Ultraslow vacancy-mediated tracer diffusion in two dimensions: The Einstein relation verified

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We study the dynamics of a charged tracer particle (TP) on a two-dimensional lattice, all sites of which except one (a vacancy) are filled with identical neutral, hard-core particles. The particles move randomly by exchanging their positions with the vacancy, subject to the hard-core exclusion. In the case when the charged TP experiences a bias due to external electric field $\mathbf{E}$ (which favors its jumps in the preferential direction), we determine exactly the limiting probability distribution of the TP position in terms of appropriate scaling variables and the leading large-n (n being the discrete time) behavior of the TP mean displacement $\overline{\mathbf{X}}_n$; the latter is shown to obey an anomalous, logarithmic law $|\overline{\mathbf{X}}_n| = \alpha_0(|\mathbf{E}|)\ln(n)$. Comparing our results with earlier predictions by Brummelhuis and Hilhorst [J. Stat. Phys. **53**, 249 (1988)] for the TP diffusivity D_n in the unbiased case, we infer that the Einstein relation $\mu_n = \beta D_n$ between the TP diffusivity and the mobility $\mu_n = \lim_{|\mathbf{E}|\to 0}(|\overline{\mathbf{X}}_n|/|\mathbf{E}|n)$ holds in the leading n order, despite the fact that both D_n and μ_n are not constant but vanish as $n\to\infty$. We also generalize our approach to the situation with very small but finite vacancy concentration ρ_v, in which case we find a ballistic-type law $|\overline{\mathbf{X}}_n| = \pi\alpha_0(|\mathbf{E}|)\rho_v n$. We demonstrate that here, again, both D_n and μ_n, calculated in the linear in ρ_v approximation, do obey the Einstein relation.

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I. INTRODUCTION

Consider a square lattice of which each site except one is filled with a hard-core particle. The empty site is referred to as a "vacancy." The particles move randomly on the lattice, their random walks being constrained by the condition that each site can be at most singly occupied. More specifically, at each moment of time $n=1,2,3,\ldots$ one particle selected with probability 1/4 among the four particles surrounding the vacancy will exchange its position with the vacancy. Next suppose that one selects one of the particles, "tags" it, and follows its trajectory $\mathbf{X}_n$. Evidently, dynamics of the tagged, the tracer particle (TP), will be quite complicated, in contrast to the standard, by definition, lattice random walk executed by the vacancy: The TP can move only when encountered by the vacancy and its successive moves will be correlated, since the vacancy will always have a greater probability to return for its next encounter from the direction it has left than from a perpendicular or opposite direction. On the other hand, it is clear that on a two-dimensional (2D) lattice the TP will make infinitely long excursions as $n\to\infty$ even in the presence of a single vacancy, since its random walk is recursive in 2D and the vacancy is certain to encounter the tracer particle many times. A natural question is, of course, what are the statistical properties of the TP random walk, its mean-square displacement $\overline{\mathbf{X}_n^2}$ from its initial position at time moment n, and the probability $P_n^{(tr)}(\mathbf{X})$ that at time n the TP appears at position $\mathbf{X}=(x_1,x_2)$?

The just described model, which represents, in fact, one of the simplest cases of the so-called "slaved diffusion processes," has been studied over the years in various guises: the "constrained dynamics" model of Palmer [1]; vacancy-mediated bulk diffusion in metals and crystals (see, e.g., [2–7]); frictional properties of dynamical percolative environments [8,9]; or dynamics of impure atoms in close-packed surface layers of metal crystals, such as, e.g., a copper [10–13]. Brummelhuis and Hilhorst [14] were the first to present an exact solution of this model in the lattice formulation. It has been shown that, in the presence of a single vacancy, the TP trajectories are remarkably confined; the mean-square displacement shows an unbounded growth, but it grows only *logarithmically* with time,

$$\overline{\mathbf{X}_n^2} \sim \frac{\ln(n)}{\pi(\pi-1)}, \quad \text{as} \quad n\to\infty, \tag{1}$$

which implies that the TP diffusivity D_n, defined as

$$D_n = \frac{\overline{\mathbf{X}_n^2}}{4n} \sim \frac{\ln(n)}{4\pi(\pi-1)n}, \tag{2}$$

is not constant but rather vanishes as time n progresses.

Moreover, it has been found [14] that at sufficiently large times, $P_n^{(tr)}(\mathbf{X})$ converges to a limiting form as a function of the scaling variable $\eta = |\mathbf{X}|/\sqrt{\ln(n)}$. Still striking, this limiting distribution is not a *Gaussian* but a modified Bessel function $K_0(\eta)$, which signifies that the successive steps of the TP, although separated by long time intervals, are effectively correlated. These results have been subsequently reproduced by means of different analytical techniques in Refs. [15–17].

Brummelhuis and Hilhorst have also generalized their analytical approach to the case of a very small but finite vacancy concentration ρ_v [18], in which case a conventional diffusive-type behavior

$$\overline{\mathbf{X}_n^2} = \frac{\rho_v n}{(\pi - 1)}, \quad \rho_v \ll 1, \quad n \to \infty \tag{3}$$

has been recovered. Note that Eq. (3) coincides with the earlier result of Nakazato and Kitahara [2] in the limit $\rho_v \ll 1$, and is well confirmed by numerical simulations [4,19].

Note that Eqs. (1)–(3) also reveal, as we have already remarked, essential correlations in successive moves of the TP. To see this, one notices that in the absence of such correlations the TP diffusion coefficient can be estimated as $D_0 \sim \omega/4$, where D_0 refers to the TP uncorrelated random walk due to a single vacancy, 4 is the coordination number of the square lattice, while ω stands for the mean frequency at which the TP performs the moves. The latter is evidently equal to the frequency at which the TP is visited by the vacancy, i.e., $\omega = \tau_n / n$ with τ_n being the mean number of such visits during time n. Since the vacancy performs a standard lattice random walk, one has $\tau_n \sim \ln(n)/\pi$ (see, e.g., Ref. [5]) and, hence, discarding the correlations in successive moves of the TP, we should find $D_0 \sim \ln(n)/4\pi n$. On comparing D_0 and D_n in Eq. (2), we observe that both show the same n-dependence but the prefactors are different, which means that correlations are marginally important—they do not change the n dependence but renormalize the numerical factors. It is customary to define the so-called correlation factor f_{corr} [4,14] as $f_{corr} = D_n / D_0$ as the property which, in essence, embodies all nontrivial physics and represents the main challenge for the theoretical analysis of diffusion in interacting particles' systems. For the model under study, one has that $f_{corr} = 1/(\pi - 1) \approx 0.467 \ldots < 1$ and, hence, correlations induce a stronger confinement of the TP trajectories due to the enhanced probability of moves in the direction opposite to the direction of the preceding move. As a matter of fact, as shown in Ref. [14], for the square lattice the "effective" probability for the TP to step in the direction opposite to its preceding move is 1/2, while the "effective" probabilities to step in a perpendicular direction or to step once more in the same direction amount only to 0.1816 and 0.1366, respectively. Note finally that the same type of arguments apply to the result in Eq. (3). Here, discarding correlations, one expects that $D_0 \sim \rho/4$ since the mean frequency of moves (which equals the mean frequency of the TP encounters with the vacancies) is proportional to the vacancy concentration. On comparing the latter estimate with the result in Eq. (3), one finds that they are related with exactly the same correlation factor.

This paper is devoted to the following, rather fundamental in our opinion, problem: Suppose that we charge the tracer particle (while the rest are kept neutral) and switch on an electric field $\mathbf{E}$. In such a situation, the TP will have asymmetric hopping probabilities and in its exchanges with the vacancy, depending on the TP and vacancy relative orientation, the TP will have a preference (or, on the contrary, a reduction of the rate) for exchanging its position with the vacancy compared to the other three neighboring particles. One might expect that in this case the TP mean displacement $\overline{\mathbf{X}_n}$ will not be exactly equal to zero and might define the TP mobility as

$$\mu_n = \lim_{|\mathbf{E}| \to 0} \frac{|\overline{\mathbf{X}_n}|}{|\mathbf{E}| n}. \tag{4}$$

Now, the question is whether or not the mobility μ_n, calculated from the TP mean displacement in the presence of an external electric field, and the diffusivity D_n, Eq. (2), deduced from the TP mean-square displacement in the absence of the field, obey the generalized Einstein relation of the form

$$\mu_n = \beta D_n, \tag{5}$$

where β denotes the reciprocal temperature.

Note that this question has been already addressed within the context of the TP diffusion in one-dimensional (1D) hard-core lattice gases with arbitrary finite vacancy concentration [3,6,7,20,21]. It has been found that Eq. (5) holds not only for the TP diffusion in a 1D hard-core gas on a finite lattice [3], but also for infinite 1D lattices with nonconserved [7] and conserved particle numbers [6,20,21]. Remarkably, in the latter case, Eq. (5) holds for n sufficiently large despite the fact that both the TP mobility and the diffusivity are not constant as $n \to \infty$ but all vanish in proportion to $1/\sqrt{n}$ [6,20,21]. As well, the validity of the Einstein relation has been corroborated for the charge carriers in semiconductors [22] and for polymeric systems in the subdiffusive regime [23,24]. On the other hand, it is well known that the Einstein relation is violated in some physical situations; for instance, it is not fulfilled for Sinai diffusion [25] or diffusion on percolation clusters, due to effects of strong temporal trapping in the dangling ends, as well as for the Scher-Lax-Montroll model of anomalous random walk [26] (see also Refs. [27] and [28] for some other examples). Hence, in principle, it is not *a priori* clear whether or not Eq. (5) should be valid for the model under study; here, the TP walk proceeds only due to encounters with a *single* vacancy, its mean-square displacement grows only *logarithmically* with time, and the diffusivity follows a much faster decay law in Eq. (2), compared to the $D_n \sim n^{-1/2}$ law obtained for the one-dimensional systems with finite vacancy concentrations.

The paper is structured as follows: In Sec. II we present a more precise formulation of the problem and introduce basic notations. In Sec. III we discuss our general approach to computation of the probability $P_n^{(tr)}(\mathbf{X})$ of finding the TP at position $\mathbf{X}$ at time moment n, and to evaluate $P_n^{(tr)}(\mathbf{X})$ in the general form as a function of some return probabilities describing the random walk executed by the vacancy. Section IV is devoted to the calculation of these return probabilities in the general case, as well as to the derivation of explicit expressions determining their asymptotical behavior. In Sec. V we present explicit asymptotical results for both the probability distribution and the TP mean displacement. We show that as $n \to \infty$, $P_n^{(tr)}(\mathbf{X})$, written in terms of two appropriate scaling variables, converges to a rather unusual limiting distribution. We also demonstrate here that the TP mobility, which is obtained in the present work in the leading n order, and the TP diffusivity in the unbiased case, calculated earlier by Brummelhuis and Hilhorst [14], do obey the Einstein re-

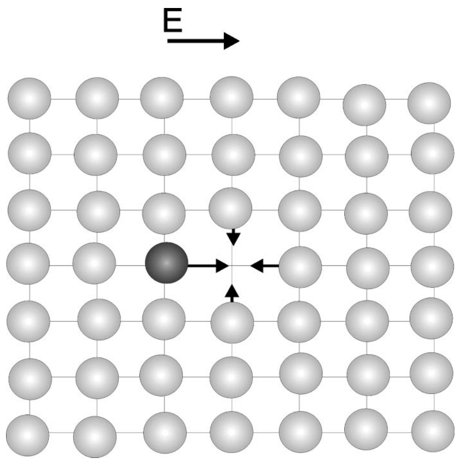

FIG. 1. Two-dimensional, infinite in both directions, square lattice in which all sites except one are filled with identical hard-core particles (gray spheres). The black sphere denotes a single tracer particle, which is subject to external field **E**, oriented in the positive x_1 direction, and thus has asymmetric hopping probabilities. The arrows of different size depict schematically the hopping probabilities; a larger arrow near the TP indicates that it has a preference for moving in the direction of the applied field.

lation. Further on, in Sec. VI we extend an approximate description of the situation with very small but finite vacancy concentration ρ_v, proposed originally in Ref. [18], over the case when the TP is subject to an external electric field, and determine the TP mobility in the leading n and ρ_v order. We also show that in this case the TP mobility and the TP diffusivity in the unbiased case do obey the Einstein relation, in the linear ρ_v approximation and in the leading n order. As well, for this situation we find the limiting probability distribution of the TP position. Finally, in Sec. VII, we conclude with a brief summary and discussion of our results.

