Boundary singularities and boundary conditions for the Fokker-Planck equations

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The boundary conditions for the Fokker-Planck equations, forward and backward ones are directly derived from the Chapman-Kolmogorov equation for M-dimensional region with boundaries. The boundaries are assumed, in addition, to be able to absorb wandering particles or to give rise to fast surface transport. It is demonstrated that the boundaries break down the symmetry of random walks in their vicinity, leading to the boundary singularities in the corresponding kinetic coefficients. Eliminating these singularities we get the desired boundary conditions. As it must be the boundary condition for the forward Fokker-Planck equation matches the mass conservation.

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I. THE CHAPMAN-KOLMOGOROV AND FOKKER-PLANCK EQUATIONS. EFFECT OF THE MEDIUM BOUNDARIES

As is well-known [1, 2] Markovian stochastic processes are completely determined by their transition probabilities which obey the Chapman-Kolmogorov equation. The Kramers-Moyal expansion can be used to determine the Fokker-Planck equation by specifying drift vector and diffusion tensor based on the assumption of vanishing higher order Kramers-Moyal coefficients.

Usually, the Fokker-Planck equations are derived implicitly assuming that the phase space of the stochastic variables under consideration extends to infinity so that so-called natural boundary conditions apply. If stochastic processes in a finite region of phase space are considered, boundary conditions are introduced a posteriori based on apparent physical arguments leading to the notion of a reflecting barrier, characterized by a vanishing normal component of the probability current, an absorbing barrier, where the probability distribution has to vanish, and boundary conditions at a discontinuity, where probability distributions and the normal components of the probability current have to be continuous. No attempts, so far, have been made to derive the Fokker-Planck equation simultaneously with appropriate boundary conditions from the Chapman-Kolmogorov equation.

It is quite evident that boundaries can strongly influence the stochastic motion of a particle in various ways depending on the microscopic interactions. As an example we mention a boundary formed by a fast diffusion layer. In such a thin layer particles are able to diffuse in the directions tangential to the boundary on a fast time scale, whereas in the bulk the particles behavior should accurately be described by the Fokker-Planck equation. The theoretical treatment of the particle diffusion requires a formulation of consistent boundary conditions which match the internal Fokker-Planck behavior to the stochastic properties of the boundary layer.

So it could be desirable to have a technique of deriving the boundary conditions applying directly to the manner of the region boundaries affecting stochastic processes. In this respect we note paper [3] devoted to the general description of random processes near boundaries causing deterministic jumps, paper [4] deriving boundary conditions for the Fokker-Planck equation describing coupled transport of photons and electrons, a serious of papers [5, 6, 7] dealing with boundary conditions for the advection-diffusion problem combining the Boltzmann and Fokker-Planck equations and their numerical implementation, and also work [8] developing diffusion models for molecular transport across membranes via ion channels and wider pores in terms of random walks affected by boundaries with complex properties. In addition paper [9] actually constructs the absorbing boundary as a limit transition of an infinite space with half-spaces different in properties substantially and work [10] implements boundary conditions for Wiener processes in path integrals. Papers [11, 12] develop a rather sophisticated moment technique for tackling the Fokker-Planck equation with mixed boundary conditions based on a special moment truncation scheme.

In the present paper we shall extend the method of deriving the Fokker-Planck equation from the Chapman-Kolmogorov equation in such a way that simultaneously consistent boundary conditions can be formulated. Our approach is based on introducing physical models for the stochastic behavior close to the boundary. We explicitly demonstrate that boundaries break the symmetry of
the random forces leading to boundary singularities in the Kramers-Moyal expansion. The cancelation of these singularities yields the appropriate boundary conditions. We explicitly derive the boundary conditions for a reflecting or absorbing barrier as well as boundaries with mixed properties, and describe the general procedure for the derivation of the boundary conditions for the case of the fast diffusion layer. It should be noted that a similar anomalous effect of the region boundaries on random processes was analyzed in papers [13, 14, 15] in numerical implementation of Wiener processes in their vicinity. Besides, paper [16] applies also to the concept of the symmetry breakdown caused, however, by external fields in constructing a generalized master equation for the classic and anomalous diffusion processes.

In principle the present approach can be extended to anomalous transport phenomena, e.g., sub- and superdiffusion, which are modeled by fractional diffusion operators. It is well-known that the formulation of boundary conditions for these processes is still a challenging problem although several approaches have been developed [17, 18, 19, 20]. The procedure outlined in the present paper might be helpful in formulating appropriate boundary conditions for these more involved processes.

The paper is organized as follows. Section II presents the problem under consideration and sketches out deriving two types of the Fokker-Planck equations based on the general Chapman-Kolmogorov equation for Markovian processes. Finally it formulates the problem of the boundary conditions and derives the general expressions that should be fulfilled at the boundaries of medium. Section III discusses the types of medium boundaries and their properties to be taken into account. Section IV introduces the equivalent lattice description of the continuous Markovian process that enables us to calculate anomalous kinetic coefficients in the vicinity of the boundary. Section V is actually the main part of the paper, it calculates the boundary singularities. The results are used in Sec. VI to obtained the desired boundary conditions for the forward and backward Fokker-Planck equations.

II. THE CHAPMAN-KOLMOGOROV AND FOKKER-PLANCK EQUATIONS

We consider stochastic dynamics of a Markovian system represented as a point \( r \) belonging to a certain domain \( Q \) in the Euclidean \( M \)-dimensional space \( \mathbb{R}^M \). The domain \( Q \) is assumed to be bounded by a smooth hypersurface \( \Upsilon \). When the detailed information about possible trajectories \( \{ r(t) \} \) of the system motion is of minor importance the conditional probability called also the Green function

\[
G(r, t | r_0, t_0) := \mathcal{P} \{ r_0, t_0 \Rightarrow r, t \}
\]

gives us the complete description of system evolution. By definition, the Green function is the probability density of finding the system at the point \( r \) at time \( t \) provided it was located at the point \( r_0 \) at the initial time \( t_0 \).

Since Markovian systems have no memory the Green function \( G(r, t | r_0, t_0) \) obeys the integral Chapman-Kolmogorov equation that represents transition of the system from the initial point \( r_0 \) to the terminal one \( r \) within the time interval \( (t_0, t) \) as a complex step via an intermediate point \( r_s \in Q \) at a certain fixed moment of time \( t_s \) with succeeding summation over all the possible positions of the intermediate point (see, e.g., Ref. [1])

\[
G(r, t | r_0, t_0) = \iiint_Q dr_s \ G(r, t | r_s, t_s) \ G(r_s, t_s | r_0, t_0). \tag{1}
\]

The time \( t_s \) may be chosen arbitrary between the initial and terminal time moments, \( t_s \in [t_0, t] \). Figure I visualizes this equation.

Since the domain boundary \( \Upsilon \) is considered to be a physical object special properties will be ascribed to it and itself can affect the system, for example, trapping it. So the symbol of triple integral is used in equation (1) to underline this feature and where appropriate it should be read as

\[
\iiint_Q dr \ldots = \iint_{Q^+} dr \ldots + \oint_{\Upsilon^+} ds \ldots + \oint_{\Upsilon_{tr}} ds \ldots
\]

where the symbol \( Q^+ \) denotes the internal points of the domain \( Q \), the boundary \( \Upsilon \) is split from the medium bulk because it can differ essentially from the medium bulk in properties, and the boundary traps \( \Upsilon_{tr} \) are singled out and treated individually by the same reasons. To simplify notations a similar rule

\[
\iint_Q dr \ldots = \iiint_{Q^+} dr \ldots + \oint_{\Upsilon} ds \ldots
\]

is also adopted. Such a split of integrals is for treating motion of the system inside the internal points \( Q^+ \), its possible anomalous transport along the boundary \( \Upsilon \), and the trap effect individually. Besides, according to the probability definition, the equality

\[
\iiint_Q dr \ G(r, t | r_0, t_0) = 1 \tag{2}
\]
holds when the integration runs over all the possible states of the system including the boundary traps \( \Upsilon_{br} \).

