A one-dimensional random walk in a multi-zone environment

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Abstract
We study a symmetric random walk (RW) in a one-dimensional environment, formed by several zones of finite width, where the probability of transition between two neighbouring points, and the corresponding diffusion coefficient, are considered to be fixed. We derive analytically the probability of finding a walker at the given position and time. The probability distribution function is found and has no Gaussian form because of the properties of adsorption in the bulk of the zones and the partial reflection at the separation points. The time dependence of the mean squared displacement of a walker is studied too, revealing the transient anomalous behaviour as compared to an ordinary RW.

Keywords: random walk, inhomogeneous environment, diffusion

(Some figures may appear in colour only in the online journal)

1. Introduction

The random walk model (RW) is applied in the majority of fields, such as polymer physics, economics, and computer sciences [1] and is generally used as a simple mathematical formulation of the diffusion process. The standard unconstrained RW is characterized by constant transition probabilities which are independent of space and time, and are the prototype example of a stochastic Gaussian process.

The RW problem in an inhomogeneous environment is of great interest since it is connected with physical phenomena such as the transport properties in fractures and porous rocks, and the diffusion of particles in gels, colloidal solutions and biological cells (see, e.g. [2] for a review). A particle performing ordinary diffusion is typically characterized by the mean square displacement \( \langle x^2 \rangle \) obeying a scaling law \( \langle x^2 \rangle \sim t \) at time \( t \) (or, equivalently, after \( t \) steps of the RW trajectory) independently of the space dimension \( d \) [3]. The presence
of inhomogeneities may lead to the anomalous diffusion regime with nonlinear power-law dependence on $t$. Numerous analytical and numerical studies have been carried out to analyze the properties of anomalous diffusion on fractal-like structures like percolation clusters [4–11]. Anomalous diffusion is found in processes like charged particle transport in amorphous semiconductors [12] or the motion of biochemical species in the crowded environment of biological cells [13]. A space dependent diffusivity is often observed in heterogeneous systems, such as in processes of Richardson diffusion in turbulence [14] or in the diffusion of tracers in bacterial and eukaryotic cells [15]. The non-ergodicity of heterogeneous diffusion processes with a space-dependent diffusion coefficient is demonstrated analytically in [16].

Restricting the volume of space available to the diffusing particles by confining boundaries causes remarkable entropic effects [17]. Numerous studies dealing with the one-dimensional RW in an environment with ‘inhomogeneities’ such as walls [18–20], a stack of permeable barriers [21–23] or finite-sized barriers [24, 25], have revealed the physically significant effects and the non-trivial behaviour with pronounced deviation away from the Gaussian one. In particular, the time dependent (transient) diffusion coefficients are observed in an inhomogeneous system with parallel walls of arbitrary permeabilities [21]. The breaking of time scale invariance is found for Brownian random walks in confined space with absorbing walls [26]. These studies also point out the difficulties in analytical description in the problems above. Taking into account certain properties of such models, we are aiming to generalize.

In the present paper, we focus our attention on the symmetric RW model with position-dependent transition probability which is equal for the left and right steps and varies within the different intervals (zones) of the coordinate axis. Actually, replacing the probabilities of transition and adhesion within each zone with their mean values, we obtain the step-like dependence in space. In particular, the zones of narrow width in our model can reproduce the walls.

Thus, we consider the RW in an environment consisting of $N$ zones with constant parameters, and reduce the problem to solving the differential equation with a diffusion coefficient which inherits the established space dependence. We concentrate our attention on finding the probability distribution function (PDF) by neglecting the local fluctuations of environment characteristics. Since the adhesion property of zones can vary, it is expected that a time dependence of the averages should differ from that in the case of uniform medium.

On the basis of the PDF found for any $N$ we calculate $\langle x^2 \rangle$ as a function of finite $t$ and investigate its anomalous behaviour within the three-zone models. Averaging PDF over time $t$, we can also estimate the probability of finding a walker in a given point of space and compare it with the performed numerical simulations. We interpret its profile peculiarities from the points of view of transport theory and mechanics.