II. THE MODEL

Consider a two-dimensional, infinite in both x_1 and x_2 directions, square lattice, every site of which except one (a vacancy) is filled by identical hard-core particles (see Fig. 1). All particles except one are electrically neutral. The charged particle, which is initially at the origin, will be referred to in what follows as the tracer particle, the TP. Its position at the lattice at time n will be denoted by $\mathbf{X}_n$. Electric field $\mathbf{E}$ of strength $E=|\mathbf{E}|$ is oriented in the positive x_1 direction. For simplicity, the charge of the TP is set equal to unity.

We suppose that every particle performs a random walk in discrete time n, constrained by the single-occupancy condition (hard-core exclusion). In consequence, only those neighboring the vacancy particles can move. In order to specify dynamics of the system, we will distinguish here between ''individual'' characteristics of the particle's motion, and ''collective'' ones. By the term ''individual'' we presume characteristics of isolated particles, while ''collective'' ones describe the resulting evolution of the entire system. We first describe the individual characteristics of particles' dynamics. We suppose that each neutral particle performs a symmetric random walk between nearest-neighboring sites. Hence, for the neutral particles all jump directions are equally probable and the jump direction probabilities are equal. The motion of the tracer particle is affected by the applied electric field such that it ''prefers'' to jump along its direction. The normalized jump direction probabilities of the (isolated) TP are given, in the usual fashion, by

$$p_\nu = Z^{-1}\exp\left[\frac{\beta}{2}(\mathbf{E}\cdot\mathbf{e}_\nu)\right], \tag{6}$$

where Z is the normalization constant, $\mathbf{e}_\nu$ is the unit vector denoting the jump direction, $\nu\in\{\pm1,\pm2\}$, and $(\mathbf{E}\cdot\mathbf{e}_\nu)$ stands for the scalar product. We adopt the notations $\mathbf{e}_{\pm 1}=(\pm1,0)$ and $\mathbf{e}_{\pm 2}=(0,\pm1)$, which means that $\mathbf{e}_1$ $(\mathbf{e}_{-1})$ is the unit vector in the positive (negative) x_1 direction, while $\mathbf{e}_2$ $(\mathbf{e}_{-2})$ is the unit vector in the positive (negative) x_2 direction. Consequently, the normalization constant Z is

$$Z=\sum_\mu \exp\left[\frac{\beta}{2}(\mathbf{E}\cdot\mathbf{e}_\mu)\right], \tag{7}$$

where the sum with the subscript μ denotes summation over all possible orientations of the vector $\mathbf{e}_\mu$, that is, $\mu=\{\pm1,\pm2\}$. Note that the jump direction probabilities defined by Eqs. (6) and (7) do preserve the standard detailed balance condition of the form

$$p_\nu \exp\left[-\frac{\beta}{2}(\mathbf{E}\cdot\mathbf{e}_\nu)\right]=p_{-\nu}\exp\left[\frac{\beta}{2}(\mathbf{E}\cdot\mathbf{e}_\nu)\right]. \tag{8}$$

Turning next to the evolution of the entire system, we first note that the choice of the ''collective'' transition probabilities q_ν is rather nontrivial. Similarly to the situation described in Ref. [29], which concerned a biased dynamics of the TP in a two-dimensional lattice gas, one expects a nonhomogeneous particles' density distribution around the TP. This implies that, in particular, simple detailed balance relation in Eq. (8) is invalid and the ''true'' detailed balance condition would also involve average particles' densities at the sites ν and $-\nu$.

As we have already remarked, hard-core exclusion hinders the hopping motion of all particles, except for four nearest-neighbors of the vacancy. That is, for only four particles adjacent to the vacancy an attempt to jump might be successful. Then, the most natural choice coherent with the individual dynamic rules is to assume that at each time step:

(i) if the TP is not adjacent to the vacancy, one particle, chosen with probability 1/4 among four nearest-neighbors of the vacancy, exchanges its position with the vacancy; and

(ii) if the TP is at the site $\mathbf{X}_n$ and the vacancy occupies an adjacent site $\mathbf{X}_n+\mathbf{e}_\nu$, then the TP exchanges its position with the vacancy with probability

$$q_{-\nu}=Z_\nu^* p_\nu, \tag{9}$$

i.e., $q_{-\nu}$ is proportional to the probability p_ν of an isolated particle, Eq. (6), which mirrors its preference for jumps in the direction of the applied field, while the probability of the exchange of positions with any of the other three adjacent neutral particles is given by

$$q_{\mu\neq-\nu}=\frac{1}{4}Z_{\nu}^{*}. \tag{10}$$

The normalization factor Z_{ν}^{*}, dependent on the initial position ν, is chosen next from the condition that the vacancy performs one jump each time step as it is prescribed in the original model of Brummelhuis and Hilhorst. Such a condition yields

$$Z_{\nu}^{*}=(3/4+p_{\nu})^{-1}. \tag{11}$$

Also note that without imposing such a condition we would introduce artificial "temporal trapping" probability, which would definitely lead to a violation of Eq. (5).

Such a choice of the dynamic rules completely defines the time evolution of the system. Note that, apart from four sites in the immediate vicinity of the tracer particle, the vacancy performs a standard, symmetric random walk. In the vicinity of the TP, the vacancy jump direction probabilities are perturbed by the TP asymmetric hopping rules. Hence, the random walk executed by the vacancy can be thought of as a particular case of the so-called "random walk with defective sites" (see Ref. [5] for more details), or as a realization of the "random walk with a hop-over site" [17].

III. PROBABILITY DISTRIBUTION FUNCTION $P_n^{(tr)}(\mathbf{X})$

A standard approach to define the properties of the TP random walk would be to start with a master equation determining the evolution of the whole configuration of particles. In doing so, similarly to the analysis of the tracer diffusion on 2D lattices in the presence of a finite vacancy concentration (see, e.g., Ref. [29]), one obtains the evolution of the joint distribution $P_n(\mathbf{X},\mathbf{Y})$ of the TP position $\mathbf{X}$ and of the vacancy position $\mathbf{Y}$ at time moment n. The property of interest, i.e., the reduced distribution function of the TP alone, will then be found from $P_n(\mathbf{X},\mathbf{Y})$ by performing lattice summation over all possible values of the variable $\mathbf{Y}$.

Here we pursue, however, a different approach, which has been first put forward in the original work of Brummelhuis and Hilhorst [14], that is, we construct the distribution function of the TP position at time n directly in terms of the return probabilities of the random walk performed by the vacancy. The only complication, compared to the unbiased case considered by Brummelhuis and Hilhorst [14], is that in our case ten different return probabilities would be involved, instead of three different ones appearing in the unbiased case. Hence, the analysis will be slightly more involved.

We begin by introducing some basic notations.

(i) Let $P_n^{(tr)}(\mathbf{X})$ be the probability that the TP, which starts its random walk at the origin, appears at the site $\mathbf{X}$ at time moment n, given that the vacancy is initially at site $\mathbf{Y}_0$.

(ii) Let $F_n^{*}(\mathbf{0}|\mathbf{Y_0})$ be the probability that the vacancy, which starts its random walk at the site $\mathbf{Y}_0$, arrives at the origin $\mathbf{0}$ for the first time at the time step n.

(iii) Let $F_n^{*}(\mathbf{0}|\mathbf{e}_{\boldsymbol{\nu}}|\mathbf{Y_0})$ be the conditional probability that the vacancy, which starts its random walk at the site $\mathbf{Y}_0$, appears at the origin for the first time at the time step n, being at time moment $n-1$ at the site $\mathbf{e}_{\boldsymbol{\nu}}$.

Further on, for any time-dependent quantity L_n we define the generating function of the form

$$L(\xi)=\sum_{n=0}^{+\infty}L_n\xi^n, \tag{12}$$

and for any space-dependent quantity $Y(\mathbf{X})$ the discrete Fourier transform

$$\tilde{Y}(\mathbf{k})=\sum_{\mathbf{X}}\exp(i(\mathbf{k}\cdot\mathbf{X}))Y(\mathbf{X}), \tag{13}$$

where the sum runs over all lattice sites.

Now, following Brummelhuis and Hilhorst [14], we write down directly the equation obeyed by the reduced probability distribution $P_n^{(tr)}(\mathbf{X})$ (cf. Ref. [16] for a study of the joint probability of the TP position and of the vacancy position in the unbiased case):

$$\begin{aligned}P_n^{(tr)}(\mathbf{X})={}&\delta_{\mathbf{X},\mathbf{0}}\left(1-\sum_{j=0}^{n}F_j^{*}(\mathbf{0}|\mathbf{Y_0})\right)+\sum_{p=1}^{+\infty}\sum_{m_1=1}^{+\infty}\cdots\sum_{m_p=1}^{+\infty}\sum_{m_{p+1}=0}^{+\infty}\delta_{m_1+\cdots+m_{p+1},n}\sum_{\nu_1}\cdots\sum_{\nu_p}\delta_{\mathbf{e}_{\boldsymbol{\nu}_1}+\cdots+\mathbf{e}_{\boldsymbol{\nu}_p},\mathbf{X}}\\&\times\left(1-\sum_{j=0}^{m_{p+1}}F_j^{*}(\mathbf{0}|-\mathbf{e}_{\boldsymbol{\nu}_\mathbf{p}})\right)F_{m_p}^{*}(\mathbf{0}|\mathbf{e}_{\boldsymbol{\nu}_\mathbf{p}}|-\mathbf{e}_{\boldsymbol{\nu}_{\mathbf{p}-\mathbf{1}}})\cdots F_{m_2}^{*}(\mathbf{0}|\mathbf{e}_{\boldsymbol{\nu}_\mathbf{2}}|-\mathbf{e}_{\boldsymbol{\nu}_\mathbf{1}})F_{m_1}^{*}(\mathbf{0}|\mathbf{e}_{\boldsymbol{\nu}_\mathbf{1}}|\mathbf{Y_0}).\end{aligned} \tag{14}$$

Next, using the definition of the generating functions and of the discrete Fourier transforms, Eqs. (12) and (13), we obtain the following matricial representation of the generating function of the TP probability distribution:

$$\tilde{P}^{(tr)}(\mathbf{k};\xi)=\frac{1}{1-\xi}\left(1+\mathcal{D}^{-1}(\mathbf{k};\xi)\sum_{\mu}U_{\mu}(\mathbf{k};\xi)F^{*}(\mathbf{0}|\mathbf{e}_{\boldsymbol{\mu}}|\mathbf{Y_0};\xi)\right). \tag{15}$$

In Eq. (15) the function $\mathcal{D}(\mathbf{k};\xi)$ stands for the determinant of the following 4×4 matrix:

$$\mathcal{D}(\mathbf{k};\xi)\equiv\det[\mathbf{I}-\mathbf{T}(\mathbf{k};\xi)], \tag{16}$$

where the matrix $\mathbf{T}(\mathbf{k};\xi)$ has the elements $(\mathbf{T}(\mathbf{k};\xi))_{\nu,\mu}$ defined by

$$(\mathbf{T}(\mathbf{k};\xi))_{\nu,\mu}=\exp(i(\mathbf{k}\cdot\mathbf{e}_{\nu}))A_{\nu,-\mu}(\xi). \tag{17}$$

