\infty} U(E,t)$, $U(E,t) = X_T(E,t)/t$. In [3] it was shown that for the infinitely large system the Einstein relation, i.e., the equation $\mu = \beta D$, holds trivially, since both D and μ are equal to zero. A somewhat stronger result has been obtained for the case when the one-dimensional lattice is a ring of length l. It was shown that here both D and μ are finite, vanish with the length of the ring as $1/l$, and obey the Einstein relation $\mu(l) = \beta D(l)$. Our result in Eq. (47) reveals that for the infinite lattice Einstein relation is valid for the time-dependent ''diffusion coefficient'' and mobility, i.e., equation $\mu(t)\{= \lim_{E\to 0}[U(E,t)/E]\} = \beta D(t)$ holds exactly, provided that the time is sufficiently large such that both Eqs. (1) and (47) are valid.

Consider next the situation when α is expected to be large, i.e., when C_0 is close to unity. Expanding the functions I_+ and I_- as

$$I_+ \approx \frac{1}{\alpha} - \frac{1}{\alpha^2} \to 0 \quad \text{when} \quad \alpha \to \infty, \tag{48}$$

and

$$I_- \approx \left(\frac{2\pi}{\alpha}\right)^{1/2} \exp(\alpha/2) \to \infty \quad \text{when} \quad \alpha \to \infty, \tag{49}$$

we arrive at the following equation:

$$\left(1 + \frac{q-pC_0}{p-q} - \frac{1}{\alpha}\right) = \frac{pq(1-C_0)^2}{(p-q)^2}\left[\sqrt{2\pi\alpha}\exp(\alpha/2) + \frac{p-qC_0}{p-q}\right]^{-1}. \tag{50}$$

One may readily notice that when α is large, the rhs of Eq. (50) tends to zero and thus we have

$$\alpha \approx \frac{p-q}{p(1-C_0)}. \tag{51}$$

Equation (51) allows formulation of the conditions when α is large, more precisely: this happens when C_0 obeys the inequality $1 > C_0 \gg q/p = \exp(-\beta E)$.

In this limit the mean displacement of the tracer particle obeys

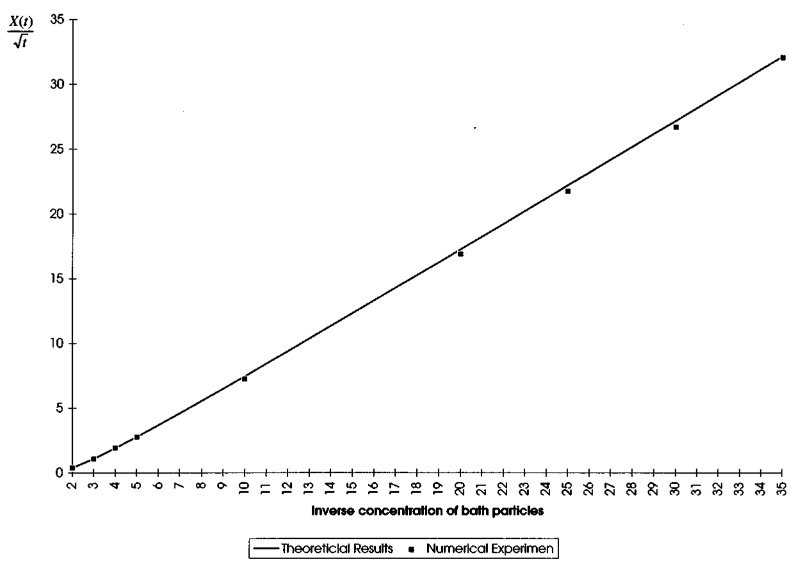

FIG. 3. Theoretical and experimental values of the prefactor in the dependence of the average tracer displacement $X(t)$ on $t^{1/2}$ vs the inverse concentration of bath particles $(q=0)$.

$$\overline{X_T(E,t)} \approx \left[\frac{(p-q)t}{p(1-C_0)}\right]^{1/2} = \left(\frac{[1-\exp(-\beta E)]t}{1-C_0}\right)^{1/2}. \tag{52}$$

Finally, let us consider the case of the directed walk in a one-dimensional lattice gas, when $p=1$ and $q=0$, which was previously examined in [39]. In this case Eq. (41) simplifies considerably and reads

$$\alpha_\infty I_+ = C_0. \tag{53}$$

When C_0 is small, $C_0 \ll 1$, we have from Eq. (53)

$$\alpha_\infty \approx \frac{2C_0^2}{\pi}, \tag{54}$$

which is consistent with the result in Eq. (47), while in the limit $C_0 \approx 1$, Eq. (53) yields

$$\alpha_\infty \approx \frac{1}{1-C_0}, \tag{55}$$

i.e., exactly the behavior in Eq. (51) with $p=1$ and $q=0$.