The layout of the paper is as follows. In the next section, we constitute the random walk rules and obtain the differential equation for PDF. The probability function and its distribution (PDF) are found in section 3. After calculating the mean square displacement in section 4, we conclude with discussion and outlook.

### 2. Formulation of RW model in $N$-zone environment

We start with the discrete RW model, which can be considered as a Markov process, where unitary step in time results in either zeroth or unitary step in space $\mathbb{Z}$. The evolution is determined here by stationary transition probability $T(x_{t+1}, x_t)$ defined as
\[ T(x_1, x_2) = p(x_2)\delta_{x_1 - x_2, -1} + q(x_2)\delta_{x_1 - x_2, 1} + r(x_2)\delta_{x_1 - x_2, 0}, \]
\[ \sum_{x_1 \in \mathbb{Z}} T(x_1, x_2) = 1, \]  
(1)

where constraint \( p(x) + q(x) + r(x) = 1 \) is fulfilled for all \( x \); \( \delta \) is the Kronecker symbol.

Functions \( p(x) \) and \( q(x) \) determine the probabilities of finding a walker at points \( x - 1 \) and \( x + 1 \) if it was at \( x \) in the previous time moment, respectively; while \( r(x) \) corresponds to the probability of adhesion (adsorption) \([19]\). In general, \( p(x), q(x) \) are regarded as arbitrary non-negative functions which do not exceed the unit.

To formulate our model, we give the finite sequence \( \{a_n\} \) of positive numbers,
\[ 0 = a_0 < a_1 < \ldots < a_{N-1} < a_N = \infty, \]  
(2)
determining the positions of walls or separation points of environment phases.

For \( x < 0 \), we reproduce the same configuration symmetric with respect to the starting point \( x = 0 \).

Using the finite set \( \{p_n\} \) of the given positive constants, we consider the RW without preference between the moves to the left and right in an heterogeneous environment with the following properties:
\[ p(x) = p_n \quad \text{for} \quad a_{n-1} < |x| < a_n; \quad p(|a_n|) = \frac{1}{2}(p_{n+1} + p_n), \]  
(3)
\[ q(x) = p(x), \quad r(x) = 1 - 2p(x). \]  
(4)

To preserve a probability meaning of the functions, we require \( p_n \leq 1/2 \).

We would like to note that the numerical simulations demonstrate a sensitivity of the particle distribution in space to the definition of transition probability at \( x = \{\pm a_n\} \). It shows an important role of the interface effect in the multi-zone problem.

The time evolution of the probability distribution function (PDF) \( P(x,t) \) in a Markov picture with our initial condition \( P(x,0) = \delta_{x,0} \) is given by equation:
\[ P(x,t+1) = \sum_{x_2 \in \mathbb{Z}} T(x_2, x)P(x_2, t), \quad \sum_{x \in \mathbb{Z}} P(x,t) = 1. \]  
(5)

The master equation with arbitrary distance \( \ell \) and time \( \tau \) between successive steps reads
\[ P(x,t+\tau) = p(x+\ell)\rho(x+\ell,t) + q(x-\ell)\rho(x-\ell,t) + r(x)\rho(x,t). \]  
(6)

To obtain a differential equation for PDF, \( \tau \) should be relatively large while \( \ell \) and \( \tau \) tend to zero simultaneously. Using a Taylor expansion of \( P(x, t) \), one gets
\[ \partial_t P(x,t) = v\partial_x[p(x) - q(x)]P(x,t) + D\partial_x^2[p(x) + q(x)]P(x,t) + O(\ell^2), \]  
(7)
where \( v \equiv \ell/\tau \) and \( D \equiv \ell^2/2\tau \) are constant drift velocity and diffusivity, respectively.