Explicitly, the matrix $\mathbf{T}(\mathbf{k};\xi)$ is given by

$$\mathbf{T}(\mathbf{k};\xi)\equiv\begin{pmatrix} e^{ik_1}A_{1,-1}(\xi) & e^{ik_1}A_{1,1}(\xi) & e^{ik_1}A_{1,-2}(\xi) & e^{ik_1}A_{1,2}(\xi)\\ e^{-ik_1}A_{-1,-1}(\xi) & e^{-ik_1}A_{-1,1}(\xi) & e^{-ik_1}A_{-1,-2}(\xi) & e^{-ik_1}A_{-1,2}(\xi)\\ e^{ik_2}A_{2,-1}(\xi) & e^{ik_2}A_{2,1}(\xi) & e^{ik_2}A_{2,-2}(\xi) & e^{ik_2}A_{2,2}(\xi)\\ e^{-ik_2}A_{-2,-1}(\xi) & e^{-ik_2}A_{-2,1}(\xi) & e^{-ik_2}A_{-2,-2}(\xi) & e^{-ik_2}A_{-2,2}(\xi)\end{pmatrix}, \tag{18}$$

where the coefficients $A_{\nu,\mu}(\xi)$, $\nu,\mu=\pm1,\pm2$, stand for

$$A_{\nu,\mu}(\xi)\equiv F^{*}(\mathbf{0}|\mathbf{e}_{\nu}|\mathbf{e}_{\mu};\xi)=\sum_{n=0}^{+\infty}F_n^{*}(\mathbf{0}|\mathbf{e}_{\nu}|\mathbf{e}_{\mu})\xi^{n}, \tag{19}$$

i.e., are the generating functions of the conditional probabilities for the first time visit of the origin by the vacancy, conditioned by constraint of the passage through a specified site on the previous step. Note that, by symmetry,

$$A_{2,\nu}(\xi)=A_{-2,\nu}(\xi),$$

$$A_{\nu,2}(\xi)=A_{\nu,-2}(\xi) \tag{20}$$

for $\nu=\pm1$, and

$$A_{2,2}(\xi)=A_{-2,-2}(\xi),$$

$$A_{2,-2}(\xi)=A_{-2,2}(\xi). \tag{21}$$

As a result of such a symmetry, we have to consider just ten independent functions $A_{\mu,\nu}(\xi)$ (note that in the unbiased case one has to deal with only three such functions [14]). Explicit expression of the determinant in Eq. (16) in terms of these generating functions is presented in the Appendix. Lastly, the matrix $U_{\mu}(\mathbf{k};\xi)$ in Eq. (15) is given by

$$U_{\mu}(\mathbf{k};\xi)\equiv\mathcal{D}(\mathbf{k};\xi)\sum_{\nu}(1-e^{-i(\mathbf{k}\cdot\mathbf{e}_{\nu})})[I-T(\mathbf{k};\xi)]^{-1}_{\nu,\mu}e^{i(\mathbf{k}\cdot\mathbf{e}_{\mu})}. \tag{22}$$

The property of interest, the TP probability distribution function, will then be obtained by inverting $\tilde{P}^{(tr)}(\mathbf{k};\xi)$ with respect to the wave vector k and to the variable ξ:

$$P_n^{(tr)}(\mathbf{X})=\frac{1}{2i\pi}\oint_{\mathcal{C}}\frac{d\xi}{\xi^{n+1}}\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}dk_1\int_{-\pi}^{\pi}dk_2 \times e^{i(\mathbf{k}\cdot\mathbf{X})}\tilde{P}^{(tr)}(\mathbf{k};\xi), \tag{23}$$

where the contour of integration $\mathcal{C}$ encircles the origin counterclockwise.

Finally, we remark that as far as we are interested in the leading large-n behavior of the probability distribution $P_n^{(tr)}(\mathbf{X})$ only, here we may constrain ourselves to the study of the asymptotic behavior of the generating function $\tilde{P}^{(tr)}(\mathbf{k};\xi)$ in the vicinity of its singular point nearest to $\xi=0$. We notice that, similarly to the unbiased case, this point is $\xi=1$ when $\mathbf{k}=\mathbf{0}$. As a matter of fact, such a behavior stems from the *a priori* nonevident fact that the vacancy, starting from a given neighboring site to the origin, is certain to eventually reach the origin. This will be demonstrated explicitly in Sec. IV [cf. Eq. (48)]. As a matter of fact, one can see from Eq. (48) and the explicit representation of $\mathcal{D}(\mathbf{0};\xi)$ presented in the appendix that $\mathcal{D}(\mathbf{0};\xi=1)\equiv0$. In consequence, expansion in powers of a small deviation $(1-\xi)$ has to be accompanied by a small-$\mathbf{k}$ expansion, exactly as it has been performed in Ref. [14].

IV. THE RETURN PROBABILITIES $F_N^{*}(\mathbf{0}|\mathbf{e}_{\mu}|\mathbf{e}_{\nu})$

As we have already remarked, the vacancy random walk between two successive visits of the lattice site occupied by the TP can be viewed as a standard, two-dimensional, symmetric random walk with some boundary conditions imposed on the four sites adjacent to the site occupied by the TP. In order to compute the return probabilities $F_n^{*}(\mathbf{0}|\mathbf{e}_{\mu}|\mathbf{e}_{\nu})$ for such a random walk, we add, in the usual fashion [5,30], an additional constraint that the site at the lattice origin is in an absorbing state. Then, the vacancy random walk can be formally represented as a lattice random walk with site-dependent probabilities of the form $p^{+}(\mathbf{s}|\mathbf{s}')=1/4+q(\mathbf{s}|\mathbf{s}')$, where $\mathbf{s}'$ is the site occupied by the vacancy at the time moment n, while $\mathbf{s}$ denotes the target, nearest-neighboring to $\mathbf{s}'$ site,

$$q(\mathbf{s}|\mathbf{s}')\equiv\begin{cases}0 & \text{if } \mathbf{s}'\notin\{\mathbf{0},\mathbf{e}_{\pm1},\mathbf{e}_{\pm2}\},\\ \delta_{\mathbf{s},\mathbf{0}}-1/4 & \text{if } \mathbf{s}'=\mathbf{0},\\ \delta q_{\nu} & \text{if } \mathbf{s}'=\mathbf{e}_{\nu} \text{ and } \mathbf{s}=\mathbf{0},\\ -\delta q_{\nu}/3 & \text{if } \mathbf{s}'=\mathbf{e}_{\nu} \text{ and } \mathbf{s}'\neq\mathbf{0},\end{cases} \tag{24}$$

where δq_{ν} is defined, according to Eqs. (9)–(11), by

$$\delta q_{\nu}\equiv\frac{p_{\nu}}{p_{\nu}+3/4}-\frac{1}{4}. \tag{25}$$

Further on, we define $P_n^{+}(\mathbf{s}|\mathbf{s_0})$ as the probability distribution associated with such a random walk starting at site $\mathbf{s_0}$ at step $n=0$.

Now, let the symbols $\mathcal{E}$, $\mathcal{A}$, and $\mathcal{B}$ define the following three events.

(1) The event $\mathcal{E}$: the vacancy, which has started its random walk at the site $\mathbf{e}_{\boldsymbol{\nu}}$, visits the origin $\mathbf{0}$ for the first time at the nth step exactly, being at the site $\mathbf{e}_{\boldsymbol{\mu}}$ at the preceding step $n-1$.

(2) The event $\mathcal{A}$: the vacancy, which started its random walk at the site $\mathbf{e}_{\boldsymbol{\nu}}$, is at the site $\mathbf{e}_{\boldsymbol{\mu}}$ at the time moment $n-1$ and the origin $\mathbf{0}$ has not been visited during the $n-1$ first steps of its walk.

(3) The event $\mathcal{B}$: the vacancy jumps from the neighboring to the origin site $\mathbf{e}_{\boldsymbol{\mu}}$ to the site $\mathbf{0}$ at the nth step exactly.

Evidently, by definition, the desired first visit probability $F_n^*(\mathbf{0}|\mathbf{e}_{\boldsymbol{\mu}}|\mathbf{e}_{\boldsymbol{\nu}})$ is just the probability of the $\mathcal{E}$ event

$$F_n^*(\mathbf{0}|\mathbf{e}_{\boldsymbol{\mu}}|\mathbf{e}_{\boldsymbol{\nu}})=\mathrm{Prob}(\mathcal{E}). \tag{26}$$

To calculate Prob($\mathcal{E}$) we first note that the probabilities of three such events obey

$$\mathrm{Prob}(\mathcal{E})=\mathrm{Prob}(\mathcal{A}\cap\mathcal{B})=\mathrm{Prob}(\mathcal{A})\mathrm{Prob}(\mathcal{B}). \tag{27}$$

On the other hand, we have that

$$\mathrm{Prob}(\mathcal{A})=P_{n-1}^{+}(\mathbf{e}_{\boldsymbol{\mu}}|\mathbf{e}_{\boldsymbol{\nu}}) \tag{28}$$

and

$$\mathrm{Prob}(\mathcal{B})=\frac{p_\mu}{3/4+p_\mu}. \tag{29}$$

Hence, by virtue of Eqs. (26)–(29), the return probability $F_n^*(\mathbf{0}|\mathbf{e}_{\boldsymbol{\mu}}|\mathbf{e}_{\boldsymbol{\nu}})$ is given explicitly by

$$F^*(\mathbf{0}|\mathbf{e}_{\boldsymbol{\mu}}|\mathbf{e}_{\boldsymbol{\nu}};\xi)=\xi\left(\frac{p_\mu}{3/4+p_\mu}\right)P^{+}(\mathbf{e}_{\boldsymbol{\mu}}|\mathbf{e}_{\boldsymbol{\nu}};\xi). \tag{30}$$

Therefore, calculation of the return probabilities $F_n^*(\mathbf{0}|\mathbf{e}_{\boldsymbol{\mu}}|\mathbf{e}_{\boldsymbol{\nu}})$ amounts to the evaluation of the probability distribution $P_n^{+}(\mathbf{s}|\mathbf{s_0})$ of the vacancy random walk in the presence of an absorbing site placed at the lattice origin. Such a probability distribution will be determined in the next section.

A. The generating function of the probability distribution $P^{+}(\mathbf{s}|\mathbf{s}_0)$

Making use of the generating function technique adapted to random walks on lattices with defective sites [5] and [31], we obtain

$$P^{+}(\mathbf{s_i}|\mathbf{s_j};\xi)=P(\mathbf{s_i}|\mathbf{s_j};\xi)+\sum_{l=-2}^{2}A(\mathbf{s_i}|\mathbf{s_l};\xi)P^{+}(\mathbf{s_l}|\mathbf{s_j};\xi), \tag{31}$$

where

$$\mathbf{s_i}\equiv\begin{cases}\mathbf{e_i}, & \text{for } i\in\{\pm1,\pm2\},\\ \mathbf{0}, & \text{for } i=0,\end{cases} \tag{32}$$

and

$$A(\mathbf{s_i}|\mathbf{s_l};\xi)\equiv\xi\sum_{\mathbf{s}'}P(\mathbf{s_i}|\mathbf{s}';\xi)q(\mathbf{s}'|\mathbf{s_l}), \tag{33}$$

$P(\mathbf{s_i}|\mathbf{s_j};\xi)$ being the generating function of the unperturbed associated random walk (that is, symmetric random walk with no defective sites).