In what follows a rather general model for the medium boundary will be studied. Here we paid attention only to the fact that the boundary traps have to be treated individually because the system after been trapped cannot leave the boundary reaming in a trap forever. As a result if the point \( r_0 \) belongs to a trap, then for any internal point \( r \) of the domain \( \mathcal{Q} \) the Green function is equal to zero:

\[
G(r, t| r_0, t_0) = 0 \quad \text{for} \quad r_0 \in \Upsilon_{br}, \ r \in \mathbb{Q}^+.
\]

Further on the Green function \( G(r, t| r_0, t_0) \) for the internal initial and terminal points \( r_0, r \in \mathbb{Q}^+ \) will be considered. Therefore the general Chapman-Kolmogorov equation \(^{14}\) can be reduced by eliminating the integration over the traps, so becoming

\[
G(r, t| r_0, t_0) = \int_{\mathcal{Q}} \int dr_G(r, t| r_0, t_0) G(r_0, t_0| r_0, t_0). \quad (3)
\]

In equation \(^3\) this elimination is pointed out by the absence of one integral matching the traps, cf. the general formulation \(^11\) of the Chapman-Kolmogorov equation. Within the given integration rule the equality matching identity \(^2\) is violated, instead, we have

\[
\int_{\mathcal{Q}} \int dr G(r, t| r_0, t_0) = 1 - \int_{\Upsilon_{br}} ds_G(s_{tr}, t| r_0, t_0) < 1, \quad (4)
\]

where the symbol \( s_{tr} \) stands for the boundary trap located at the point \( s \in \Upsilon \).

In order to obtain the Fokker-Planck equations two additional assumptions must be adopted. The former is the short time confinement meaning that on small time scales the system cannot jump over long distances or in terms of the Green function its first and second moments converge and

\[
\lim_{{t \to t_0 + 0}} \int_{\mathcal{Q}} \int dr G(r, t| r_0, t_0)|r - r_0|^p = 0, \quad p = 1, 2. \quad (5)
\]

The latter is the medium local homogeneity. In other words, the medium where the Markovian process develops, i.e. the domain \( \mathcal{Q} \) should be endowed with characteristics being actually some smooth fields determined inside \( \mathbb{Q}^+ \) or at \( \Upsilon \) individually. As a result the Green function \( G(r, t| r_0, t_0) \) has to be smooth with respect to all its arguments for \( t > t_0 \) and \( r, r_0 \in \mathbb{Q}^+ \).

Because the intermediate time \( t_* \) entering the Chapman-Kolmogorov equation is any fixed value between the initial and terminal time moments, \( t_0 < t_* < t \), there is a freedom to choose it for special reasons. In particular, the passage to one of the limits \( t_* \to t_0 + 0 \) or \( t_* \to t - 0 \) gives rise to either the backward or forward Fokker-Planck equation, respectively (Fig. \(^11\)).

A. The backward Fokker-Planck equation

To implement the limit \( t_* \to t_0 + 0 \) let us choose an arbitrary small time scale \( \tau \) and consider the Chapman-Kolmogorov equation for \( t_* = t_0 + \tau \) and an internal point \( r_0 \). Then according to the adopted assumptions the first multiplier \( G(r, t| r_*, t_0) \) on the right-hand side of \(^3\) is a smooth function of both the argument \( r_* \) and \( t_* \) whereas the second one \( G(r_*, t_0| r_0, t_0) \) exhibits strong variations on small spatial scales. So we can expand the function

\[
G(r, t| r_0 + \mathbf{R}, t_0 + \tau)
\]

in the Taylor series with respect to the variables \( \tau \) and \( \mathbf{R} = r_* - r_0 \). The required accuracy is the first order in the time step \( \tau \) and the second order in \( \mathbf{R} \) because the characteristic spatial displacement of the system during time \( \tau \) is of order \( \tau^{1/2} \). Within this accuracy it is

\[
G(r, t| r_0 + \mathbf{R}, t_0 + \tau) = G(r, t| r_0, t_0) + \tau \frac{\partial G(r, t| r_0, t_0)}{\partial t_0} + \sum_{i=1}^M \mathcal{R}^i \nabla_i^0 G(r, t| r_0, t_0) + \frac{1}{2} \sum_{i,j=1}^M \mathcal{G}^{ij}(r_0, t_0, \tau) \nabla_i^0 \nabla_j^0 G(r, t| r_0, t_0), \quad (6)
\]

where the operator \( \nabla_i^0 = \partial / \partial x_i^0 \) acts only on the argument \( r_0 \) of the Green function. The substitution of expansion \(^4\) into the Chapman-Kolmogorov equation \(^3\) reduces it to the following

\[
-\tau \frac{\partial G(r, t| r_0, t_0)}{\partial t_0} = -\mathcal{R}(r_0, t_0, \tau) G(r, t| r_0, t_0)
\]

\[
+ \sum_{i=1}^M \mathcal{U}^i(r_0, t_0, \tau) \nabla_i^0 G(r, t| r_0, t_0)
\]

\[
+ \sum_{i,j=1}^M \mathcal{L}^{ij}(r_0, t_0, \tau) \nabla_i^0 \nabla_j^0 G(r, t| r_0, t_0),
\quad (7)
\]

where the quantities

\[
\mathcal{R}(r_0, t_0, \tau) = 1 - \int_{\mathcal{Q}} dR G(r_0 + \mathbf{R}, t_0 + \tau| r_0, t_0), \quad (8)
\]

\[
\mathcal{U}^i(r_0, t_0, \tau) = \int_{\mathcal{Q}} dR R^i G(r_0 + \mathbf{R}, t_0 + \tau| r_0, t_0), \quad (9)
\]

\[
\mathcal{L}^{ij}(r_0, t_0, \tau) = \frac{1}{2} \int_{\mathcal{Q}} dR R^i R^j G(r_0 + \mathbf{R}, t_0 + \tau| r_0, t_0)
\quad (10)
\]

have been introduced. Besides, the first term on the right-hand side of \(^3\) has been assumed to be small and tend to zero as \( \tau \to 0 \) which is justified based on the results to be obtained.
For an internal point \( \mathbf{r}_0 \) and, thus, separated from the boundary \( \Sigma \) by finite distance the time step \( \tau \) can be chosen so small that it is possible to construct a neighborhood of the point \( \mathbf{r}_0 \) with the following properties. First, deviation of the Green function \( G(\mathbf{r}_0 + \mathbf{R}, t_0 + \tau | \mathbf{r}_0, t_0) \) from zero outside this neighborhood is ignorable due to the first assumption about the short time confinement. Second, inside it the medium can be regarded as the homogeneous space \( \mathbb{R}^M \) by virtue of the second assumption on the local homogeneity. In this case actually replicating the proof of the Law of Large Numbers using the generation function notion (see, e.g., Ref. [1]) it is possible to demonstrate that quantities (9) and (10) scale linearly with \( \tau \). The difference of quantity (8) from zero is ignorable. Therefore for internal points we can introduce the drift velocity \( \mathbf{v}^i(\mathbf{r}, t) \) and the diffusion tensor \( D^{ij}(\mathbf{r}, t) \) by the expressions

\[
v^i(\mathbf{r}, t) = \lim_{\tau \to +0} \frac{1}{\tau} \int_{Q^+} d\mathbf{R} R^i G(\mathbf{r} + \mathbf{R}, t + \tau | \mathbf{r}, t), \tag{11}\]

\[
D^{ij}(\mathbf{r}, t) = \lim_{\tau \to +0} \frac{1}{2\tau} \int_{Q^+} d\mathbf{R} R^i R^j G(\mathbf{r} + \mathbf{R}, t + \tau | \mathbf{r}, t). \tag{12}\]

Then for the internal points the division of equation (7) by \( \tau \) and the succeeding passage to the limit \( \tau \to +0 \) yield the backward Fokker-Planck equation

\[
-\frac{\partial G(\mathbf{r}, t|\mathbf{r}_0, t_0)}{\partial t_0} = \mathcal{L}_{FPB} \left\{ G(\mathbf{r}, t|\mathbf{r}_0, t_0) \right\}, \tag{13}\]

where the backward Fokker-Planck operator is

\[
\mathcal{L}_{FPB} := \sum_{i,j=1}^M D^{ij}(\mathbf{r}_0, t_0, \tau) \nabla_i v^0_j + \sum_{i=1}^M v^i(\mathbf{r}_0, t_0, \tau) \nabla_i v^0. \tag{14}\]

We note that the backward Fokker-Planck equation acts on the second spatial argument of the Green function \( G(\mathbf{r}, t|\mathbf{r}_0, t_0) \).

This Fokker-Planck equation should be supplemented with the initial condition and the boundary condition. By construction, at the initial time \( t_0 \) the system was located at the internal point \( \mathbf{r}_0 \), so the initial condition just writes the Green function in the form of the Dirac \( \delta \)-function

\[
G(\mathbf{r}, t|\mathbf{r}_0, t_0)|_{t=t_0} = \delta(\mathbf{r} - \mathbf{r}_0). \tag{15}\]

The boundary condition interrelates the values of the Green function and its derivatives at the internal points adjacent to the domain boundary \( \Sigma \), i.e. values obtained by continuation \( \mathbf{r}_0 \to \mathbf{s} \) from some internal point \( \mathbf{r}_0 \in Q^M \) to a boundary point \( \mathbf{s} \in \Sigma \).