Omitting terms of order \( O(\ell^2) \) and fixing \( v = 1 \) and \( D = 1/2 \), we obtain the differential equation of the RW in diffusion approximation:
\[ \partial_t P(x,t) = \partial_x^2[D(x)P(x,t)], \quad D(x) = \sum_{n=1}^{N} p_n \chi_n(x), \]  
(8)
where diffusivity function \( D(x) \) coincides with \( p(x) \), and
\( \chi_1(x) = \begin{cases} 
1, & |x| < a_1 \\
1/2, & |x| = a_1 \\
0/2, & |x| = a_{n-1}, a_n \\
0, & \text{otherwise}
\end{cases} \)
\( \chi_{n>1}(x) = \begin{cases} 
1, & a_{n-1} < |x| < a_n \\
1/2, & |x| = a_{n-1}, a_n \\
0, & \text{otherwise}
\end{cases} \) (9)

The characteristic functions \( \{\chi_n\} \) of the intervals are orthogonal and have the properties:

\[ \sum_{n=1}^{\infty} \chi_n(x) = 1, \quad |x| < \infty; \quad \chi_n(x)\chi_m(x) = 0, \quad n \neq m; \] (10)

\[ \int_{-\infty}^{\infty} \chi_n(x)\chi_m(x)dx = 2(a_n - a_{n-1})\delta_{n,m}, \quad n, m < N. \] (11)

However, in the continuous limit functions \( \delta_{x,y} \) and \( \chi_n(x) \) should be replaced with distributions, using the Dirac \( \delta \)-function and the Heaviside \( \theta \)-function. We find that

\[ P(x,0) = \delta(x), \quad D(x) = p_1 + \sum_{n=1}^{N-1} \alpha_n \theta(|x| - a_n), \] (12)

where \( \alpha_n = p_{n+1} - p_n, |\alpha_n| < 1/2; \) and \( \theta(x) = [1 + \text{sign}(x)]/2. \)

Although \( D(x) \) contains information on geometry and phases of environment as ‘input’, the PDF is evolving in space-time and determines a normalized statistical measure \( \mu_t \) for a fixed \( t \):

\[ d\mu_t = P(x,t)dx, \quad \int d\mu_t = 1. \] (13)

In practice, we compute the probability of finding a walker at point \( x \) at time \( t \),

\[ \Pr(x,t) = \frac{1}{t} \int_0^t P(x,\tau)d\tau, \] (14)

that is the frequency of visiting a point \( x \) in time \( t \).

### 3. Finding a solution

In order to develop an approach with \( p_n > 0 \), let us consider the functions

\[ D(\alpha, x) = \sum_{n=1}^{N} (p_n)^\alpha \chi_n(x), \quad D(0,x) = 1, \] (15)

which are generated by the diffusivity function \( D(x) \equiv D(1,x) \) and depend on both \( x \) and \( \{p_n\} \) simultaneously, which requires specific rules of differential calculus.

Due to orthogonality of basis \( \{\chi_n(x)\} \), one has

\[ D(\alpha, x)D(\beta, x) = D(\alpha + \beta, x), \quad x \in \mathbb{R}/\{\pm a_n\}. \] (16)

Differentiation (integration) of \( D(\alpha, x) \) in space \( x \) is mainly related by a change of the basis, while exponents of parameters \( \{p_n\} \) stay unchanged. One has

\[ D'(\alpha + \beta, x) = D'(\alpha, x)D(\beta, x) + D(\alpha, x)D'(\beta, x), \] (17)

where the prime symbol means differentiation with respect to the coordinate.

Numerical coefficients in the last formula are subjects of the relation:
\((p_{n+1})^{\alpha+\beta} - (p_n)^{\alpha+\beta} = \frac{1}{2} \left[ (p_{n+1})^{\alpha} - (p_n)^{\alpha} \right] \left[ (p_{n+1})^{\beta} + (p_n)^{\beta} \right] + \frac{1}{2} \left[ (p_{n+1})^{\alpha} + (p_n)^{\alpha} \right] \left[ (p_{n+1})^{\beta} - (p_n)^{\beta} \right] \),

where \(1/2\) and the sign ‘+’ in brackets result from the \(\theta\)-function in \(D\), while the ‘-’ results from \(D'\) containing the \(\delta\)-function.