Further on, Eq. (31) can be recast into the following matricial form:

$$\mathbf{P}^{+}=(\mathbf{1}-\mathbf{A})^{-1}\mathbf{P}, \tag{34}$$

in which equation $\mathbf{P}$, $\mathbf{P}^{+}$, $\mathbf{A}$ stand for the 5×5 matrices with the elements defined by

$$\mathbf{P}_{i,j}=P(\mathbf{s_i}|\mathbf{s_j};\xi),\quad \mathbf{P}^{+}_{i,j}=P^{+}(\mathbf{s_i}|\mathbf{s_j};\xi),\quad \mathbf{A}_{i,j}=A(\mathbf{s_i}|\mathbf{s_j};\xi), \tag{35}$$

where $i,j=0,+1,-1,+2,-2$. Next, using an evident relation [5]

$$P(\mathbf{s_k}|\mathbf{s_l};\xi)=\delta_{k,l}+\frac{\xi}{4}\sum_{\nu}P(\mathbf{s_k}|\mathbf{s_l}+\mathbf{e}_{\boldsymbol{\nu}};\xi), \tag{36}$$

and the symmetry properties of a standard random walk, one can readily show that:

(i) for $\mathbf{s_l}\neq\mathbf{s_0}$ and $\mathbf{s_k}\neq\mathbf{s_0}$,

$$A(\mathbf{s_k}|\mathbf{s_l};\xi)=\frac{4}{3}\;\delta q_l(P(\mathbf{0}|\mathbf{0};\xi)-1-P(\mathbf{s_k}|\mathbf{s_l};\xi)+\delta_{l,k}); \tag{37}$$

(ii) for $\mathbf{s_l}\neq\mathbf{s_0}$ and $\mathbf{s_k}=\mathbf{s_0}$,

$$A(\mathbf{s_0}|\mathbf{s_l};\xi)=\frac{4}{3}\xi\delta q_l\left(P(\mathbf{0}|\mathbf{0};\xi)-\frac{1}{\xi^2}[P(\mathbf{0}|\mathbf{0};\xi)-1]\right); \tag{38}$$

(iii) for $\mathbf{s_l}=\mathbf{s_0}$,

$$A(\mathbf{s_k}|\mathbf{s_0};\xi)=\delta_{k,0}-(1-\xi)P(\mathbf{s_k}|\mathbf{0};\xi). \tag{39}$$

Consequently, the matrices $\mathbf{A}$ and $\mathbf{P}$ in Eq. (34) are given by

$$\mathbf{A}=\begin{pmatrix} a & \delta q_1 f & \delta q_{-1} f & \delta q_2 f & \delta q_2 f\\ b & 0 & \delta q_{-1} e & \delta q_2 c & \delta q_2 c\\ b & \delta q_1 e & 0 & \delta q_2 c & \delta q_2 c\\ b & \delta q_1 c & \delta q_{-1} c & 0 & \delta q_2 e\\ b & \delta q_1 c & \delta q_{-1} c & \delta q_2 e & 0\end{pmatrix}, \tag{40}$$

where

$$a \equiv 1-(1-\xi)G(\xi),$$

$$b \equiv \frac{1-\xi}{\xi}[1-G(\xi)],$$

$$e \equiv \frac{4}{3}[2g(\xi)-1],$$

$$c \equiv \frac{4}{3}\left[-1+\frac{2}{\xi^2}+2G(\xi)\left(1-\frac{1}{\xi^2}\right)-g(\xi)\right],$$

$$f \equiv \frac{4}{3}\xi\left(G(\xi)-\frac{G(\xi)-1}{\xi^2}\right), \tag{41}$$

and

$$\mathbf{P}=\begin{pmatrix} G(\xi) & [G(\xi)-1]/\xi & [G(\xi)-1]/\xi & [G(\xi)-1]/\xi & [G(\xi)-1]/\xi \\ [G(\xi)-1]/\xi & G(\xi) & G(\xi)-2g(\xi) & \tau(\xi) & \tau(\xi) \\ [G(\xi)-1]/\xi & G(\xi)-2g(\xi) & G(\xi) & \tau(\xi) & \tau(\xi) \\ [G(\xi)-1]/\xi & \tau(\xi) & \tau(\xi) & G(\xi) & G(\xi)-2g(\xi) \\ [G(\xi)-1]/\xi & \tau(\xi) & \tau(\xi) & G(\xi)-2g(\xi) & G(\xi) \end{pmatrix}, \tag{42}$$

with

$$G(\xi) \equiv P(\mathbf{0}|\mathbf{0};\xi), \quad g(\xi) \equiv -\frac{1}{2}[P(\mathbf{e_1}|-\mathbf{e_1};\xi)-P(\mathbf{0}|\mathbf{0};\xi)],$$

$$\tau(\xi) \equiv \left(\frac{2}{\xi^2}-1\right)G(\xi)-\frac{2}{\xi^2}+g(\xi). \tag{43}$$

Note that Eqs. (40) and (42) now define the P^+ matrix explicitly, and hence, define the generating function of the probability distribution $P^+(\mathbf{s}|\mathbf{s_0})$.

B. Asymptotic behavior of the generating functions of the return probabilities in the vicinity of $\xi=1$

As we have already remarked, here we constrain our consideration to the analysis of the leading in n behavior; this amounts to consideration of the leading in the limit $\xi \to 1^-$ behavior of the corresponding generating functions. Expanding $G(\xi)$ and $g(\xi)$ in the vicinity of the singular point $\xi=1$ (cf. Refs. [5] and [14,32,33]), we have

$$G(\xi)=\frac{1}{\pi}\ln\frac{8}{1-\xi}-\frac{1}{2\pi}(1-\xi)\ln(1-\xi)+\mathcal{O}(1-\xi),$$

$$\xi \to 1^- \tag{44}$$

and

$$g(\xi)=\left(2-\frac{4}{\pi}\right)+\frac{2}{\pi}(1-\xi)\ln(1-\xi)+\mathcal{O}[(1-\xi)],$$

$$\xi \to 1^-. \tag{45}$$

Consequently, we find by solving the matricial equation (34) that the generating functions of the return probabilities obey

$$A_{\nu,\mu}(\xi)=\frac{A^{(1)}_{\nu,\mu}(u)}{S(u)}-\frac{A^{(2)}_{\nu,\mu}(u)}{S^2(u)}(\ln(1-\xi))^{-1}+\mathcal{O}(1-\xi), \tag{46}$$

where $u \equiv \exp(\beta E/2)$, $A^{(1)}_{\nu,\mu}(u)$ and $A^{(2)}_{\nu,\mu}(u)$ are some rational fractions (all listed explicitly in the Appendix), while

$$\begin{aligned} S(u) \equiv \{&(\pi-2)u^6+(2\pi^2-6\pi+12)u^5 \\ &+(8\pi^2-25\pi+34)u^4-(4\pi^2-60\pi+88)u^3 \\ &+(8\pi^2-25\pi+34)u^2+(2\pi^2-6\pi+12)u+\pi-2\}. \end{aligned} \tag{47}$$

It follows from Eq. (46) and explicit expressions for $A_{\nu,\mu}(\xi)$ presented in the Appendix that, in particular, the generating functions of the return probabilities fulfill

$$A_{1,-1}(1^-)+A_{-1,-1}(1^-)+2A_{2,-1}(1^-)=1,$$

$$A_{1,1}(1^-)+A_{-1,1}(1^-)+2A_{2,1}(1^-)=1,$$

$$A_{1,2}(1^-)+A_{-1,2}(1^-)+A_{-2,2}(1^-)+A_{2,2}(1^-)=1, \tag{48}$$

which relations imply that the vacancy, starting its random walk from a given, neighboring the origin site, is *certain* to return eventually to the origin.

V. THE TP MEAN DISPLACEMENT AND THE PROBABILITY DISTRIBUTION

In this section we proceed as follows: Taking advantage of the asymptotical expansion obtained in the previous section, we first determine the small $(1-\xi)$ behavior of the generating function $\widetilde{P}^{(tr)}(\mathbf{k};\xi)$, accompanied by the small-$\mathbf{k}$ expansion. Next, we evaluate the generating function of the TP mean displacement by differentiating the obtained asymptotical expression for $\widetilde{P}^{(tr)}(\mathbf{k};\xi)$ with respect to the components of the wave vector and analyze its large-n behavior. Lastly, we invert the asymptotical expansion of the generating function $\widetilde{P}^{(tr)}(\mathbf{k};\xi)$ and obtain the corresponding probability distribution $P_n^{(tr)}(\mathbf{X})$ in a certain scaling limit.

A. Asymptotic expansion of the generating function $\widetilde{P}^{(tr)}(\mathbf{k};\xi)$

Using the explicit representation of the determinant $\mathcal{D}(\mathbf{k};\xi)$ in Eq. (16) in terms of the generating functions of the return probabilities $A_{\nu,\mu}(\xi)$ presented in the Appendix, as well as the asymptotical expansions in Eq. (46), we find that in the vicinity of $\xi=1$ and for small values of the wave vector k, $\mathcal{D}(\mathbf{k};\xi)$ is given by

$$\mathcal{D}(\mathbf{k};\xi)=i\mathcal{F}_1(u)k_1+\mathcal{F}_2(u)k_1^2+\mathcal{F}_3(u)k_2^2 -\mathcal{F}_4(u)\ln^{-1}(1-\xi)+\cdots, \tag{49}$$

where we have used the shortenings

$$\mathcal{F}_1(u)\equiv-\frac{(\pi-2)(u-1)(1+u)^5[u^2+2(2\pi-3)u+1]}{[u^2+2(\pi-1)u+1]S(u)}, \tag{50}$$

$$\mathcal{F}_2(u)\equiv\frac{(\pi-2)(1+u)^4(u^2+1)[u^2+2(2\pi-3)u+1]}{2[u^2+2(\pi-1)u+1]S(u)}, \tag{51}$$

$$\mathcal{F}_3(u)\equiv\frac{u(\pi-2)(1+u)^4[(2\pi-3)u^2+2u+2\pi-3]}{[u^2+2(\pi-1)u+1]S(u)}, \tag{52}$$

and

$$\mathcal{F}_4(u)\equiv\frac{\pi(\pi-2)(1+u)^4[(2\pi-3)u^2+2u+2\pi-3][u^2+2(2\pi-3)u+1]}{[u^2+2(\pi-1)u+1]S(u)}, \tag{53}$$

and assumed, for simplicity, that the starting point $\mathbf{Y}_0$ of the vacancy random walk is $\mathbf{Y}_0=\mathbf{e}_{-1}$. On the other hand, we find that

$$\sum_{\boldsymbol{\nu}} U_{\boldsymbol{\nu}}(\mathbf{k};\xi)F^*(\mathbf{0}|\mathbf{e}_{\boldsymbol{\nu}}|-\mathbf{e}_{\mathbf{1}};\xi)=-i\mathcal{F}_1(u)k_1-\mathcal{F}_2(u)k_1^2 -\mathcal{F}_3(u)k_2^2+\cdots. \tag{54}$$

Consequently, in the small-$\mathbf{k}$ limit and $\xi\to1^-$, the generating function $\widetilde{P}^{(tr)}(\mathbf{k};\xi)$ obeys

$$\widetilde{P}^{(tr)}(\mathbf{k};\xi)=\frac{1}{1-\xi}\left\{1-\left(-i\alpha_0k_1+\frac{1}{2}\alpha_1k_1^2+\frac{1}{2}\alpha_2k_2^2\right)\times\ln(1-\xi)\right\}^{-1}, \tag{55}$$

where the coefficients

$$\alpha_0(E)\equiv\pi^{-1}\sinh(\beta E/2)[(2\pi-3)\cosh(\beta E/2)+1]^{-1},$$

$$\alpha_1(E)\equiv\pi^{-1}\cosh(\beta E/2)[(2\pi-3)\cosh(\beta E/2)+1]^{-1}, \tag{56}$$

$$\alpha_2(E)\equiv\pi^{-1}[\cosh(\beta E/2)+2\pi-3]^{-1}$$

are all functions of the field strength E and of the temperature only.