**B. The boundary condition problem for the backward Fokker-Planck equation and the vector of boundary singularity**

The direct implementation of the passage to the boundary points, however, raises a certain problem. Expansion (7) exhibits irregular behavior within the joint passage to limits \( \tau \to +0 \) and \( \mathbf{r}_0 \to \mathbf{s} \). When the former \( \tau \to +0 \) precedes the latter \( \mathbf{r}_0 \to \mathbf{s} \) no boundary conditions are got at all.

In the opposite order, i.e. when the passage \( \mathbf{r}_0 \to \mathbf{s} \) is performed first, the kinetic coefficients (8)–(10) change the scaling type; now they vary with time \( \tau \) as \( \sqrt{\tau} \) at the leading order. The matter is that a path of Markovian system is not smooth at every point and its characteristic variations on small time scales about \( \tau \) are proportional to \( \sqrt{\tau} \). For the internal points of the domain \( Q \) the path deviations in opposite directions are equiprobable within accuracy \( \sqrt{\tau} \). As a result the coefficient \( \mathcal{U}^i(\mathbf{r}, t, \tau) \) becomes a linear function of the argument \( \tau \). In some sense the given anomaly in the Markovian dynamics is hidden at the internal points and reflected only in the linear \( \tau \)-dependence of the second order moments \( \mathcal{L}^{ij}(\mathbf{r}_0, t_0, \tau) \) of the Green function \( G(\mathbf{r}, t|\mathbf{r}_0, t_0) \). The medium boundary \( \Sigma \) breaks down this symmetry because, in particular, it prevents the system from getting the points on the opposite side. Since the system displacement remains the same magnitude the terms \( \mathcal{U}^i(\mathbf{r}, t, \tau) \) acquire the root square dependence on the argument \( \tau \). In a certain sense the medium boundary reveals this anomaly (Fig. 2). The succeeding division of expansion (7) by \( \tau \) gives rise to singularities of the type \( \tau^{-1/2} \) which will be referred to as boundary singularities.

The medium boundary can affect the system dynamics in a more complex way, here, however, we currently confine our speculations only to the effect of its impermeability. Since the boundary \( \Sigma \) confines the system motion only in the normal direction it is quite natural to expect that the boundary singularities quantified in terms of di-
verging components $\Omega^i(s, t, \tau)/\tau$ will form a vector object $b$ that is determined by mutual effect of two factors. The former is the spatial orientation of the medium boundary $\mathcal{Y}$ described by its unit normal $n$. The latter is the spatial arrangement and intensity of random Langevin forces governing stochastic motion of the given system. They are characterized by the diffusion tensor $D^{ij}(r, t)$. Within a scalar cofactor we have only one possibility to construct the vector $b = \{b^i\}$ using the two objects,

$$b^i = \sum_{j=1}^{M} D^{ij} n^j \quad (16)$$

or, in the vector form

$$b = D \cdot n \quad (17)$$

The validity of this construction will be justified in the present paper and $b$ will be referred to as the vector of boundary singularities. To be rigorous it should be noted that in the general case the correct expression for the vector of boundary singularities should use the operator $D^j_i$ obtained from the diffusion tensor $D^{ij}$ by lowering one of its indices, namely, $b^i = \sum_{j=1}^{M} D^j_i n^j$ (such details are discussed in Sec. IV A). However dealing with orthonormal bases as it is the case at the initial stage of the current consideration the tensors $D^{ij}$ and $D^j_i$ coincide with other in the component magnitudes. So in order not to overload the reader perception and the mathematical constructions expressions similar to (16) will be used where appropriate.

The notion of the boundary singularity vector enables us to write immediately the desired boundary condition when the medium boundary just confines the system motion. In this case the first and third terms on the right-hand side of expansion (7) are absent and the corresponding singularity caused by the sequence of transitions $r_0 \to s$ and then $\tau \to 0$ takes the form

$$\frac{1}{\sqrt{\tau}} \sum_{i=1}^{M} b^i(s) \nabla_i^0 G(r, t|r_0, t_0)_{|r_0 \to s} = \frac{1}{\sqrt{\tau}} \sum_{i,j=1}^{M} D^{ij}(s, t_0) n^j(s) \nabla_i^0 G(r, t|r_0, t_0)_{|r_0 \to s} .$$

Naturally, for the internal points $r$ and $r_0$ the Green function $G(r, t|r_0, t_0)$ cannot exhibit any singularity whence it follows that the cofactor of the singularity $\tau^{-1/2}$ must be equal to zero, i.e.

$$\sum_{i,j=1}^{M} D^{ij}(s, t_0) n^j(s) \nabla_i^0 G(r, t|r_0, t_0)_{|r_0 \to s} = 0 .$$

It is the very know expression for the boundary condition of the backward Fokker-Planck equation which is typically obtained in another way applying to physical meaning of the Green function (see, e.g., Ref. [1]).

The present paper is devoted to deriving the boundary conditions for the Fokker-Planck equation applying to the notion of the boundary singularities. A more general situation will be studied justifying also these qualitative speculations. Currently we can state that the boundary condition for the backward Fokker-Planck equation should stem from the requirement for the boundary singularity terms to vanish in expansion (17), i.e. when $r_0 \in \mathcal{Y}$

$$- \mathcal{R}(r_0, t_0, \tau) G(r, t|r_0, t_0) + \sum_{i=1}^{M} \mathcal{M}^i(r_0, t_0, \tau) \nabla_i^0 G(r, t|r_0, t_0) + \sum_{i,j=1}^{M} \mathcal{G}^{ij}(r_0, t_0, \tau) \nabla_i^0 \nabla_j^0 G(r, t|r_0, t_0) = 0 \quad (18)$$

where the symbol $\mathcal{R}$ labels the components of the corresponding kinetic coefficients scaling as $\tau^{1/2}$. It should be pointed out that in expression (18) the argument $r_0$ is an arbitrary point of a thing layer $\mathcal{T}_\tau$ adjacent to the boundary $\mathcal{Y}$, which is designated by the symbol $\xi$. When $\tau \to 0$ its thickness also tends to zero (as $\tau^{1/2}$), however, before passing to the limit $\tau \to 0$ the layer $\mathcal{T}_\tau$ remains volumetric.

Now let us discuss similar problems with respect to the forward Fokker-Planck equation matching the other possibility of passage to the limit case in the Chapman-Kolmogorov equation (3).

C. The forward Fokker-Planck equation

The Chapman-Kolmogorov equation (3) also allows for the limit where the intermediate point tends to the terminal one, i.e. $t_\kappa = t - \tau$ with $\tau \to +0$. In this case the former cofactor $G(r, t|r_\kappa, t)$ on the right-hand side of (3) exhibits strong variations on small spatial scales whereas the latter one $G(r_\kappa, t - \tau|r_0, t_0)$ becomes a smooth function of the argument $r_\kappa$. Now, however, applying directly to an expansion similar to that have been used in deriving the backward Fokker-Planck equation is not appropriate. The matter is that in this way the integration runs over the initial point $r_\kappa$ of the Green function $G(r, t|r_\kappa, t - \tau)$ and appearing coefficients similar to quantities (5)–(10) lose their meaning. In particular, an integral similar to (11) can deviate from unit essentially.

To overcome this problem the Pontryagin technique is applied [21]. It is rather similar to the Kramers-Moyal approach (see, e.g., [2]) but is more suitable for tackling the boundary singularity. Let us consider at the first step some arbitrary smooth function $\phi(r)$ determined in the domain $Q$ and integrate with it both the sides of the
Chapman-Kolmogorov equation \textsuperscript{3}. In this way we get

\[
\iint_{\mathcal{Q}} dr \phi(r) G(r, t_s + \tau| r_0, t_0) = \int \int \int d\mathbf{r} d\mathbf{r}_s \phi(\mathbf{r}) G(\mathbf{r}, t_s + \tau| \mathbf{r}_s, t_s) G(\mathbf{r}_s, t_s| r_0, t_0).
\]

(19)

For a rather small time scale \(\tau\) the Green function

\[ G(\mathbf{r}, t_s + \tau| \mathbf{r}_s, t_s) \]

is practically located within some small neighborhood of the point \(\mathbf{r}_s\). Thereby the function \(\phi(\mathbf{r})\) can be expanded in the Taylor series near the point \(\mathbf{r}_s\) with respect to the variable \(\mathbf{R} = \mathbf{r} - \mathbf{r}_s\).

\[ \phi(\mathbf{r}) = \phi(\mathbf{r}_s) + \sum_{i=1}^{M} R^i \nabla_i^* \phi(\mathbf{r}_s) + \frac{1}{2} \sum_{i,j=1}^{M} R^i R^j \nabla_i^* \nabla_j^* \phi(\mathbf{r}_s). \]