To find the PDF, we first concentrate the geometrical data in the new coordinate \([27]\)

\[ y(x) = \int_0^x D(-1/2, x')dx'. \] (19)

Although there exists one-to-one correspondence between \(x\) and \(y\), the derivatives of \(y(x)\) are singular, in general, at the points \(x = \{\pm a_n\}\).

Integrating (19), we obtain that \(y(x) = \text{sign}(x) Y(-1/2, |x|)\), where

\[ Y(\alpha, x) \equiv \frac{1}{2} \sum_{n=1}^N (p_n)^\alpha \left( a_n - a_{n-1} + |x - a_{n-1}| - |x - a_n| \right), \quad x \geq 0. \] (20)

At this stage, let us define the new functions \(\tilde{D}(\alpha, y(x)) = D(\alpha, x)\):

\[ \tilde{D}(\alpha, y) = \sum_{n=1}^N (p_n)^\alpha \tilde{\chi}_n(y). \] (21)

where \(\tilde{\chi}_n(y) = \theta(|y| - b_{n-1}) - \theta(|y| - b_n)\) and \(b_n \equiv y(a_n)\).

Then, introducing distribution \(\tilde{P}(y, t)\), we rewrite the statistical measure as

\[ d\mu_t = \tilde{P}(y, t)dy = \tilde{P}(y(x), t)\tilde{D}(-1/2, y(x))dx. \] (22)

Substituting the redefined \(P(x, t)\) and \(\partial_\gamma \tilde{D}(-1/2, y)\partial_\gamma\) into (8), we have

\[ \partial_\gamma \tilde{P} - \partial_\gamma^2 \tilde{P} = \kappa \partial_\gamma (\beta \tilde{P}), \quad \tilde{P}(y, 0) = \delta(y), \] (23)

where the constant \(\kappa\) regulates an interface effect between zones.

The right hand side of (23) can be reduced to the form of \(\beta(y) = \tilde{D}(-1/2, y)\partial_\gamma \tilde{D}(1/2, y)\).

Computations lead to expressions:

\[ \beta(y) = \text{sign}(y) \sum_{n=1}^{N-1} \beta_n \delta(|y| - b_n), \quad \beta_n = \frac{p_{n+1} - p_n}{2\sqrt{p_n p_{n+1}}}, \] (24)

\[ B(y) = \sum_{n=1}^{N-1} \beta_n \theta(|y| - b_n), \partial_\gamma B(y) = \beta(y). \] (25)

Taking into account the specific properties of \(D\)-functions, which should be investigated in more detail, the form of \(\beta_n\) can vary, which also influences the value of \(\kappa\). However, a sign of \(\beta_n\) is defined by the difference \(p_{n+1} - p_n\). Moreover, \(B(y)\) is not a logarithmic function here, although \(\beta(y)\) is similar to its log-derivative by construction.

We have already found that the bulk diffusion mainly depends on \(y(x)\). The remaining problem is to account for the surface effect determined by \(\beta(y)\) and \(\kappa\). We attempt to find \(\tilde{P}(y, t)\) within the perturbative scheme, when
\[ P(y, t) = \varphi(y, t) + \sum_{n=1}^{\infty} \kappa S_n(y, t), \quad \text{(26)} \]

where

\[ \varphi(y, t) = \frac{1}{\sqrt{4\pi t}} \exp \left( -\frac{y^2}{4t} \right) \quad \text{(27)} \]

is Gaussian distribution resulting in probability (14):

\[ \Phi(y, t) = \frac{1}{\sqrt{4\pi t}} \exp \left( -\frac{y^2}{4t} \right) + \frac{|y|}{2t} \left[ \text{erf} \left( \frac{|y|}{2\sqrt{t}} \right) - 1 \right]. \quad \text{(28)} \]