B. The TP mean displacement for arbitrary field strength E

As a matter of fact, the leading large-n asymptotical behavior of the TP mean displacement can be obtained directly from Eq. (55) since the generating function of the TP mean displacement, i.e.,

$$\overline{\mathbf{X}}(\xi)\equiv\sum_{n=0}^{+\infty}\overline{\mathbf{X}}_n\xi^n \tag{57}$$

obeys (see, e.g., Ref. [4])

$$\overline{\mathbf{X}}(\xi)=-i\left(\frac{\partial\widetilde{P}^{(tr)}}{\partial k_1}(\mathbf{0};\xi)\mathbf{e}_{\mathbf{1}}+\frac{\partial\widetilde{P}^{(tr)}}{\partial k_2}(\mathbf{0};\xi)\mathbf{e}_{\mathbf{2}}\right). \tag{58}$$

Consequently, differentiating the expression on the right-hand side of Eq. (55) with respect to the components of the wave vector $\mathbf{k}$, we find that the asymptotical behavior of the generating function of the TP mean displacement in the vicinity of $\xi=1^-$ follows

$$\overline{\mathbf{X}}(\xi)\sim\left(\frac{\alpha_0(E)}{1-\xi}\ln\frac{1}{1-\xi}\right)\mathbf{e}_{\mathbf{1}}. \tag{59}$$

Further on, using the discrete Tauberian theorem (cf. Ref. [5]) and Eq. (56), we find the following general force-velocity relation for the system under study,

$$\overline{\mathbf{X}}_n \sim (\alpha_0(E)\ln n)\mathbf{e_1} = \left(\frac{1}{\pi}\,\frac{\sinh(\beta E/2)}{(2\pi-3)\cosh(\beta E/2)+1}\ln n\right)\mathbf{e_1}, \quad \text{as} \quad n\to\infty, \tag{60}$$

which shows that the TP mean displacement grows *logarithmically* with n. Consequently, one may claim that the typical displacement along the x_1 direction scales as $\ln(n)$ as $n\to\infty$. On the other hand, typical displacement in the x_2 direction is expected to grow only in proportion to $\sqrt{\ln(n)}$, as in the unbiased case [14]. These claims will be confirmed in what follows by the form of the scaling variables involved in the limiting distribution.

Consider next the behavior of the coefficient $\alpha_0(E)$ in the limit $E\to 0$. Here, we find from Eq. (56) that

$$\alpha_0(E)=\frac{\beta E}{4\pi(\pi-1)}+\mathcal{O}(E^3), \tag{61}$$

and hence, the mobility μ_n, defined in Eq. (4), follows

$$\mu_n \sim \frac{\beta}{4\pi(\pi-1)}\,\frac{\ln(n)}{n}, \quad \text{as} \quad n\to\infty. \tag{62}$$

Comparing next the result in Eq. (62) with that for the diffusivity D_n, Eq. (2), derived by Brummelhuis and Hilhorst [14] in the unbiased case, we infer that the TP mobility and diffusivity do obey, at least in the leading n order, the generalized Einstein relation of the form $\mu_n=\beta D_n$ [3]. Note that this cannot be, of course, an *a priori* expected result, in view of an intricate nature of the random walks involved and anomalous, *logarithmic* confinement of the random walk trajectories.

C. Probability distribution $P_n^{(tr)}(\mathbf{X})$

We turn next to calculation of the asymptotic forms of the probability distribution $P_n^{(tr)}(\mathbf{X})$. Inverting $\tilde{P}^{(tr)}(\mathbf{k};\xi)$ with respect to $\mathbf{k}$, we notice first that in the limit $\xi\to 1^-$ the integrand is sharply peaked around $\mathbf{k}=0$, such that the bulk contribution to the integral comes from the values $k_1=0$ and $k_2=0$; this implies that we can extend the limits of integration from $\pm\pi$ to $\pm\infty$, which yields in the limit $\xi\to 1^-$:

$$\begin{aligned} P^{(tr)}(\mathbf{X};\xi) \sim & \frac{1}{(1-\xi)(2\pi)^2}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dk_1 dk_2 \\ & \times \exp(-ik_1x_1-ik_2x_2) \\ & \times\left\{1-\left(-i\alpha_0(E)k_1+\frac{1}{2}\alpha_1(E)k_1^2 \right.\right. \\ & \left.\left. +\frac{1}{2}\alpha_2(E)k_2^2\right)\ln(1-\xi)\right\}^{-1}. \end{aligned} \tag{63}$$

Further on, using the integral equality

$$\begin{aligned} &\left\{1-\left(-i\alpha_0(E)k_1+\frac{1}{2}\alpha_1(E)k_1^2+\frac{1}{2}\alpha_2(E)k_2^2\right)\ln(1-\xi)\right\}^{-1} \\ &= \int_0^{+\infty} dv\, \exp\left[-v\left\{1-\left(-i\alpha_0(E)k_1+\frac{1}{2}\alpha_1(E)k_1^2 \right.\right.\right. \\ &\left.\left.\left. +\frac{1}{2}\alpha_2(E)k_2^2\right)\ln(1-\xi)\right\}\right], \end{aligned} \tag{64}$$

we cast the integral in Eq. (63) into the form

$$\begin{aligned} P^{(tr)}(\mathbf{X};\xi) \sim & \frac{1}{(1-\xi)(2\pi)^2}\int_0^{+\infty} dv\, \exp(-v) \\ & \times\int_{-\infty}^{+\infty} dk_1 \int_{-\infty}^{+\infty} dk_2 \exp(-ik_2x_2) \\ & \times \exp\left(\frac{v}{2}(\alpha_1(E)k_1^2+\alpha_2(E)k_2^2)\ln(1-\xi)\right. \\ & \left. -ik_1[x_1+v\,\alpha_0(E)\ln(1-\xi)]\right). \end{aligned} \tag{65}$$

Note now that in order to evaluate explicitly the Gaussian integral in Eq. (65), we have to consider separately two cases: when (a) the external field in infinitely strong, $E=\infty$ (which implies $\alpha_2=0$), such that the TP performs a totally directed walk, and (b) when E is bounded, $E<\infty$ (and hence, $\alpha_2>0$).

1. Directed walk, $E=\infty$

We start with the simplest case when the TP performs a totally directed walk under the influence of an infinitely strong field. In this case, the probability distribution is defined for non-negative x_1 values only, and Eq. (65) reduces to

$$\begin{aligned} P^{(tr)}(\mathbf{X};\xi) \sim & \frac{\delta(x_2)\,\theta(x_1)}{2\pi(1-\xi)}\int_0^{+\infty} dv\, \exp(-v) \\ & \times\int_{-\infty}^{+\infty} dk_1 \exp\left(\frac{v}{2}\alpha_1(E)k_1^2\ln(1-\xi)\right. \\ & \left. -ik_1[x_1+v\,\alpha_0(E)\ln(1-\xi)]\right), \end{aligned} \tag{66}$$

where $\theta(x_1)$ denotes the Heaviside theta function. Performing the integrals, we find that, in the limit $\xi\to 1^-$, the generating function $P^{(tr)}(\mathbf{X};\xi)$ obeys

$$\begin{aligned} P^{(tr)}(\mathbf{X};\xi) \sim & -\delta(x_2)\,\theta(x_1) \\ & \times\frac{\pi(2\pi-3)}{(1-\xi)\ln(1-\xi)}\exp\left(\frac{\pi(2\pi-3)}{\ln(1-\xi)}x_1\right). \end{aligned} \tag{67}$$

Applying next the discrete Tauberian theorem [5,34], we find, eventually,

$$P_n^{(tr)}(\mathbf{X}) \sim \delta(x_2)\,\theta(x_1)\frac{\pi(2\pi-3)}{\ln(n)}\exp\left(-\frac{\pi(2\pi-3)}{\ln(n)}x_1\right), \tag{68}$$

which means that in the totally directed case, in the large-n and large-x_1 limit, the scaled variable $\eta_\infty \equiv \pi(2\pi-3)x_1/\ln(n)$ is asymptotically distributed according to

$$P(\eta_\infty) = \theta(\eta_\infty)\exp(-\eta_\infty), \tag{69}$$

i.e., has an exponential scaling function.

2. Arbitrary bounded field $E<\infty$

In this case the coefficient $\alpha_2>0$ and the probability distribution is defined also for negative values of x_1; as well, $P^{(tr)}(\mathbf{X};\xi)$ is defined also for nonzero values of x_2. In this general case, we find, performing integrations over the components of the wave vector, that $P^{(tr)}(\mathbf{X};\xi)$ attains, as $\xi\to 1^-$, the following form:

$$\begin{aligned}P^{(tr)}(\mathbf{X};\xi) \sim &-\left(2\pi(1-\xi)\ln(1-\xi)\sqrt{\alpha_1(E)\alpha_2(E)}\right)^{-1}\\ &\times\int_0^{+\infty} dv\,\exp(-v)\exp\left\{\frac{1}{2v\,\ln(1-\xi)}\right.\\ &\times\left[\left(\frac{x_1}{\alpha_1(E)}+v\frac{\alpha_0(E)}{\alpha_1(E)}\ln(1-\xi)\right)^2\right.\\ &\left.\left.+\left(\frac{x_2}{\alpha_2(E)}\right)^2\right]\right\}.\end{aligned} \tag{70}$$

The integral in the latter equation can be calculated exactly, which yields

$$\begin{aligned}P^{(tr)}(\mathbf{X};\xi) \sim &-\left(\pi(1-\xi)\ln(1-\xi)\sqrt{\alpha_1(E)\alpha_2(E)}\right)^{-1}\\ &\times\exp\left(\frac{\alpha_0(E)}{\alpha_1(E)}x_1\right)K_0\left[\eta_E\left(\frac{1}{1-\xi}\right)\right],\end{aligned} \tag{71}$$

where K_0 is the modified Bessel (McDonald) function of zeroth order, and

$$\eta_E(\lambda) \equiv \sqrt{\frac{2}{\ln(\lambda)}+\frac{\alpha_0^2(E)}{\alpha_1(E)}}\sqrt{\frac{x_1^2}{\alpha_1(E)}+\frac{x_2^2}{\alpha_2(E)}}. \tag{72}$$

Finally, using the discrete Tauberian theorem [5,34], we find from Eq. (72) that in the large-n and large-X limits, the probability distribution $P_n^{(tr)}(\mathbf{X})$ obeys

$$\begin{aligned}P_n^{(tr)}(\mathbf{X}) \sim &\left(\pi\sqrt{\alpha_1(E)\alpha_2(E)}\ln(n)\right)^{-1}\\ &\times\exp\left(\frac{\alpha_0(E)}{\alpha_1(E)}x_1\right)K_0[\eta_E(n)].\end{aligned} \tag{73}$$

Note that in the unbiased case, i.e., when $E=0$, the probability distribution $P_n^{(tr)}(\mathbf{X})$ defined by Eqs. (72) and (73) reduces to the form predicted earlier by Brummelhuis and Hilhorst [14].