Beside, since the Green function \(G(\mathbf{r}, t_s + \tau| r_0, t_0)\) depends smoothly on \(\tau\) the expansion

\[ G(\mathbf{r}, t_s + \tau| r_0, t_0) = G(\mathbf{r}, t_s| r_0, t_0) + \tau \frac{\partial G(\mathbf{r}, t_s| r_0, t_0)}{\partial t_s} \]

is also justified for a small value of \(\tau\). Then the substitution of the last two expressions into equation (19) with succeeding integration over \(\mathbf{R}\) and the replacement of the dummy variable \(\mathbf{r}_s\) by \(\mathbf{r}\) as well as \(t_s\) by \(t\) yields

\[
\int \int \int_{\mathcal{Q}} d\mathbf{r} \phi(\mathbf{r}) \left[ \frac{\partial G(\mathbf{r}, t| r_0, t_0)}{\partial t} \right] \\
= \int \int \int_{\mathcal{Q}} d\mathbf{r} \left\{ \phi(\mathbf{r}) \left[ -\mathfrak{A}(\mathbf{r}, t, \tau) G(\mathbf{r}, t| r_0, t_0) \right] + \sum_{i=1}^{M} \nabla_i \phi(\mathbf{r}) \left[ \mathfrak{A}^i(\mathbf{r}, t, \tau) G(\mathbf{r}, t| r_0, t_0) \right] \right. \\
+ \left. \sum_{i,j=1}^{M} \nabla_i \nabla_j \phi(\mathbf{r}) \left[ \mathfrak{A}^{ij}(\mathbf{r}, t, \tau) G(\mathbf{r}, t| r_0, t_0) \right] \right\}.
\]

(20)

Here the coefficients \(\mathfrak{A}(\mathbf{r}, t, \tau), \mathfrak{A}^i(\mathbf{r}, t, \tau)\) and \(\mathfrak{A}^{ij}(\mathbf{r}, t, \tau)\) again exhibit anomalous behavior within a narrow layer \(\Upsilon\) adjacent to the medium boundary \(\Upsilon\) (Fig. 3). As should be expected and in accordance with results to be obtained the thickness of this layer scales with time \(\tau\) as \(\tau^{1/2}\). These coefficients themselves also scale as \(\tau^{1/2}\). As a result the corresponding part of integral (20) scales as \(\tau\). Thereby after dividing both of the sides of (20) by \(\tau\) with the following passage to the limit \(\tau \to 0\) the contribution to (20) caused by integration over this layer remains finite. Therefore to analyze the properties of the integral relation (20) the domain \(\mathcal{Q}\) is split into this layer of boundary singularities and the internal part. After the passage to the limit \(\tau \to 0\) this division matches treating individually the boundary \(\Upsilon\) and the internal points with regular behavior of the kinetic coefficients.

\[
\int \int \int_{\mathcal{Q}} d\mathbf{r} \ldots = \oint_{\mathcal{Y}} ds \ldots + \int \int \int_{\mathcal{Q}^+} d\mathbf{r} \ldots
\]

(21)

Let us consider the second term first. Inside the region \(\mathcal{Q}^+\) the kinetic coefficients \(\mathfrak{A}^i(\mathbf{r}, t, \tau)\) and \(\mathfrak{A}^{ij}(\mathbf{r}, t, \tau)\) behave in regular way, i.e. they scale as \(\tau\) according formulae (11) and (12), whereas the term \(\mathfrak{A}(\mathbf{r}, t, \tau)\) vanishes at all. So dividing the corresponding part of the integral relation (20) by \(\tau\) and passing to the limit \(\tau \to 0\) we have

\[
\int \int \int_{\mathcal{Q}^+} d\mathbf{r} \phi(\mathbf{r}) \left[ \frac{\partial G(\mathbf{r}, t| r_0, t_0)}{\partial t} \right] \\
= \int \int \int_{\mathcal{Q}^+} d\mathbf{r} \left\{ \sum_{i=1}^{M} \nabla_i \phi(\mathbf{r}) \left[ v^i(\mathbf{r}, t, \tau) G(\mathbf{r}, t| r_0, t_0) \right] \\
+ \sum_{i,j=1}^{M} \nabla_i \nabla_j \phi(\mathbf{r}) \left[ D^{ij}(\mathbf{r}, t, \tau) G(\mathbf{r}, t| r_0, t_0) \right] \right\}.
\]

(22)

Using the Gauss divergence theorem this integral in turn is split into two parts, surface and volume ones:

\[
\int \int \int_{\mathcal{Q}^+} d\mathbf{r} \ldots = \oint_{\mathcal{Y}} ds \ldots + \int \int \int_{\mathcal{Q}^+} d\mathbf{r} \ldots
\]

(23)
The volume integral has the form
\[ \int_{\mathbb{Q}^+} d\mathbf{r} \phi(r) \left[ \frac{\partial G(r, t|\mathbf{r}_0, t_0)}{\partial t} \right] \]
\[ = \int_{\mathbb{Q}^+} d\mathbf{r} \phi(r) \left\{ - \sum_{i=1}^{M} \nabla_i \left[ v^i(r, t, \tau) G(r, t|\mathbf{r}_0, t_0) \right] ight. \]
\[ + \sum_{i,j=1}^{M} \nabla_i \nabla_j \left[ D^{ij}(r, t, \tau) G(r, t|\mathbf{r}_0, t_0) \right] \} \}
\[ = \mathcal{L}_{FP} \{ G(r, t|\mathbf{r}_0, t_0) \} \]  \hspace{1cm} (24)

The latter equality immediately gives rise to the forward Fokker-Planck equation.

Indeed, currently \( \phi(r) \) is an arbitrary smooth function and no addition constraints will be imposed further on it for the internal points of the domain \( \mathbb{Q} \). So applying to local variations of \( \phi(r) \) at an arbitrary internal point \( r \) (Fig. 3) we see that the left and right sides of (24) should be equal to each other for the points \( r \in \mathbb{Q}^+ \) individually, getting the forward Fokker-Planck equation
\[ \frac{\partial G(r, t|\mathbf{r}_0, t_0)}{\partial t} = \mathcal{L}_{FP} \{ G(r, t|\mathbf{r}_0, t_0) \} \]  \hspace{1cm} (25)

with the forward Fokker-Planck operator
\[ \mathcal{L}_{FP} \{ \} := \sum_{i=1}^{M} \nabla_i \]
\[ \times \left[ \sum_{j=1}^{M} \nabla_j \left( D^{ij}(r, t, \tau) \right) \right] - v^i(r, t, \tau) \} \]  \hspace{1cm} (26)

Here the symbol \( \Diamond \) stands for a function acted by this operator. It should be also pointed out that the Fokker-Planck operator acts on the first spatial argument of the Green function.

The forward Fokker-Planck equation can be also written in the conservation form
\[ \frac{\partial G(r, t|\mathbf{r}_0, t_0)}{\partial t} + \sum_{i,j=1}^{M} \nabla_i \mathbf{J}^i \{ G(r, t|\mathbf{r}_0, t_0) \} = 0 , \]  \hspace{1cm} (27)

with the probability flux operator \( \mathbf{J} = \{ \mathbf{J}^i \}_{i=1}^{M} \)
\[ \mathbf{J}^i \{ \} := - \sum_{j=1}^{M} \nabla_j \left( D^{ij}(r, t, \tau) \right) \Diamond + v^i(r, t, \tau) \} \Diamond \]  \hspace{1cm} (28)

The forward Fokker-Planck is naturally supplemented with the same initial condition (15).

### D. Boundary relations for the forward Fokker-Planck equation

Splits (21) and (23) give rise to two additional terms. The former one is related to the first split and is the integral over the layer \( \mathcal{T}_r \) of boundary singularities
\[ \oint_{\mathcal{T}_r} d\mathbf{r} G(s, t|\mathbf{r}_0, t_0) \sum_{i,j=1}^{M} \nabla_i \phi(s) * \mathbf{U}^i(r, t, \tau) \left[ D^{ij}(s, t, \tau) G(s, t|\mathbf{r}_0, t_0) \right] \]
\[ - \phi(s) * \mathbf{R}(r, t, \tau) + \sum_{i,j=1}^{M} \nabla_i \nabla_j \phi(s) * \mathbf{D}^{ij}(r, t, \tau) \} \} \right\} \]  \hspace{1cm} (29)

Here the symbol \( d\mathbf{r} \) as well as presence of the argument \( r \) in the singular components of the kinetic coefficients takes into account the fact that before the passage to the limit \( \tau \to 0 \) the layer \( \mathcal{T}_r \) is volumetric. The Green function \( G(r, t|\mathbf{r}_0, t_0) \) as well as the test function \( \phi(r) \) and its derivatives exhibits minor variations across the layer \( \mathcal{T}_r \) so their argument \( r \) have been replaced by the corresponding nearest point \( s \) laying on the boundary \( \mathcal{T} \).