A possible solution of the inhomogeneous equation \( \partial_t S_1 - \partial_x^2 S_1 = \partial_x (\beta \varphi) \) is the function

\[ S_1(y, t) = -B(y) \varphi(y, t) - \mathcal{F}(y, t), \]

where

\[ \mathcal{F}(y, t) = -\frac{1}{2} \sum_{n=1}^{N-1} \beta_n [\varphi(y - b_n, t) + \varphi(y + b_n, t)]. \quad \text{(29)} \]

Finding \( \mathcal{F}(y, t) \) from the auxiliary equation \( \partial_t \mathcal{F} - \partial_x^2 \mathcal{F} = \beta \partial_x \varphi \), we contract \( \beta \partial_x \varphi \) and \( \varphi \) playing the role of fundamental solution to the diffusion equation with the use of the formula:

\[ \int_0^t \exp \left( \frac{y_1^2}{4(t - \tau)} - \frac{y_2^2}{4\tau} \right) \frac{d\tau}{\sqrt{(t - \tau)\tau^3}} = \frac{4\pi}{y_2^2} \sqrt{\frac{\pi}{2t}} \exp \left[ -\frac{(|y_1| + |y_2|)^2}{4t} \right]. \quad \text{(30)} \]

Limiting ourselves by accounting for the first-order correction, we obtain our main result for the PDF:

\[
P(x, t) = \varphi(y(x), t)[1 - \kappa B(y(x))]D(-1/2, x) + \frac{\kappa}{2} \sum_{n=1}^{N-1} \beta_n [\varphi(y(x) - b_n, t) + \varphi(y(x) + b_n, t)]D(-1/2, x). \quad \text{(31)}
\]

This formula looks applicable at \(|\beta_n| < 1\) because the correction is of the same order of magnitude as \(\varphi\). The PDF of the ordinary RW is restored at \(2p_n = 1\) for all \(n\), when \(\beta_n = 0\) and \(y(x) = \sqrt{2x}\).

Of course, the number of independent zones decreases if the neighbouring zones have the same value of \(p_n\) and, therefore, are joint. The interface point \(x = a_n\) between zones with \(p_n\) and \(p_{n+1} = p_n\) becomes regular.

Note that (31) is similar to the amplitude squared in the WKB approximation of quantum mechanics, and the points \(x = \{\pm a_n\}\) are connected with the turns, induced by a potential in the Schrödinger equation. In principal, a ‘potential’ [27] in our model could appear by excluding the term \(\partial_x^2\mathcal{F}\) in (23) and would be determined by the Schwarzian derivative of the function (A.2)

\[ f(y) = \int_0^y \tilde{D}(1/2, y')dy'. \quad \text{(32)} \]

In order to get an expression for probability \(Pr(x, t)\), we should simply replace the function \(\varphi(y, t)\) with \(\Phi(y, t)\) in (31). To test our calculations, we compare the obtained \(Pr(x, t)\) with numerical simulations. Data are presented in figure 1. The analytical solution at \(\kappa = 1\) is in agreement here with the RW developing in the three-zone environment. However, one needs
to account for higher-order corrections to reproduce better the considerable changes of the probability profile at short $\Delta x$.

4. Variance

To investigate the walker diffusion, let us calculate the variance $\langle x^2 \rangle$, that is,

$$\Lambda(t) \equiv \int x^2 d\mu; \quad \langle x \rangle \equiv \int x d\mu = 0.$$  

(33)

Note that $\Lambda(t)$ is linear in $t$ in the case of purely Gaussian distribution.