3. Limiting probability distribution function

Now, we recollect that the scaling behavior expected is $x_1 \sim \ln(n)$ (for $E>0$) and $x_2 \sim \sqrt{\ln(n)}$. In order to obtain from Eqs. (72) and (73) the limiting probability distribution, we introduce two scaling variables:

$$\begin{aligned}\eta_1 &\equiv x_1/\alpha_0(E)\ln(n),\\ \eta_2 &\equiv x_2/\sqrt{2\alpha_2(E)\ln(n)}.\end{aligned} \tag{74}$$

Note that η_1 becomes η_∞ in the special case $E=\infty$. In terms of these scaling variables $\eta_E(n)$ in Eq. (72) takes the form

$$\begin{aligned}\eta_E(n) = \frac{\alpha_0^2(E)}{\alpha_1(E)}\ \ln(n)|\eta_1|\left\{1+\frac{\alpha_1(E)}{\alpha_0^2(E)\ln(n)}\left[1+\left(\frac{\eta_2}{\eta_1}\right)^2\right]\right.\\ \left.+\mathcal{O}[1/\ln^2(n)]\right\}.\end{aligned} \tag{75}$$

Note now that for arbitrary fixed η_1 and η_2, the argument of the Bessel function $\eta_E(n)$ written in terms of the scaling variables tends to infinity as $n\to\infty$. Consequently, using the limiting behavior of the modified Bessel function

$$K_0(y) = \left(\frac{\pi}{2y}\right)^{1/2}\exp(-y)[1+\mathcal{O}(1/y)], \tag{76}$$

we find that the probability distribution $P_n^{(tr)}(\mathbf{X})$, written in terms of the scaling variables, converges as $n\to\infty$ to the limiting form

$$P_n^{(tr)}(\mathbf{X}) \underset{n\to\infty}{\sim} \begin{cases}[2\pi\alpha_2(E)\,\alpha_0^2(E)\,\eta_1\ln^3(n)]^{-1/2}\exp(-\eta_1-\eta_2^2/\eta_1) & \text{for}\quad \eta_1\geqslant 0,\\ 0, \quad \text{for} \quad \eta_1<0,\end{cases} \tag{77}$$

or, equivalently, that the scaling variables η_1 and η_2 have the following, rather unusual limiting joint distribution function:

$$P(\eta_1,\eta_2) = \frac{\theta(\eta_1)}{\sqrt{\pi\eta_1}}\exp\left(-\eta_1-\frac{\eta_2^2}{\eta_1}\right). \tag{78}$$

We note that this distribution is properly normalized and yields, of course, the same result for the TP mean displacement as the approach based on differentiation of the asymptotical expansion of the generating function. We also remark that the reduced distributions $P(\eta_1)=\int d\eta_2 P(\eta_1,\eta_2)$ and $P(\eta_2)=\int d\eta_1 P(\eta_1,\eta_2)$ take the form

$$P(\eta_1) = \theta(\eta_1)\exp(-\eta_1),$$

$$P(\eta_2)=\exp(-2|\eta_2|), \tag{79}$$

and hence the reduced distribution $P(\eta_1)$ appears to be exactly the same as in the case $E=\infty$.

VI. FINITE VACANCY CONCENTRATION

In this last section we turn to the situation when vacancies are present at a very small, but finite concentration ρ_v. We base our analysis on the model and approximate analytical approach proposed by Brummelhuis and Hilhorst in Ref. [18], generalizing it over the case when the TP experiences a bias due to external electric field. In their approach, Brummelhuis and Hilhorst decoupled the joint probability distribution of the TP and vacancies into the product of pair distribution functions. This approximation is appropriate when $\rho_v \ll 1$ and yields meaningful results for the TP mean square displacement in which the prefactor is evaluated only to the leading order in the concentration of vacancies. As a matter of fact, such an approximation is tantamount to the so-called Smoluchowski approach, well-known in the literature on the evolution of the reaction-diffusion systems (see, e.g., Ref. [35] and references therein). Making use of their approach and the results of previous sections concerning the form of the pair distribution functions in the biased case, we determine the TP mean displacement in the presence of an external electric field. This mean displacement is shown to grow linearly with time, and we calculate the prefactor in this dependence in the linear with ρ_v approximation. We verify the validity of the Einstein relation for this model and also present an estimate of the limiting probability distribution.

The model of Ref. [18] is defined as follows. Consider a finite lattice of size $L\times L$ with periodic boundary conditions, containing M vacancies. The mean concentration of the vacancies is thus $\rho_v=M/L^2$, and is supposed to be very small, $\rho_v \ll 1$. The TP is initially located at the origin and initial positions of the vacancies are denoted by $\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)}$, which all are different from each other and from $\mathbf{0}$. All other sites are filled with neutral hard-core particles. Note that additionally to the definition of the model in Ref. [18] we also suppose the TP is charged and is subject to external electric field $\mathbf{E}$, which is oriented in the positive x_1 direction.

Further on, the particles' dynamics in Ref. [18] is defined in the following way. Similar to the single vacancy case, Brummelhuis and Hilhorst stipulate that at each time step, all vacancies exchange their positions with either of the neighboring particles, such that each vacancy makes a step each time step. Note that when many vacancies are present, it may of course appear that two or more vacancies occupy adjacent sites or have common neighboring particles, in which case their random walks will interfere. This requires, in turn, definition of complementary dynamic rules describing evolution of configurations with vacancies appearing at adjacent sites. Such a definition is of course possible, but is not, however, necessary, since in view of the decoupling approximation underlying the model solution only consideration of the pair distribution functions is required. As also noticed in Ref. [18], the situations in which two vacancies appear at the adjacent sites or have common neighbors contribute only to $\mathcal{O}(\rho_v^2)$ and thus go beyond their approximation. Consequently, such details can be safely neglected when one focuses on the linear ρ_v approximation only.

Now, we briefly outline the basic steps involved in the approach by Brummelhuis and Hilhorst [18]. Let $\mathcal{P}_n^{(tr)}(\mathbf{X}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)})$ denote the probability of finding at time moment n the TP at position $\mathbf{X}$ as a result of its interaction with all M vacancies. This probability can be represented as

$$\begin{aligned}&\mathcal{P}_n^{(tr)}(\mathbf{X}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)})\\&\quad=\sum_{\mathbf{X}_0^{(1)}}\cdots\sum_{\mathbf{X}_0^{(M)}}\delta_{\mathbf{X},\mathbf{X}_0^{(1)}+\cdots+\mathbf{X}_0^{(M)}}\mathcal{P}_n^{(tr)}\\&\qquad\times(\mathbf{X}_0^{(1)},\mathbf{X}_0^{(2)},\cdots,\mathbf{X}_0^{(M)}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\cdots,\mathbf{Y}_0^{(M)}),\end{aligned} \tag{80}$$

where $\mathcal{P}_n^{(tr)}(\mathbf{X}_0^{(1)},\mathbf{X}_0^{(2)},\ldots,\mathbf{X}_0^{(M)}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)})$ stands for the conditional probability that within the time interval n the TP has displaced to the position $\mathbf{X}_0^{(1)}$ due to interactions with the first vacancy, to the position $\mathbf{X}_0^{(2)}$ due to the interactions with the second vacancy and etc.

Next, the main assumption of Ref. [18] is that all the vacancies contribute independently to the TP displacement. That is, events in which two or more vacancies appear simultaneously at the sites adjacent to the TP are simply being discarded. Under such an assumption, the conditional probability $\mathcal{P}_n^{(tr)}(\mathbf{X}_0^{(1)},\mathbf{X}_0^{(2)},\ldots,\mathbf{X}_0^{(M)}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)})$ can be approximated as a product of two-particle distribution functions

$$\begin{aligned}&\mathcal{P}_n^{(tr)}(\mathbf{X}_0^{(1)},\mathbf{X}_0^{(2)},\ldots,\mathbf{X}_0^{(M)}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)})\\&\quad\approx\prod_{j=1}^{M}P_n^{(tr)}(\mathbf{X}_0^{(j)}|\mathbf{Y}_0^{(j)}),\end{aligned} \tag{81}$$

where $P_n^{(tr)}(\mathbf{X}_0^{(j)}|\mathbf{Y}_0^{(j)})$ denotes the probability of finding the TP at the site $\mathbf{X}_0^{(j)}$ at time moment n due to interactions with a vacancy initially at $\mathbf{Y}_0^{(j)}$ in a system with a *single* vacancy. As we have already remarked, the situations in which two or more vacancies appear at the adjacent sites or have common neighbors contribute only to $\mathcal{O}(\rho_v^2)$. Consequently, the approximation in Eq. (81) would yield correct results to the order $\mathcal{O}(\rho_v)$, and is quite reasonable when $\rho_v \ll 1$.

Further on, combining Eqs. (80) and (81), and averaging $\mathcal{P}_n^{(tr)}(\mathbf{X}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)})$ over initial vacancy configurations, one has [18]

$$\begin{aligned}&\langle\mathcal{P}_n^{(tr)}(\mathbf{X}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)})\rangle\\&\quad\approx\sum_{\mathbf{X}_0^{(1)}}\cdots\sum_{\mathbf{X}_0^{(M)}}\delta_{\mathbf{X},\mathbf{X}_0^{(1)}+\cdots+\mathbf{X}_0^{(M)}}\prod_{j=1}^{M}\langle P_n^{(tr)}(\mathbf{X}_0^{(j)}|\mathbf{Y}_0^{(j)})\rangle.\end{aligned} \tag{82}$$

Now, defining the Fourier transformed averaged distributions as

$$\widetilde{\mathcal{P}}_n^{(tr)}(\mathbf{k},M,L)=\sum_{\mathbf{X}}\exp[i(\mathbf{k}\cdot\mathbf{X})]\times\langle\mathcal{P}_n^{(tr)}(\mathbf{X}|\mathbf{Y}_0^{(1)},\mathbf{Y}_0^{(2)},\ldots,\mathbf{Y}_0^{(M)})\rangle \tag{83}$$

and

$$\widetilde{P}_n^{(tr)}(\mathbf{k})=\sum_{\mathbf{X}}\exp[i(\mathbf{k}\cdot\mathbf{X})]\langle P_n^{(tr)}(\mathbf{X}|\mathbf{Y}_0^{(1)})\rangle, \tag{84}$$

and performing the corresponding summations, one finds that

$$\widetilde{\mathcal{P}}_n^{(tr)}(\mathbf{k},M,L)\approx(\widetilde{P}_n^{(tr)}(\mathbf{k}))^M. \tag{85}$$

Turning next to the limit $L,M\to\infty$ (while the ratio $M/L^2=\rho_v$ is kept fixed), we obtain

$$\widetilde{\mathcal{P}}_n^{(tr)}(\mathbf{k},\rho_v)=\lim_{L,M\to\infty}\widetilde{\mathcal{P}}_n^{(tr)}(\mathbf{k},M,L)\approx\exp(-\rho_v\Omega_n(\mathbf{k})), \tag{86}$$

where

$$\Omega_n(\mathbf{k})\equiv\sum_{j=0}^{n}\sum_{\nu}\Delta_{n-j}(\mathbf{k}|\mathbf{e}_\nu)\sum_{\mathbf{Y}\neq\mathbf{0}}F_j^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Y}), \tag{87}$$

$$\Delta_n(\mathbf{k}|\mathbf{e}_\nu)=1-\widetilde{P}_n^{(tr)}(\mathbf{k}|-\mathbf{e}_\nu)\exp[i(\mathbf{k}\cdot\mathbf{e}_\nu)], \tag{88}$$

$F_j^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Y})$ are conditional return probabilities, defined in Sec. III, and $\widetilde{P}_n^{(tr)}(\mathbf{k}|-\mathbf{e}_\nu)$ is the Fourier transformed single-vacancy probability distribution $P_n^{(tr)}(\mathbf{X}|-\mathbf{e}_\nu)$. The latter can be readily obtained by applying the discrete Fourier transformation to the relation

$$P_n^{(tr)}(\mathbf{X}|\mathbf{Y})=\delta_{\mathbf{X},\mathbf{0}}\left(1-\sum_{j=0}^{n}F_j^*(\mathbf{0}|\mathbf{Y})\right)+\sum_{j=0}^{n}\sum_{\nu}P_{n-j}^{(tr)}(\mathbf{X}-\mathbf{e}_\nu|-\mathbf{e}_\nu)F_j^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Y}) \tag{89}$$

and choosing $\mathbf{Y}=-\mathbf{e}_\nu$.