The latter term is due to the part of expression (22) remaining after integration using the convergence theorem and can be written in the form
\[ \oint_{\mathcal{T}_r} ds \sum_{i,j=1}^{M} \nabla_j \phi(s) n^i(s) \left[ D^{ij}(s, t, \tau) G(s, t|\mathbf{r}_0, t_0) \right] \]
\[ = - \oint_{\mathcal{T}_r} ds \phi(s) \sum_{i=1}^{M} n^i(s) J^i \{ G(s, t|\mathbf{r}_0, t_0) \} \]  \hspace{1cm} (30)

where \( n(s) = \{ n^i(s) \} \) is the unit normal to the boundary \( \mathcal{T} \) at point \( s \) directed inwards the domain \( \mathbb{Q} \).

Leaping ahead we note that the appropriate choice of the boundary values of the test function \( \phi(s) \) and its derivatives fulfils equality (29) and, at the next step, gives rise to the required boundary condition for the forward Fokker-Planck equation. Let us demonstrate this for the impermeable boundary using the notion of the boundary singularity vector \( \mathbf{b} \). Namely, we again assume that for an internal point \( r \) located in the vicinity of a boundary point \( s \), i.e. \( \mathbf{r} \in s \)
\[ \mathbf{U}^i(r, t, \tau) \propto \mathbf{b}^i(s) = \sum_{j=1}^{M} D^{ij}(s, t) n^j(s) \]  \hspace{1cm} (31)

In this case only the first term in equality (29) remains and it is fulfilled when
\[ \sum_{i,j=1}^{M} D^{ij}(s, t) n^i(s) \nabla_j \phi(s) = 0 . \]  \hspace{1cm} (32)

Equality (31) just relates the boundary values of the test function \( \phi(s) \) with its derivative along the boundary normal \( n(s) \). So for an arbitrary smooth function \( \phi_T(s) \) determined at the boundary \( \mathcal{T} \) it is possible to construct the appropriate function \( \phi(r) \) determined in the domain \( \mathbb{Q} \) and meeting equality (31) (see Fig. 3). So in the given case the left-hand side and, thus, the right-hand side of expression (31) becomes zero. Since the integral on the
right-hand side of (30) contains an arbitrary function \( \phi(s) \) determined at the boundary \( \Upsilon \) the equality

\[
\sum_{i=1}^{M} n^i(s) J^i \{ G(s, t| r_0, t_0) \} = 0 \tag{32}
\]

holds for every point of the boundary \( \Upsilon \) individually. This expression meaning the zero value of the probability flux in the direction normal to the boundary \( \Upsilon \) matches well the physical seance of its impermeability.

However, to derive the boundary conditions for the Fokker-Planck equations more sophisticated constructions are necessary. Besides, in order to take into account other possible properties of the medium boundary its model should be specified.

### III. BOUNDARY TYPES

In the present paper, to be specific, we consider three typical examples of medium boundaries. They are (i) the impermeable boundary, (ii) the boundary absorbing particles, and (iii) the boundary with a thin adjacent layer characterized by extremely high values of the kinetic coefficients, the fast diffusion boundary (Fig. 4).

The first type matches a medium whose boundary is similar to its bulk in properties, the boundary points differ from internal ones only by the absence of medium points on one side. As a result a random walker hopping over the medium points just cannot pass through the boundary returning to the medium bulk after getting it.

The second type is similar to the first one except for the fact that the walker can be trapped at the boundary and will not return to the medium anymore. In this case the corresponding boundary conditions are typically used in describing the first passage time problem or diffusion in solids with fixed boundary values of impurity concentration \( C_s \) (see, e.g., Ref. [1]). Generally the boundary absorption is described by the rate \( \sigma C_s \), where \( \sigma \) is a certain kinetic coefficient.

The third type boundaries are widely met, for example, in polycrystals or nanoparticle agglomerates. The grain boundaries contain a huge amount of defects and as a result the diffusion coefficient inside the grain boundaries can exceed its value in the crystal bulk by many orders. Therefore impurity propagation in polycrystals is governed mainly by grain boundary diffusion (for a review see, e.g., Ref. [22] and references therein). In terms of random walks the effect of the fast diffusion layer is reduced to extremely long spatial jumps made by an walker inside it. It is natural to characterize such a boundary layers by its thickness \( \lambda \) about the atomic spacing and the ratio of the diffusion coefficients inside the boundary layer and in the regular crystal lattice \( \varrho \gg 1 \).

### IV. EQUIVALENT LATTICE REPRESENTATION OF RANDOM WALKS NEAR THE MEDIUM BOUNDARY

The derivation of the Fokker-Planck equations, the forward and backward ones, requires calculation of three quantities \( R(r, t, \tau) \), \( U(r, t, \tau) \), and \( Z^{ij}(r, t, \tau) \) specified by expressions (5)–(10). They are the moments of the system displacement \( R \) during the time \( \tau \) treated as an arbitrary small value. In order to obtain the desired boundary conditions these quantities should be found in the vicinity of the medium boundary \( \Upsilon \) or, more precisely, in its neighborhood \( \Upsilon_r \) of thickness about \( (D\tau)^{1/2} \), where \( D \) is the characteristic value of the diffusion tensor components. To study the boundary effects it suffices to consider a rather small region wherein the medium and its boundary are practically homogeneous in properties and, in addition, the boundary geometry is approximated well by some hyperplane. In this region the system motion will be imitated by random walks on a lattice constructed as follows.

First, the elementary steps of the random walks on it are characterized by a time \( \tau_a \) such that

\[
\tau_a \ll \tau \tag{33}
\]

and the arrangement of the lattice nodes, i.e., their spacings \( \{a_i\} \) and the spatial orientation should give us again the same diffusion tensor \( D \) as well as the drift field \( \nu \) for the internal points on time scales \( \tau_a \ll t \ll \tau \). The individual hops of a random walker between the neighboring nodes actually represent a collection of mutually independent Langevin forces governing the random system motion in the given continuum. Second, the boundary \( \Upsilon \) is represented as a layer of nodes \( \Upsilon_0 \) between which the walker can migrate via elementary hops. In other words, the aforementioned collection of mutually independent Langevin forces has to contain components acting along the boundary \( \Upsilon \) and one component moving the walker towards or from \( \Upsilon \). Other characteristics of this effective lattice may be chosen for the sake of convenience. At final stage we should pass to the limit \( \tau_a \to 0 \) returning to the continuous description.
A. Diffusion tensor representations

In order to construct the required lattice let us consider Markovian random walks \( \{ \mathbf{r}(t) \} \) in \( M \)-dimensional Euclidean half-space \( \mathbb{R}^M_+ \) made of vectors

\[
\mathbf{r} = \{ x^1, x^2, \ldots, x^M \}
\]

such that

\[
\mathbf{r} \cdot \mathbf{n} := \sum_{i=1}^{M} x^i n^i \geq 0,
\]

where \( \mathbf{n} = \{ n^1, n^2, \ldots, n^M \} \) is a certain unit vector. The boundary of \( \mathbb{R}^M_+ \), i.e. the hyperplane \( \mathcal{Y} = \{ \mathbf{r} \cdot \mathbf{n} = 0 \} \) perpendicular to the vector \( \mathbf{n} \) is, in its turn, the Euclidean space \( \mathbb{R}^{M-1} \) of dimension \( M - 1 \). The half-space \( \mathbb{R}^M_+ \) and, correspondingly, the hyperplane \( \mathcal{Y} \) are assumed to be homogeneous. The latter means the local properties of the random walks under consideration to be independent of position in space; naturally the boundary and internal points are not equivalent. In particular, the diffusion tensor \( \mathbf{D} \) and drift vector \( \mathbf{v} \) are the same at all the internal points of the half-space \( \mathbb{R}^M_+ \).

In this case the components of the drift vector and diffusion tensor are determined by the expressions (cf. formulæ (35-36))

\[
v^i = \frac{1}{\tau} \langle \delta X^i(t, \tau) \rangle, \tag{34}
\]

\[
D^{ij} = \frac{1}{2\tau} \left\langle \left[ \delta X^i(t, \tau) - v^i \tau \right] \left[ \delta X^j(t, \tau) - v^j \tau \right] \right\rangle. \tag{35}
\]

Here the random variable \( \delta X^i(t, \tau) := x^i(t + \tau) - x^i(t) \) and \( \mathbf{r} = \{ x^i \} \) is an arbitrary internal point, the observation time interval \( \tau \) should be chosen to be small enough that the length scale \( \langle \mathbf{D}_\tau \rangle^{1/2} \) be much less then the distance between the point \( \mathbf{r} \) and the boundary \( \mathcal{Y} \), i.e. \( D_\tau \ll \| \mathbf{r} \| \mathbf{n} \|^2 \), and the triangular brackets \( \langle \ldots \rangle \) stands for averaging over all the random trajectories passing through the point \( \mathbf{r} \) at time \( t \). It should be noted that due to the space homogeneity the passage to the limit \( \tau \to 0 \) can be omitted which is necessary in the general case.