In our case, one has

$$\Lambda_0(t) = \Lambda_0(t) + \kappa \Lambda_1(t) + O(\kappa),$$

(34)

Although function $x(y)$ can be presented similarly to (20), it is useful to rewrite it in integrals in terms of $\{\tilde{\chi}_n(y)\}$. We find that

$$[x(y)]^2 = y^2 A_2(y) + |y| A_1(y) + A_0(y), \quad A_n(y) = \sum_{n=1}^{N} A_{n,n} \tilde{\chi}_n(y);$$

(35)

where numerical coefficients are

$$A_{2,n} = p_n, \quad A_{1,n} = 2(\sqrt{p_n} c_n - p_n b_{n-1}), \quad A_{0,n} = (c_n - \sqrt{p_n} b_{n-1})^2,$$

(36)

$$c_n = \sum_{m=1}^{n-1} \sqrt{p_m} (b_m - b_{m-1}).$$

(37)

Note that $A_2(y)$ coincides with diffusivity $\bar{D}(y)$.

Combining the environment parameters $A_{n,n}$ and time dependent integrals, we write down the variance components:
\[ \Lambda_0(t) = 2 \sum_{i=0}^{N} \sum_{n=1}^{N} A_{in} [U_s(b_i, t) - U_s(b_{i-1}, t)] , \]  
(38)

\[ \Lambda_1(t) = -2 \sum_{i=0}^{N} \sum_{n=2}^{N} A_{in} B_n [U_s(b_i, t) - U_s(b_{i-1}, t)] \]
\[ + \sum_{i=0}^{N} \sum_{n=1}^{N-1} \sum_{m=1}^{N} A_{in} \beta_m (V_s(b_i, t, t \mid b_m) - V_s(b_{i-1}, t, t \mid b_m)) , \]
(39)

where \( B_n = \sum_{m=1}^{n-1} \beta_n \) for \( n \geq 2 \), and

\[ U_s(b, t) \equiv \int_0^b y^s \varphi(y, t) dy , \]
(40)

\[ V_s(B, t \mid b) \equiv \int_0^b y^s [\varphi(|y - b|) + \varphi(|y + b|)] dy . \]
(41)

The Gaussian integrals yield

\[ U_0(b, t) = \frac{1}{2} \text{erf} \left( \frac{b}{2 \sqrt{t}} \right) , \quad U_1(b, t) = \sqrt{\frac{t}{\pi}} \left[ 1 - \exp \left( -\frac{b^2}{4t} \right) \right] , \]
\[ U_2(b, t) = t \text{erf} \left( \frac{b}{2 \sqrt{t}} \right) - b \sqrt{\frac{t}{\pi}} \exp \left( -\frac{b^2}{4t} \right) . \]
(42)

Using \( U_s(b, t) \), we also get

\[ V_0(B, t \mid b) = U_0(B + 2b, t) - \theta(b - B) U_0(2b - B, t) \]
\[ + \theta(B - b) [U_0(B, t) - 2U_0(b, t)] , \]
(43)

\[ V_1(B, t \mid b) = U_1(B + 2b, t) - 2U_1(2b, t) + 4bU_0(2b, t) - 2bU_0(B + 2b, t) \]
\[ + \theta(b - B) [U_1(2b - B, t) - 2bU_0(2b - B, t) + 2bU_0(b, t)] \]
\[ + \theta(B - b) U_1(B, t) \],
(44)

\[ V_2(B, t \mid b) = U_2(B + 2b, t) - 2U_1(2b, t) - 4bU_1(B + 2b, t) \]
\[ + 4b^2U_0(B + 2b, t) \]
\[ - \theta(b - B) [U_2(2b - B, t) - 4bU_1(2b - B, t) \]
\[ + 4b^2U_0(2b - B, t)] \]
\[ + \theta(B - b) [U_2(B, t) - 2U_2(b, t) + 4bU_1(b, t) \]
\[ - 4b^2U_0(b, t)] , \]
(45)

where \( \theta(0) = 1/2 \) is assumed.