Note now that the presented derivation is quite general and valid for the arbitrary choice of p_ν (q_ν). We focus now on the case under study, i.e., when the TP experiences a constant bias due to external electric field, and stipulate that q_ν obeys Eqs. (6)–(10). For such a choice of q_ν we find that the generating function of $\Omega_n(\mathbf{k})$ is given by

$$\Omega(\mathbf{k};\xi)=\sum_{\nu}\Delta(\mathbf{k}|\mathbf{e}_\nu;\xi)\sum_{\mathbf{Y}\neq\mathbf{0}}F^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Y};\xi). \tag{90}$$

Further on, turning to the asymptotical limit $\xi\to1^-$, $\mathbf{k}\to\mathbf{0}$ and making use of the results of the previous sections, we have that $\Delta(\mathbf{k}|\mathbf{e}_\nu;\xi)$ follows

$$\Delta(\mathbf{k}|\mathbf{e}_\nu;\xi)\equiv\frac{1}{1-\xi}\Bigg\{1-\exp[i(\mathbf{k}\cdot\mathbf{e}_\nu)]\times\left[1-\ln(1-\xi)\left(-i\alpha_0(E)k_1+\frac{1}{2}\alpha_1(E)k_1^2+\frac{1}{2}\alpha_2(E)k_2^2\right)\right]^{-1}\Bigg\}+\cdots. \tag{91}$$

Consider next the form of $\Sigma_{\mathbf{Y}\neq\mathbf{0}}F^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Y};\xi)$ in the limit $\xi\to1^-$, $\mathbf{k}\to\mathbf{0}$. This sum can be evaluated rather straightforwardly by taking advantage of the results of Sec. III. We have then

$$\sum_{\mathbf{Y}\neq\mathbf{0}}F^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Y};\xi)=\xi\left(\frac{p_\nu}{3/4+p_\nu}\right)\sum_{\mathbf{Y}\neq\mathbf{0}}P^+(\mathbf{e}_\nu|\mathbf{Y};\xi)=\xi\left(\frac{p_\nu}{3/4+p_\nu}\right)\mathcal{B}_\nu^t(\mathbf{1}-\mathbf{A})^{-1}\sum_{\mathbf{Y}\neq\mathbf{0}}\mathcal{B}(\mathbf{Y};\xi), \tag{92}$$

where $\mathcal{B}_\nu$ is the νth basis vector, $\mathcal{B}_\nu^t$ denotes the transposition of $\mathcal{B}_\nu$, and $\mathcal{B}(\mathbf{Y};\xi)$ is the vector, whose elements are $[P(\mathbf{s_i}|\mathbf{Y};\xi)]_i$, $i=0,1,-1,2,-2$. Explicitly, the basis vectors are given by

$$\mathcal{B}_\mathbf{0}\equiv\begin{pmatrix}1\\0\\0\\0\\0\end{pmatrix},\quad \mathcal{B}_\mathbf{1}\equiv\begin{pmatrix}0\\1\\0\\0\\0\end{pmatrix},\quad \mathcal{B}_{-1}\equiv\begin{pmatrix}0\\0\\1\\0\\0\end{pmatrix},\quad \mathcal{B}_2\equiv\begin{pmatrix}0\\0\\0\\1\\0\end{pmatrix},\quad \mathcal{B}_{-\mathbf{2}}\equiv\begin{pmatrix}0\\0\\0\\0\\1\end{pmatrix}. \tag{93}$$

Further on, using an evident symmetry relation

$$P(s_i|\mathbf{Y}_i;\xi)=P(\mathbf{Y}_i|s_i;\xi), \tag{94}$$

as well as the relation in Eq. (36), we obtain

$$\sum_{\mathbf{Y}\neq\mathbf{0}}\mathcal{B}(\mathbf{y};\xi)=\left(\frac{1}{1-\xi}-G(\xi)\right)\mathcal{B}_\mathbf{0}+\left(\frac{1}{1-\xi}-\frac{1}{\xi}[G(\xi)-1]\right)\times(\mathcal{B}_\mathbf{1}+\mathcal{B}_{-\mathbf{1}}+\mathcal{B}_\mathbf{2}+\mathcal{B}_{-\mathbf{2}}). \tag{95}$$

Then, combining Eqs. (92), (95) and (40), (41), (44), and performing some straightforward but cumbersome calculations, we find that in the limit $\xi\to1^-$ and $\mathbf{k}\to\mathbf{0}$, the sum $\Sigma_{\mathbf{Y}\neq\mathbf{0}}F^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Y};\xi)$ is given by

$$\sum_{\mathbf{Y}\neq\mathbf{0}}F^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Y};\xi)=-\frac{\pi}{(1-\xi)\ln(1-\xi)}+\cdots, \tag{96}$$

which is, remarkably, independent of u and ν in the leading ξ order. Consequently, in the limit $\xi \to 1^-$ and $\mathbf{k}\to\mathbf{0}$, the generating function $\Omega(\mathbf{k};\xi)$ obeys

$$\Omega(\mathbf{k};\xi)\approx\frac{\pi}{(1-\xi)^2}\frac{-i\alpha_0(E)k_1+\frac{1}{2}\alpha_1(E)k_1^2+\frac{1}{2}\alpha_2(E)k_2^2}{1-\ln(1-\xi)\left(-i\alpha_0(E)k_1+\frac{1}{2}\alpha_1(E)k_1^2+\frac{1}{2}\alpha_2(E)k_2^2\right)}. \tag{97}$$

Next, using the discrete Tauberian theorem, we obtain from the latter equation that in the limit $n\to\infty$ and $\mathbf{k}\to\mathbf{0}$,

$$\Omega_n(\mathbf{k})\approx\pi\frac{\left(-i\alpha_0(E)k_1+\frac{1}{2}\alpha_1(E)k_1^2+\frac{1}{2}\alpha_2(E)k_2^2\right)}{1+\ln(n)\left(-i\alpha_0(E)k_1+\frac{1}{2}\alpha_1(E)k_1^2+\frac{1}{2}\alpha_2(E)k_2^2\right)}\; n. \tag{98}$$

Finally, inverting Eq. (86) with respect to the wave vector,

$$\mathcal{P}_n^{(tr)}(\mathbf{X},\rho_v)\approx\frac{1}{4\pi^2}\int_{-\pi}^{\pi}dk_1\int_{-\pi}^{\pi}dk_2 \times\exp(-i(\mathbf{k}\cdot\mathbf{X})-\rho_v\Omega_n(\mathbf{k})), \tag{99}$$

and taking advantage of Eq. (58), we find that the leading, large-n behavior of the TP mean displacement is given by

$$\overline{\mathbf{X}}_n\sim(\pi\alpha_0(E)\rho_v n)\mathbf{e_1}=\frac{\sinh(\beta E/2)}{(2\pi-3)\cosh(\beta E/2)+1}\rho_v n\mathbf{e_1}, \tag{100}$$

i.e., grows linearly with time. This signifies that the TP mobility attains a constant value at sufficiently large times n,

$$\mu_n=\lim_{|E|\to 0}\frac{|\overline{\mathbf{X}}_n|}{|\mathbf{E}|n}=\frac{\beta\rho_v}{4(\pi-1)}. \tag{101}$$

Comparing Eq. (101) and the result of Brummelhuis and Hilhorst [18] for the TP diffusivity in absence of the field, Eq. (3), we notice that again the Einstein relation is fulfilled.

Lastly, using Eqs. (98) and (99) we derive the limiting probability distribution function. We find then that in the scaling limit $n\to\infty$, $\rho_v\to 0$ and $\rho_v n/\ln(n)$ fixed, the limiting probability distribution written in terms of the scaling variables η_1 and η_2, Eqs. (74), obeys

$$P(\eta_1,\eta_2)=\delta(\eta_1)\delta(\eta_2)\exp(-\sigma)+\frac{\theta(\eta_1)}{\sqrt{\pi}} \times\exp\left(-\sigma-\eta_1-\frac{\eta_2^2}{\eta_1}\right)I_1(2\sqrt{\sigma\eta_1}), \tag{102}$$

where $I_1(x)$ is the modified Bessel function of the first order.

VII. CONCLUSION

In conclusion, we have studied the dynamics of a charged tracer particle diffusing on a two-dimensional lattice, all sites of which except one (a vacancy) are filled with identical neutral, hard-core particles. The system evolves in discrete time n, $n=0,1,2,\ldots$, by particles exchanging their positions with the vacancy, subject to the condition that each site can be at most singly occupied. The charged TP experiences a bias due to an external field $\mathbf{E}$, which favors its jumps in the preferential direction. We determine exactly, for arbitrary strength of the field $E=|\mathbf{E}|$, the leading large-n behavior of the TP mean displacement $\overline{\mathbf{X}}_n$, which is not zero here due to external bias, and the limiting probability distribution of the TP position. We have shown that the TP trajectories are anomalously confined and their mean displacement grows with time only logarithmically, $\overline{\mathbf{X}}_n=[\alpha_0(E)\ln(n)]\ \mathbf{e}_1$ as $n\to\infty$. On comparing our results with the earlier analysis of the TP diffusivity D_n in the unbiased case by Brummelhuis and Hilhorst [14], we have demonstrated that, remarkably, the Einstein relation $\mu_n=\beta D_n$ between the diffusivity and the mobility μ_n of the TP holds in the leading n order, despite the fact that both D_n and μ_n tend to zero as $n\to\infty$. Note, however, that validity of the Einstein relation for the system under study relies heavily on the proper normalization of the vacancy transition probabilities [see Eqs. (9)–(11)]. In the absence of such a normalization, artificial "temporal trapping" effects may emerge, which will result ultimately in the violation of the Einstein relation for the system under study (see also Refs. [27] and [28] for physical situations in which such type of effects is observed). We have also presented a generalization of an approximate description of the TP dynamics on a two-dimensional lattice with small but finite vacancy concentration ρ_v [18] for systems with external bias. In this case we have found for the TP mean displacement a ballistic-type law of the form $\overline{\mathbf{X}}_n = [\pi\alpha_0(E)\rho_v n]\mathbf{e}_1$. We have shown that here, again, both D_n and μ_n calculated in the linear in ρ_v approximation do obey the Einstein relation.