In what follows nonorthogonal bases will be used. So, keeping in mind the tensor notation (see, e.g. Ref. [23]), the upper and lower indices will be distinguished. In these terms \( \{ x^i \} \) or just \( x^i \) is a vector, whereas, the collection of the basis vectors \( \mathbf{e}_i \) is a covector. According to definitions (35) and (36) the objects \( D^{ij} \) and \( v^i \) are contravariant tensors. In addition, if the basis \( \mathbf{e} \) has the form \( \mathbf{e} = \mathbf{e}_\mathcal{Y} \oplus \mathbf{e} \), where \( \mathbf{e}_\mathcal{Y} \) is the basis of the hyperplane \( \mathcal{Y} \) and the vector \( \mathbf{e} \) does not lie in it, then the Greek letters will label the tensor indices corresponding to the hyperplane \( \mathcal{Y} \) to simplify perceiving this fact.

In order to deal with the diffusion tensor in a nonorthogonal basis \( \mathbf{e} = \{ \mathbf{e}_i \} \) the metric tensor is also necessary. It is defined as

\[
g_{ij} := (\mathbf{e}_i \cdot \mathbf{e}_j) \tag{36}
\]

and is the kernel of the scalar product of two vectors \( \mathbf{r} \) and \( \bar{\mathbf{r}} \), namely,

\[
(\mathbf{r} \cdot \bar{\mathbf{r}}) := \sum_{i,j=1}^{M} g_{ij} x^i \bar{x}^j. \tag{37}
\]

For an orthonormal basis the metric tensor \( g_{ij} = \delta_{ij} \), where \( \delta_{ij} \) is the Kronecker delta. The metric tensor \( g_{ij} \) defines the conversion of contravariant tensors into covariant ones, in particular,

\[
D^i_j = \sum_{k=1}^{M} D^{ik} g_{kj} \quad \text{and} \quad D^i_i = \sum_{k=1}^{M} g_{ik} D^{kj} \tag{38}
\]

Due to the diffusion tensor \( D^{ij} \) as well as the metric tensor \( g_{ij} \) being symmetric the tensor \( D_{ij} \) is also symmetric, whereas the tensors \( D^i_j \) and \( D^i_i \) are identical and are denoted further as \( D^i_j \). The tensor \( D^i_j \) can be regarded as a certain operator \( \hat{D} \) acting in the space \( \mathbb{R}^M \) and the tensor \( D_{ij} \) specifies a quadratic form

\[
\mathbf{r} \cdot \hat{D} \mathbf{r} = \sum_{i,j,k=1}^{M} g_{ij} x^i D^i_k x^k = \sum_{i,j=1}^{M} D_{ij} x^i x^j. \tag{39}
\]

The quadratic form (39) is positive definite. To demonstrate this a random variable

\[
\delta L = \sum_{p=1}^{M} \left[ \delta X^p(t, \tau) - v^p \tau \right] (\mathbf{e}_p \cdot \ell) \]

\[
= \sum_{p,i=1}^{M} \left[ \delta X^p(t, \tau) - v^p \tau \right] g_{pi} \ell^i
\]

is considered, where \( \ell = \sum_{i=1}^{M} \mathbf{e}_i \ell^i \) is an arbitrary vector in the space \( \mathbb{R}^M \) and the metric tensor definition (36) has been taken into account. Whence we have a chain of equalities

\[
0 < \langle |\delta L| \rangle^2 = \sum_{p,p',i,i'=1}^{M} g_{pi} g_{p'i'} \ell^i \ell^{i'}
\]

\[
\times \left\langle \left[ \delta X^p(t, \tau) - v^p \tau \right] \left[ \delta X^{p'}(t, \tau) - v^{p'} \tau \right] \right\rangle
\]

\[
= \sum_{p,p',i,i'=1}^{M} 2\tau D^{pp'} g_{pi} g_{p'i'} \ell^i \ell^{i'}
\]

\[
= \sum_{i,i'=1}^{M} 2\tau D_{ii'} \ell^i \ell^{i'} = \sum_{p,p',i,i'=1}^{M} 2\tau D^{ii'} l_i l_i'.
\]
So for any arbitrary vector \( \ell \) and covector \( l_i \) the inequalities
\[
\sum_{i,j=1}^{M} D_{ij} \ell^i l^j > 0, \quad \sum_{i=1}^{M} D^{ij} l_i \ell_j > 0 \tag{40}
\]
hold. The covector and vector representations of the same object are related as \( l_i = \sum_{j=1}^{M} g_{ij} \ell^j; \) within orthonormal bases they are identical.

Due to the symmetry of the tensor \( D_{ij} \) and the quadratic form \([39]\) being positive definite all the eigenvalues of the operator \( \hat{D} \) are real positive quantities and its eigenvectors form a basis in the space \( \mathbb{R}^M \) which can be chosen to be orthonormal one, see, e.g., Ref. [24]. In this basis the diffusion tensor takes the diagonal form. Thereby the corresponding eigenvectors and eigenvalues specify the directions and intensity of the mutually independent Langevin forces governing random walks in the medium under consideration. Unfortunately, in the general case where all the eigenvalues are nondegenerate this basis is unique. So it cannot be used in constructing the desired basis vector of the space \( \mathbb{R}^M \) parallel to the hyperplane \( \Upsilon \). In order to overcome this one can meet a situation when none of the basis vectors is parallel to the hyperplane \( \Upsilon \). In the case when none of the basis vectors is parallel to the hyperplane \( \Upsilon \), in order to overcome this problem we will construct a special nonorthogonal basis applying to the following statement.

**Proposition 1** Let \( \mathbb{R}^{M+} = \{ r \cdot \mathbf{n} > 0 \} \) be a homogeneous half-space bounded by the hyperplane \( \Upsilon = \{ r \cdot \mathbf{n} = 0 \} \) and \( \varepsilon = \{ \mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_M \} \) be a fixed arbitrary basis of \( \mathbb{R}^M \). In this basis the components of the diffusion tensor \( \{ D^{ij} \} \) as well as the metric tensor \( \{ g_{ij} \} \) are given. Then there is a basis \( \mathbf{b} = b_{\Upsilon} \oplus \mathbf{b}_M \) with the following properties.

First, it is composed of a certain orthonormal basis \( \mathbf{b}_\Upsilon \) of the hyperplane \( \Upsilon \) and a unit vector \( \mathbf{b}_M \) not belonging to \( \Upsilon \) that is determined by the expression
\[
\mathbf{b}_M = \frac{1}{\omega} \sum_{i=1}^{M} \mathbf{e}_i D_{ij} n^j. \tag{41}
\]

Here according to the construction of the half-space \( \mathbb{R}^{M+} \) \( \mathbf{n} = \{ n^1, n^2, \ldots, n^M \} \) is the unit vector normal to the hyperplane \( \Upsilon \) and the normalization factor
\[
\omega = \left[ \sum_{i,j,p,k=1}^{M} g_{ij} D_{p}^{i} D_{k}^{j} n^p n^k \right]^{1/2}. \tag{42}
\]

Second, in the basis \( \mathbf{b} \) the diffusion tensor takes the diagonal form
\[
[D] = \begin{bmatrix} D_1 & 0 & \cdots & 0 \\ 0 & D_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & D_M \end{bmatrix}, \tag{43}
\]

where all its diagonal components are positive quantities, \( \{ D_i > 0 \} \), with the value \( D_M \) being given by the expression
\[
D_M = \omega^2 \left[ \sum_{i,j=1}^{M} D_{ij} n^i n^j \right]^{-1}. \tag{44}
\]