V. NUMERICAL SIMULATIONS

In order to check the analytical predictions of Sec. IV and V Monte Carlo (MC) simulations have been performed. The simulation algorithm was defined as follows: The total number of particles in the system was held constant at 399 (398 bath particles and one tracer). We constructed a one-dimensional regular lattice of unit spacing and length $2L+1$, sites of which were labeled by integers on the interval $[-L,L]$. For each C_p, the length was chosen as $L=399/C_p$. The number of particles and, thus, L was chosen to be large enough so that over the time scale of the simulations the mean vacancy density near $L_\pm$ was unaffected by the dynamics of the tracer which always occupied the lattice site 0 at $t=0$. At the zero moment of MC time particles were placed randomly on the lattice with the prescribed mean concentration and the constraint that no two particles can simultaneously occupy the same site. The tracer particle was placed at the origin. The subsequent particle dynamics employed in simulations follows the definitions of Sec. II closely. At each MC time step we select, at random, one particle and let it choose a potential jump direction. If the selected particle is a bath particle, it chooses the direction of the jump — to the right or to the left, with the probability 1/2. If the selected particle is the tracer — it chooses the hop to the right with probability p and the hop to the left with probability q, $q=1-p$. For any particle the jump is instantly fulfilled if at this moment of time the adjacent site in the chosen direction is vacant.

In simulations we followed the time evolution of the displacement of the tracer particle and plotted it versus the ''physical time,'' which is the time needed for each particle to move once, on average. Figure 2 presents typical behavior of the average displacement calculated for fixed q and C_0 (the actual parameter for the presented results are $q=0$ and $C_0=1/3$, the results for other values of C_0 and q are similar) plotted versus $\sqrt{t}$. The dotted line in this figure shows the evolution of the deviation from the mean average displacement $(\overline{\sigma^2})^{1/2}$ which shows growth in proportion to $t^{1/4}$.

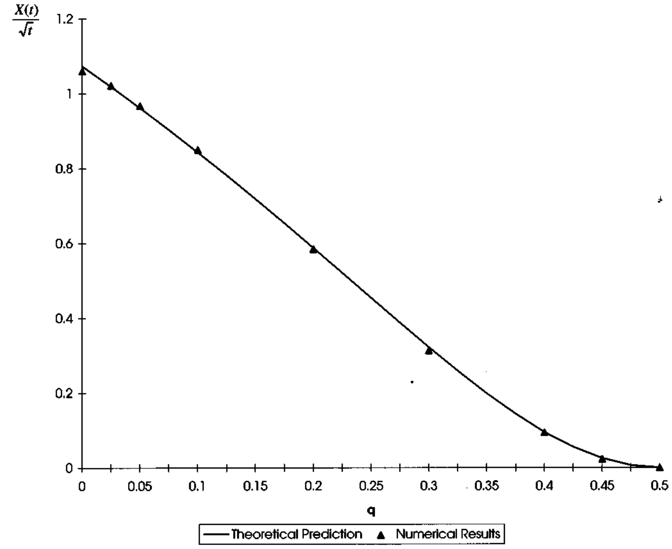

FIG. 4. Theoretical and experimental values of the prefactor in the dependence of the average tracer displacement $X(t)$ on $t^{1/2}$ vs q $(C=1/3)$.

Numerical results for the time evolution of the mean displacement, performed for different values of parameters C_0 and p, were used to obtain a numerical evaluation of the prefactor in Eq. (3) as a function of C_0 and p. In Fig. 3 we plot, for the particular case of totally directed walk $q=0$, the prefactor α versus the inverse concentration of vacancies. The solid line represents the results of our analytic calculations while the squares show the numerical results. In Fig. 4, for fixed concentration of the vacancies $C_0=1/3$ we present the comparison between the analytical predictions of the prefactor α and the numerical MC results.

VI. CONCLUSIONS

To conclude, we have examined the behavior of the mean displacement of a driven tracer particle moving in a symmetric hard-core lattice gas. We have shown that the mean displacement grows in proportion to $\sqrt{t}$, i.e., the hard-core interactions hinder the ballistic motion of the tracer and introduce effective frictional forces. The prefactors in the growth law are determined implicitly, in a form of the transcendental equation, for arbitrary magnitude of the driving force and arbitrary concentration of the lattice-gas particles. In several asymptotic limits we find explicit formulas for these prefactors. Our analytical findings are in a very good agreement with the results of the numerical simulations.

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