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APPENDIX

In this Appendix we list some explicit expressions skipped in the body of the manuscript. First of all, explicit form of the determinant $\mathcal{D}(\mathbf{k};\xi)$ in Eq. (16) in terms of the generating functions of the return probabilities $A_{\nu,\mu} = A_{\nu,\mu}(\xi)$ reads

$$\begin{aligned}
\mathcal{D}(\mathbf{k};\xi) = {} & 1 - A_{2,2}^2 + 2A_{-1,-1}A_{2,1}A_{1,2}A_{-2,2} + 2A_{1,-1}A_{2,1}A_{-1,2}A_{2,2} - 2A_{2,-1}A_{-2,2}A_{1,2}A_{-1,1} - A_{1,-1}A_{-1,1}A_{2,2}^2 \\
& + A_{1,-1}A_{-1,1}A_{-2,2}^2 + A_{1,-1}A_{-1,1} - A_{-1,-1}A_{1,1} - A_{-1,-1}A_{1,1}A_{-2,2}^2 + A_{-1,-1}A_{1,1}A_{2,2}^2 - 2A_{-1,-1}A_{2,1}A_{1,2}A_{2,2} \\
& + 2A_{2,-1}A_{2,2}A_{1,2}A_{-1,1} - 2A_{1,-1}A_{2,1}A_{-1,2}A_{-2,2} - 2A_{2,-1}A_{2,2}A_{1,1}A_{-1,2} + 2A_{2,-1}A_{-2,2}A_{1,1}A_{-1,2} + A_{-2,2}^2 \\
& + 2(A_{2,-1}A_{1,2}A_{-1,1} + A_{1,-1}A_{2,1}A_{-1,2} - A_{-1,-1}A_{2,1}A_{1,2} - A_{1,-1}A_{-1,1}A_{-2,2} - A_{-2,2} + A_{-1,-1}A_{1,1}A_{-2,2} \\
& - A_{2,-1}A_{1,1}A_{-1,2})\cos k_2 + (A_{-1,1}A_{2,2}^2 - A_{-1,1} + 2A_{2,1}A_{-1,2}A_{-2,2} - 2A_{2,1}A_{-1,2}A_{2,2} - A_{-1,1}A_{-2,2}^2)e^{-ik_1} \\
& + (2A_{2,-1}A_{-2,2}A_{1,2} - 2A_{2,-1}A_{2,2}A_{1,2} + A_{1,-1}A_{2,2}^2 - A_{1,-1} - A_{1,-1}A_{-2,2}^2)e^{ik_1} + 2(A_{1,-1}A_{-2,2} \\
& - A_{2,-1}A_{1,2})e^{ik_1}\cos k_2 + 2(-A_{2,1}A_{-1,2} + A_{-1,1}A_{-2,2})e^{-ik_1}\cos k_2 .
\end{aligned}$$

Next, the coefficients in Eq. (46) defining asymptotical behavior of the generating functions of the return probabilities are given explicitly by

$$A_{1,-1}^{(1)}(u) = u^2(u+1)^2[(\pi-2)u^2 - 2(\pi^2-3\pi-2)u + \pi - 2],$$

$$A_{1,-1}^{(2)}(u) = -\pi u^2(u+1)^2(u^2+2u+2\pi-3)((2\pi-3)u^2+2u+1[(\pi-2)u^2+4u+\pi-2]^2,$$

$$A_{-1,-1}^{(1)}(u) = (4\pi^2-15\pi+14)u^4 - (6\pi^2-56\pi+80)u^3 + (8\pi^2-34\pi+52)u^2 + (2\pi^2-8\pi+16)u + \pi - 2,$$

$$A_{-1,-1}^{(2)}(u) = -\pi(u+1)^2[(2\pi-3)u^2+2u+1]^2[(\pi-2)u^2+4u+\pi-2]^2,$$

$$A_{2,-1}^{(1)}(u) = u(\pi-2)(u+1)^2[(2\pi-3)u^2+2u+1],$$

$$\begin{aligned}
A_{2,-1}^{(2)}(u) = {} & -\pi u(u+1)^2[(2\pi-3)u^2+2u+1][(\pi-2)u^2+4u+\pi-2][(\pi^2-4\pi+6)u^4+(2\pi^2-6\pi+8)u^3 \\
& -(2\pi^2-20\pi+28)u^2+(2\pi^2-6\pi+8)u+\pi^2-4\pi+6],
\end{aligned}$$

$$A_{1,1}^{(1)}(u) = u^2[(\pi-2)u^4 + (2\pi^2-8\pi+16)u^3 + (8\pi^2-34\pi+52)u^2 - (6\pi^2-56\pi+80)u + 4\pi^2 - 15\pi + 14],$$

$$A_{1,1}^{(2)}(u) = -u^2\pi(u+1)^2(u^2+2u+2\pi-3)^2[(\pi-2)u^2+4u+\pi-2]^2,$$

$$A_{-1,1}^{(1)}(u) = (u+1)^2[(\pi-2)u^2 - 2(\pi^2-3\pi-2)u + \pi - 2],$$

$$A_{-1,1}^{(2)}(u) = -\pi(u+1)^2(u^2+2u+2\pi-3)[(2\pi-3)u^2+2u+1][(\pi-2)u^2+4u+\pi-2]^2,$$

$$A_{2,1}^{(1)}(u) = (\pi-2)u(u+1)^2(u^2+2u+2\pi-3),$$

$$\begin{aligned}
A_{2,1}^{(2)}(u) = {} & -\pi u(u+1)^2(u^2+2u+2\pi-3)[(\pi-2)u^2+4u+\pi-2][(\pi^2-4\pi+6)u^4+(2\pi^2-6\pi+8)u^3 \\
& -(2\pi^2-20\pi+28)u^2+(2\pi^2-6\pi+8)u+\pi^2-4\pi+6],
\end{aligned}$$

$$A_{1,2}^{(1)}(u) = u^2(\pi-2)(u+1)^2(u^2+2u+2\pi-3),$$

$$A_{1,2}^{(2)}(u)=-\pi u^2\,(u+1)^2(u^2+2u+2\pi-3)[(\pi-2)u^2+4u+\pi-2][(\pi^2-4\pi+6)u^4+(2\pi^2-6\pi+8)u^3-(2\pi^2-20\pi+28)u^2+(2\pi^2-6\pi+8)u+\pi^2-4\pi+6],$$

$$A_{-1,1}^{(1)}(u)=(\pi-2)(u+1)^2[(2\pi-3)u^2+2u+1],$$

$$A_{-1,1}^{(2)}(u)=-\pi\,(u+1)^2[(2\pi-3)u^2+2u+1][(\pi-2)u^2+4u+\pi-2][(\pi^2-4\pi+6)u^4+(2\pi^2-6\pi+8)u^3-(2\pi^2-20\pi+28)u^2+(2\pi^2-6\pi+8)u+\pi^2-4\pi+6],$$

$$A_{-2,2}^{(1)}(u)=-u[u^2+(2\pi-2)u+1]^{-1}(u+1)^2[(\pi-6)u^4-8u^3+(4\pi^3-16\pi^2-2\pi+28)u^2-8u+\pi-6],$$

$$A_{-2,2}^{(2)}(u)=-\pi\,u(u+1)^2[(\pi^2-4\pi+6)u^4+(2\pi^2-6\pi+8)u^3-(2\pi^2-20\pi+28)u^2+(2\pi^2-6\pi+8)u+\pi^2-4\pi+6]^2,$$

$$A_{2,2}^{(1)}(u)=u[u^2+(2\pi-2)u+1]^{-1}[(2\pi^2-9\pi+14)u^6+(4\pi^3-20\pi^2+46\pi-28)u^5+(12\pi^3-66\pi^2+169\pi-142)u^4-(16\pi^3-168\pi^2+412\pi-312)u^3+(12\pi^3-66\pi^2+169\pi-142)u^2+(4\pi^3-20\pi^2+46\pi-28)u+2\pi^2-9\pi+14],$$

$$A_{2,2}^{(2)}(u)=-\pi\,u(u+1)^2[(\pi^2-4\pi+6)u^4+(2\pi^2-6\pi+8)u^3-(2\pi^2-20\pi+28)u^2+(2\pi^2-6\pi+8)u+\pi^2-4\pi+6]^2.$$

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[1] R.G. Palmer, Lect. Notes Phys. **275**, 275 (1987).
[2] K. Nakazato and K. Kitahara, Prog. Theor. Phys. **64**, 2261 (1980).
[3] P. Ferrari, S. Goldstein, and J.L. Lebowitz, in *Statistical Physics and Dynamical Systems*, edited by J. Fritz, A. Jaffe, and D. Szasz (Birkhäuser, Boston, 1985), p. 405.
[4] K.W. Kehr and K. Binder, in *Application of the Monte Carlo Method in Statistical Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1987), and references therein.
[5] B.D. Hughes, *Random Walks and Random Environments* (Oxford Science, Oxford, 1995).
[6] S.F. Burlatsky, G. Oshanin, M. Moreau, and W.P. Reinhardt, Phys. Rev. E **54**, 3165 (1996).
[7] O. Bénichou, A.M. Cazabat, A. Lemarchand, M. Moreau, and G. Oshanin, J. Stat. Phys. **97**, 351 (1999).
[8] R. Granek and A. Nitzan, J. Chem. Phys. **92**, 1329 (1990).
[9] O. Bénichou, J. Klafter, M. Moreau, and G. Oshanin, Phys. Rev. E **62**, 3327 (2000).
[10] R. van Gastel, E. Somfai, S.B. van Albada, W. van Saarloos, and J.W.M. Frenken, Phys. Rev. Lett. **86**, 1562 (2001).
[11] J.W.M. Frenken, R. van Gastel, S.B. van Albada, E. Somfai, and W. van Saarloos, in *Proceedings of the NATO Advanced Research Workshop on "Collective Diffusion on Surfaces: Collective Behaviour and the Role of Adatom Interactions,"* edited by M.C. Tringides and Z. Chvoj (Kluwer, Dordrecht, 2001).
[12] R. van Gastel, E. Somfai, W. van Saarloos, and J.W.M. Frenken, Nature (London) **408**, 665 (2000).
[13] O. Bénichou and G. Oshanin, Phys. Rev. E **64**, R020103 (2001).
[14] M.J.A.M. Brummelhuis and H.J. Hilhorst, J. Stat. Phys. **53**, 249 (1988); see also: M. Brummelhuis, Ph.D. thesis, Leiden University, The Netherlands, 1991.
[15] T.J. Newman, Phys. Rev. B **59**, 13754 (1999).
[16] Z. Toroczkai, Int. J. Mod. Phys. B **11**, 3343 (1997).
[17] R.K.P. Zia and Z. Toroczkai, J. Phys. A **31**, 9667 (1998).
[18] M.J.A.M. Brummelhuis and H.J. Hilhorst, Physica A **156**, 575 (1989).
[19] Ajay and R.G. Palmer, J. Phys. A **23**, 2139 (1990).
[20] C. Landim, S. Olla, and S.B. Volchan, Commun. Math. Phys. **192**, 287 (1998).
[21] G. Oshanin, J. De Coninck, M. Moreau, and S.F. Burlatsky, in *Instabilities and Non-Equilibrium Structures VII*, edited by E. Tirapegui (Kluwer Academic, Dordrecht, in press); e-print cond-mat/9910243.
[22] Q. Gu, E.A. Schiff, S. Grebner, F. Wang, and R. Schwartz, Phys. Rev. Lett. **76**, 3196 (1996).
[23] F. Amblard, A.C. Maggs, B. Yurke, A.N. Pargellis, and S. Leibler, Phys. Rev. Lett. **77**, 4470 (1996).
[24] E. Barkai and J. Klafter, Phys. Rev. Lett. **81**, 1134 (1998).
[25] Ya.B. Sinai, Theor. Probab. Appl. **27**, 247 (1982); H. Kesten, M.V. Kozlov, and F. Spitzer, Compos. Math. **30**, 145 (1975); B. Derrida and Y. Pomeau, Phys. Rev. Lett. **48**, 627 (1982).
[26] E. Barkai and V.N. Fleurov, Phys. Rev. E **58**, 1296 (1998).
[27] J. Kurchan, J. Phys. A **31**, 3719 (1998).
[28] L.F. Cugliandolo, D.S. Dean, and J. Kurchan, Phys. Rev. Lett. **79**, 2168 (1997).
[29] O. Bénichou, A.M. Cazabat, J. De Coninck, M. Moreau, and G. Oshanin, Phys. Rev. Lett. **84**, 511 (2000); Phys. Rev. B **63**, 235413 (2001).
[30] N.G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, New York, 1981).
[31] E.W. Montroll, J. Math. Phys. **10**, 753 (1969); Proc. Symp. Appl. Math. **16**, 193 (1964).
[32] W. McCrea and F. Whipple, Proc. R. Soc. Edinburgh **60**, 281 (1940).
[33] F. Spitzer, *Principles of Random Walk* (Van Nostrand, Princeton, NJ, 1964).
[34] W. Feller, *An Introduction to Probability Theory and its Applications*, 2nd ed. (Wiley, New York, 1970), Vols. 1 and 2.
[35] O. Bénichou, M. Moreau, and G. Oshanin, Phys. Rev. E **61**, 3388 (2000).