Third, let, in addition, the initial basis be of the form \( \varepsilon = \varepsilon_\Upsilon \oplus \mathbf{n} \), where \( \varepsilon_\Upsilon = \{ \mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_M \} \) is a certain basis of the hyperplane \( \Upsilon \), and \( \hat{U}_\Upsilon = \| \nu^{\alpha}_\Upsilon \| \) be the transformation of the hyperplane \( \Upsilon \) mapping the basis \( \mathbf{b}_\Upsilon \) onto the basis \( \varepsilon_\Upsilon \), i.e., \( \mathbf{b}_\Upsilon \stackrel{\hat{U}_\Upsilon}{\to} \varepsilon_\Upsilon \). By mapping \( \mathbf{b}_M \to \mathbf{n} \) the transformation \( \hat{U}_\Upsilon \) is complemented to a certain transformation \( \hat{U} \) of the compleat space \( \mathbb{R}^M \), namely, if \( r \) is an arbitrary vector of the space \( \mathbb{R}^M \) with the coordinates specified by its expansion over the bases \( \varepsilon \) and \( \mathbf{b} \):
\[
r = \sum_{\gamma=1}^{M-1} \mathbf{e}_\gamma x^\gamma + \mathbf{n} x^M = \sum_{\gamma=1}^{M-1} \mathbf{b}_\gamma \zeta^\gamma + \mathbf{b}_M \zeta^M, \tag{45}
\]
then its coordinates are related by the expressions
\[
\zeta^\alpha = \sum_{\gamma=1}^{M-1} \alpha^{\alpha}_{\gamma} \left( x^\gamma - \frac{1}{D_M^{\alpha M}} \right), \tag{46a}
\]
\[
\zeta^M = \frac{\omega}{D_M^{MM}} x^M, \tag{46b}
\]
and for the inverse transformation
\[
x^\alpha = \sum_{\gamma=1}^{M-1} \bar{\alpha}^{\alpha}_{\gamma} \zeta^\gamma + \frac{1}{\omega} D_M^{\alpha M} \zeta^M, \tag{46c}
\]
\[
x^M = \frac{D_M^{MM}}{\omega} \zeta^M. \tag{46d}
\]
Here \( \hat{\bar{U}}^{-1}_\Upsilon = \| \bar{\nu}^{\alpha}_\Upsilon \| \) is the operator inverse to the operator \( \hat{U}_\Upsilon \), i.e. meeting the identity \( \sum_{\gamma=1}^{M-1} \bar{\alpha}^{\alpha}_{\gamma} \nu^\gamma = \delta_{\alpha}^\beta \). Besides, the equality
\[
\sum_{\gamma=1}^{M-1} \bar{\alpha}^{\alpha}_{\gamma} \bar{\nu}^{\beta}_{\gamma} D_\gamma = D^{\alpha \beta} - \frac{1}{D_M^{MM}} D_M^{\alpha M} D_M^{\beta M} \tag{47}
\]
holds.

Since the proof of this proposition requires just formal mathematical manipulations related weakly to the subject matter of the paper it is presented in the individual Appendix A.

**Comments on Proposition 1** First, it is worthwhile to note that the basis vector \( \mathbf{b}_M \) constructed by expression (41) is actually the vector \( \mathbf{b} \) of boundary singularities (expression (10)) normalized to unity.

Second, for the initial basis \( \varepsilon \) of the general form actually expression (47) persuades us to introduce the surface diffusion tensor
\[
\mathcal{D}^{ij} := D^{ij} - \sum_{p,k=1}^{M} D_{p}^{i} D_{k}^{j} n^p n^k \frac{D_M^{\alpha M} D_M^{\beta M}}{\sum_{p,k=1}^{M} D_{p}^{k} n^p n^k}. \tag{48}
\]
that describes the system random motion along the hyperplane \( \Upsilon \). Indeed, in a basis \( b_\gamma \oplus n \) the components of this tensor belonging to the hyperplane \( \Upsilon \) coincide with ones given by expression (17) and are equal to zero when one of its indices matches the vector \( n \).

Third, when the initial basis \( e \) is orthonormal the expressions of Proposition 1 can be simplified. Indeed, in this case the metric tensor \( g_{ij} := (e_i, e_j) = \delta_{ij} \) is the unit matrix and it is possible not to distinguish between the upper and lower tensor indices, in particular, all the components \( D_{ij} = D'_j = D'^{ij} \) are identical. If, in addition, the initial basis has the form \( e = \epsilon_\Upsilon \oplus n \) expressions (41)–(44) become

\[
 b_M = \frac{1}{\omega} \left[ \sum_{\gamma=1}^{M-1} e_\gamma D_\gamma M + n D_{MM} \right],
\]

where the coefficient

\[
 \omega = \sqrt{\sum_{\gamma=1}^{M-1} D^2_\gamma M + D^2_{MM}}
\]

and the value

\[
 D_M = \frac{1}{D_{MM}} \sum_{\gamma=1}^{M-1} D^2_\gamma M - D_{MM}.
\]

Besides, the inverse transformation matrix \( \| \tilde{u}_{\alpha \beta} \| \) coincides with the direct transformation matrix transposed, i.e. \( \tilde{u}_{\alpha \beta} = u_{\beta \alpha} \). □

Proposition 1 prompts us to use the basis \( b = \{ b_\gamma \} \) in describing random walks in the half-space \( \mathbb{R}^{M+} \). For its internal points the continuous random walks are represented as a collection of mutually independent one-dimensional Markovian processes \( \{ \xi^i(t) \} \)

\[
 r(t) = b_i \xi^i(t) = b_i \int_0^t dt' \xi^i(t'),
\]

where the Langevin random forces \( \{ \xi^i(t) \} \) meet the correlations

\[
 \langle \xi^i(t) \rangle = v^i,
\]

\[
 \langle \xi^i(t) \xi^{i'}(t') \rangle = 2 D_{i i'} \delta(t - t'),
\]

and \( \{ v^i \} \) are the components of the drift velocity \( v = b_i v^i \) in the basis \( b \). As could be shown directly these random forces lead to expressions (54) and (55).

### B. Equivalent lattice random walks

The desired lattice is constructed as follows (see also Fig. 5 for illustration). At the first step a set of nodes

![Fig. 5: The lattice random walks imitating continuous Markovian process in the half-space \( \mathbb{R}^{M+} \). Here \( \Upsilon \) is the boundary of \( \mathbb{R}^{M+} \), the axes \( x^1, x^2 \) are chosen to be directed along the vectors \( b_1, b_2 \) of the basis \( b_\gamma \), the axis \( x^3 \) is normal to the plane \( \Upsilon \), whereas the basic vector \( b_3 \) is not normal to it in the general case. The values \( a_1, a_2, a_3 \) are the lattice spacings and grey arrows show possible hops to the nearest neighbors.](image)

\( \{ a_\Upsilon \} \) is fixed on the boundary \( \Upsilon \) such that

\[
 a_\Upsilon (n_\Upsilon) = \sum_{\alpha=1}^{M-1} b_\alpha a_\alpha n_\alpha,
\]

where \( n_\Upsilon = \{ n_1, n_2, \ldots, n_{M-1} \} \) is a collection of integers taking values in \( \mathbb{Z} \) and the lattice spacings \( a_\alpha \) are chosen to be equal to

\[
 a_\alpha = \sqrt{2 \tau _\alpha M D_{\alpha}}.
\]

Here \( \tau _\alpha \) is any small time scale meeting inequality (33) and being the time step of lattice random walks; an walker hops to one of the nearest neighbors in time \( \tau _\alpha \). Such jumps are illustrated by grey arrows in Fig. 5. These nodes are regarded as the boundary layer \( \Upsilon_0 \) of the lattice to be constructed. Then the layer \( \Upsilon_0 \) as a whole is shifted inwards the region \( \mathbb{R}^{M+} \) by the vector \( a_M b_M \), where

\[
 a_M = \sqrt{2 \tau _\alpha M D_M}.
\]

Then this new layer \( \Upsilon_1 \) in turn is shifted by the same vector \( \mathbb{R}^{M+} \), giving rise to the next layer \( \Upsilon_2 \) of nodes and so on. In this way we construct the system of layers \( \{ \Upsilon_k \} \) making up the desired lattice and exactly random walks on this lattice will imitate the continuous process in the half-space \( \mathbb{R}^{M+} \).

Let us now specify the probability of hops from an internal node \( n \) to one of its nearest neighbors \( n' \) along
a basis vector $b_i$ by the expression

$$P_{mn'} = \frac{1}{2M} + \frac{\tau_n}{2a_i} v^i \chi_i.$$  \hspace{1cm} (57)

Here the random value $\chi_i = \pm 1$ takes into accounts the possibility of jumps along the vector $b_i$ or in the opposite direction. The sequence of such hops with time step $\tau_n$ represents equivalently the continuous process rather far from the boundary $\mathcal{Y}$. Indeed, due to the law of large numbers (see, e.g. [26]) two Markovian processes are identical if on a rather small time scale both of them lead to the same mean and mean-square values of the system displacement. By virtue of (57) one hop of the walker is characterized by the following mean values of its displacement $\delta r = b_i \delta \xi_i$

$$\sum_{n'} P_{mn'} \delta c_{nm'} = \tau_n v^i,$$  \hspace{1cm} (58)

$$\sum_{n'} P_{mn'} \delta c_{nm'} \delta c_{nm'} = 2 \tau_n D i_{ij},$$  \hspace{1cm} (59)

where the sums run over all the nearest neighbors $n'$ of the node $n$. According to (54) and (55) actually the same mean values of the system displacement during the time interval $\tau_n$ are given by the continuous random process. Rigorously speaking, the latter mean value and one corresponding to the continuous random process are not identical, but their difference

$$(b_i \cdot b_j) v^i v^j \tau_a^2$$

is of the second order in the time scale $\tau_a$ whereas the leading terms are of the first order. Thereby choosing the time scale $\tau_a$ to be sufficiently small we can make this difference ignorable.