Analyzing \( \Lambda(t) \), let us introduce effective diffusivities \( \Lambda(t)/2t \) and \( \partial_t \Lambda(t)/2 \). Thus, if \( p_n = p \) for all \( n \), these coincide with \( p \).

We also consider the second-order derivative of \( \Lambda(t) \), denoted by \( C \) and connected with the velocity autocorrelation function according to Kubo’s relation [28, 29]:

\[ \frac{1}{2} \frac{d\langle \dot{x}^2(t) \rangle}{dt} = \int_0^t \langle \dot{x}(t') \dot{x}(0) \rangle dt' , \quad t \to \infty , \]
(46)
where $x(t)$ is the continuous stochastic coordinate with $\langle x(t) \rangle = 0$ and $\langle \dot{x}(t) \rangle = 0$.

The results based on our formulae are sketched in figure 2. We see on the left panel that there are the time intervals where the effective diffusivities are decreasing and increasing. These may correspond, respectively, to transient regimes of subdiffusion and superdiffusion, represented by $C < 0$ and $C > 0$ on the right panel. We conclude that a role of the $n$th zone in the diffusion picture depends mainly on the adsorption effect which is proportional to probability $r_n = 1 - 2p_n$. Moreover, the model situations under consideration demonstrate the inaccessibility of the regime with $p_3$ in a given time interval. However, by putting $b_N \to \infty$ before tending $t$ to infinity, it is expected that only terms with $U_2(b_N, t)/t \to 1$ should survive at $t \to \infty$ in a strong mathematical sense. However, we found that this limit is reached slowly because of the structure of the environment. In other words, there is always a non-vanishing probability of walker capture by the $n$th zone with $r_n > r_N$. This determines the time delay which may be estimated. Moreover, we assume an existence of different time scales which should be accurately defined [30] for a deeper understanding.

On the other hand, the right panel of figure 2 illustrates that the correlation $C$ is relaxed with time, and information about the early stage of evolution, developed in region near the origin, is lost. In the case when a worker stays within the infinitely wide $N$th zone for a long time, an impact of a whole zone structure decreases in its history.

It is interesting to note that the stage with $C < 0$ is often connected with a presence of a liquid-like state in a many-particle system [29]. This state emerges here due to a specifically located zone with $2p = 0.4$ and could be intuitively foreseen, although the sufficient conditions required for its appearance are still unclear to us. We can only say that the zones with relatively small $p_n$ keep a walker in a trap for a short time, so after a while the walker is able to diffuse away.

5. Discussion

Initially, we formulated the model of a one-dimensional RW with space dependent transition probability, which is identical for the left and right steps. We describe a wandering in space with the finite-sized zones having adsorption properties in the bulk and partial reflection at the boundary points. It generalizes a problem of RW with various barriers [19, 20, 24] and allows us to speak about the heterogeneous environment. By locating the $N$ zones $x \in (-a_n, -a_{n-1}) \cup (a_{n-1}, a_n)$ densely along the coordinate axis, the transition probability in the $n$th zone is determined by

![Figure 2. Left panel: time dependence of effective diffusivities $\Lambda/2t$ (solid line) and $\partial_t \Lambda/2$ (dashed line) for two sets of parameters as in figure 1. Right panel: dependence of $C \equiv \partial^2 \Lambda/2$ on $t$. Gray curves are for the model with $p_1 = 0.2$, while black ones are for the model with $p_1 = 0.3$.](image-url)
constant parameter $p_n$, except at the separation points where its value changes. This assumption is crucial for finding an analytical solution to the model equations in diffusion approximation at the large number of walker steps. The step-like dependence of the diffusion coefficient at $x$ prompts us to introduce the new coordinate $y(x)$, in terms of which the probability distribution is constructed with the use of a Gaussian one (31). Nevertheless, the distribution function obtained is non-Gaussian because of the complexity of the environment and surface effects at singular points $\{\pm a_n\}$ where the derivatives of functions with respect to $x$ diverge.

It seems to be difficult to describe analytically an effect of an infinitely thin zone (a wall) without additional suggestions. A similar problem arises in zone interface description. Comparing the numerical RW simulations with discrete $x \in \mathbb{Z}$ and analytical solutions in the continuous limit, we might effectively displace a position $a_n$ of a point-like barrier up to $a_n \pm 1/2$ in order to obtain the finitely wide border. Another possibility is to use the solutions with a gap [25] which are not considered here.

Actually, our model describes the diffusion process, taking into account the long-range properties of environment and neglecting local fluctuations $\delta D(x) \equiv D(x) - \bar{D}(x)$ of smooth-varied diffusivity $D(x)$, where

$$
D(x) = \sum_{n=1}^{N} D_n \chi_n(x), \quad D_n = \frac{1}{2(a_n - a_{n-1})} \int_{-\infty}^{\infty} D(x) \chi_n(x) \, dx.
$$

(47)

Analyzing the results presented in figure 1, we can clarify the physical reasons for the non-trivial distribution of the particles emanating from the origin.

The explanation for remarkable probability changes is based on a role of walker adhesion, which is forced by the environment and related with probability $r_n = 1 - 2p_n$. The sequence of zones with different values of $p_n$ is also significant: the sign of the difference $p_{n+1} - p_n$ is responsible for the preferable direction of the walk on the interface of neighbouring zones indexed by $n$ and $n + 1$. The relative time of the walker being in the $n$th zone depends on the number $n$, width $a_n - a_{n-1}$, and $r_n$. Thus, the adhesion effect can be evaluated by characteristic time and length. Nevertheless, a long-time tail of the variance corresponds to the ordinary diffusion with $\langle x^2 \rangle \sim t$ at $t \to \infty$.

Alternatively, this can be treated in terms of mechanics by introducing an effective walker ‘mass’ $m_n = 1/2p_n$ for each zone of the environment. Considering a macroscopic ensemble of the particles, we can interpret the mass changes as the result of geometrically dependent interaction among particles, which is not specified in our picture but leads to the appearance of the different states or phases confined within the given intervals.

It is expected that the Fourier transform $\tilde{P}(k,t)$ of the PDF can give us the one-particle distribution function in momentum space $k$, accounting for the phase transitions in our case, in accordance with the ideas of Bloch and Balescu. Indeed, replacing $t$ and $p_n$ with inverse temperature $1/T$ and $1/2m_n$, respectively, the PDF of the ordinary diffusion process,

$$
\tilde{P}(k,t) \propto e^{-k^2 pt},
$$

(48)

plays the role of Boltzmann distribution, which is a starting point for deriving thermodynamic functions and relations for a many-particle ensemble.

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Appendix. Potential model

Let us substitute $\mathcal{P}(y, t) = \exp \left[ -B(y)/2 \right] \Pi(y, t)$ in (23) at $\kappa = 1$. One gets

$$-\partial_t \Pi = -\partial_y^2 \Pi + V^2.$$  \hspace{1cm} (A.1)

The potential $V$ can be presented as

$$V(y) \equiv -\frac{1}{2} \left( \beta - \frac{1}{2} \beta^2 \right) = -\frac{1}{2} S(f),$$  \hspace{1cm} (A.2)

where $\beta(y)$ and $f(y)$ are given by (24) and (32), respectively. We use the formal notation for the Schwarzian derivative $S(f) \equiv \left( f''/f' \right)' - \left( f''/f' \right)^2/2$; and relation $\beta = f''/f'$.

Note that the form of (A.2) is similar to the potential of the super-symmetric problem [31]. The function $u(y) \equiv 1/\sqrt{f} = \tilde{D}(-1/4, y)$ is a solution to the stationary equation

$$u'' + \frac{1}{2}(S(f))u = 0.$$  \hspace{1cm} (A.3)

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