C. Properties of the boundary layer $\mathcal{Y}_0$

In order to describe the boundary effects on random walks special properties should be ascribed to the nodes of the boundary layer $\mathcal{Y}_0$. It is worthwhile to noted that it is the place where the model of the medium boundary does appear for the first time.

Keeping in mind the boundary types discussed in Sec. [33] first, each boundary node is regarded as a unit of two elements, the lattice node itself and a trap. If a walker jumps to a trap it will never return to the lattice nodes. The introduction of traps mimics the absorption effect of medium boundaries. Second, possible fast diffusion inside a thin layer adjacent to medium boundaries is imitated in terms of multiple steps over the boundary nodes during the time interval $\tau_a$. These constructions are illustrated in Fig. [6]

For the walker located at a certain boundary node the probabilities of hopping to the internal neighboring node, $P_t$, or being trapped, $P_{tr}$, are specified as

$$P_t = \frac{1 - \sigma_a}{M}, \quad P_{tr} = \frac{\sigma_a}{M},$$  \hspace{1cm} (60)

FIG. 6: Characteristic properties of random walks in the boundary layer $\mathcal{Y}_0$. The left inset visualizes possible hops from the boundary layer. The main fragment illustrates the walker jumps inside the boundary layer $\mathcal{Y}_0$ which can be complex and comprise many elementary hops. The latter feature imitates possible fast diffusion inside a certain thin layer adjacent to crystal boundaries

where the coefficient $\sigma_a$ quantifies the trapping (absorption) effect. Leaping ahead, we note that the coefficient $\sigma_a$ can be assumed to be a small value because its magnitude $\sigma_a \to 0$ as $\tau_a \to 0$ within the collection of lattices leading to the equivalent description of the random walks on time scales $\tau_a \ll t \ll \tau$. These probabilities have been chosen to constitute the probability of walker motion along the direction of the basis vector $b_M$ equal to the same value for the internal points,

$$P_t + P_{tr} = \frac{1}{M}.$$  \hspace{1cm} (61)

Therefore the probability for the walker being initially at a boundary node $n_\mathcal{Y}$ to make a jump within the boundary layer $\mathcal{Y}_0$ is

$$P_\mathcal{Y} = \frac{M - 1}{M}. $$  \hspace{1cm} (61)

At first, let us consider the case where such jumps are the elementary hops to one $n_\mathcal{Y}'$ of the nearest neighboring nodes in $\mathcal{Y}_0$. Then, following actually construction (57) its conditional probability is written as

$$P_{n\mathcal{Y}n_\mathcal{Y}'}^{(1)} = \frac{1}{2(M - 1)} + \frac{M}{(M - 1)} \frac{\tau_a}{2\sigma_a} v_\mathcal{Y}^2 \chi_{\mathcal{Y}}.$$  \hspace{1cm} (62)

Here, as before, the value $\chi_{\mathcal{Y}} = \pm 1$ is ascribed to the walker hop along the basis vector $b_{\mathcal{Y}}$. In the opposite direction, $v_{\mathcal{Y}}^2$ are the components of the drift velocity inside the boundary layer in the basis $b_{\mathcal{Y}}$. It should be noted that regular drift inside the boundary layer and the medium can be different in nature, which is allowed for by the index $\mathcal{Y}$ at the boundary components of the
drift velocity. The adopted expression (62), as it must, obeys equalities similar to expressions (55), (59), namely, for the displacement \( \delta r_\tau = b_\alpha \delta \zeta^\alpha \) along the boundary \( \Upsilon \)

\[
P_T \sum_{m \in \Upsilon} P^{(1)}_{n_x m} \delta \zeta_\alpha \delta \zeta_m = \tau_a v^\alpha_\Upsilon,
\]

(63)

\[
P_T \sum_{m \in \Upsilon} P^{(1)}_{n_x m} \delta \zeta_\alpha \delta \zeta_m = 2 \tau_a D_\alpha \delta \zeta_\beta.
\]

(64)

The fast diffusion inside the boundary layer \( \Upsilon \) is imitated by complex jumps made up of \( g \) successive elementary hops within the time \( \tau_a \). In this case the walker can get not only the nearest neighboring nodes but also relatively distant ones. The conditional probability of such a \( g \)-fold jump from node \( n_\Upsilon \) to node \( n'_\Upsilon \) is given by the expression

\[
P^{(g)}_{n_x n'_\Upsilon} = \sum_{m_1, m_2, \ldots, m_g \in \Upsilon} P^{(1)}_{n_x m_1} \times P^{(1)}_{m_1 m_2} \times \cdots \times P^{(1)}_{m_{g-1} m_g}.
\]

(65)

By virtue of (63) and (64) the probability function \( P^{(g)}_{n_x n'_\Upsilon} \) of \( g \)-fold jumps gives the following values for the first and second moments of the walker displacement \( \delta r_\tau = \sum_{n=1}^{M-1} b_\alpha \delta \zeta^\alpha \) in the layer \( \Upsilon_0 \)

\[
P_T \sum_{m \in \Upsilon} P^{(g)}_{n_x m} \delta \zeta_\alpha = g \tau_a v^\alpha_\Upsilon,
\]

(66)

\[
P_T \sum_{m \in \Upsilon} P^{(g)}_{n_x m} \delta \zeta_\alpha \delta \zeta_m = 2 (g \tau_a) D_\alpha \delta \zeta_\beta
\]

(67)

In expression (67) we again have ignored terms of order \( g^2 \tau_a^2 \) because the displacement of a walker along the boundary \( \Upsilon \) caused by its migration inside the layer \( \Upsilon_0 \) is considerable only for \( g \gg 1 \) as will be seen further. In latter case the conditional probability \( (63) \) of transition from the node \( n_\Upsilon \) to the node

\[n'_\Upsilon = n_\Upsilon + \sum_\alpha b_\alpha m_\alpha \, \{m_\alpha \text{ are integers}\}
\]

can be approximated by the Gaussian distribution

\[
P^{(g)}_{n_x n'_\Upsilon} = \left( \frac{M-1}{2\pi g} \right)^{M-1} \exp \left\{ - \frac{(M-1)^2}{2g} \sum_{\alpha=1}^{M-1} \left[ m_\alpha - \frac{gM \tau_a v^\alpha_\Upsilon}{(M-1) a_\alpha} \right]^2 \right\}
\]

(68)

by virtue of the law of large numbers and expressions (58a), (60), (67).

The desired lattice random walks imitating the continuous Markovian process in the vicinity of the medium boundary \( \Upsilon \) is constructed.

V. BOUNDARY SINGULARITIES

As discussed in Sec. II B the medium boundary \( \Upsilon \) breaks down the symmetry of random walks in its vicinity, which is reflected in the anomalous behavior of the means quantities (8)–(10) near the boundary \( \Upsilon \). To quantify this effect it is necessary to calculate the given integrals near the boundary \( \Upsilon \) for any small time interval \( \tau \).

Quantities (8)–(10) comprise two types of quantities differing in scaling with respect to \( \tau \); regular components proportional to \( \tau \) and anomalous one scaling as \( \sqrt{\tau} \). In the present section only the latter terms are under consideration. In deriving the Fokker-Planck equations the division of them by \( \tau \) gives rise to the singularity \( (\tau)^{-1/2} \). Exactly their cofactors quantify the influence of the boundary on Markovian processes and setting them equal to zero we can relate the boundary values of the Green function \( G(r,t|\tau_0, t_0) \) to the physical properties of the medium boundaries.

Assuming the time scale \( \tau \) to be sufficiently small the medium in a certain neighborhood \( Q_\alpha \) of a boundary point \( s \in \Upsilon \) is treated as a homogeneous continuum with time independent characteristics and the corresponding fragment of the boundary \( \Upsilon \) is approximated by a hyperplane. In this case it is natural to choose the coordinate system related to a basis \( \varepsilon = \varepsilon_\tau \oplus n \), which, in particular, reduces the number of the Green function arguments,

\[
G(r, x^M|\tau) := G(r, t_0 + \tau|\{0_\Upsilon, x^M_0\}, t_0).
\]

The system origin was located at the hyperplane \( \Upsilon \) such that the vector \( r_0 = \{0_\Upsilon, x^M_0\} \) can have only one component \( x^M_0 \) determining the distance between the point \( r_0 \) and the hyperplane \( \Upsilon \). Then using the general definitions (8)–(10) of the quantities \( \mathcal{R}(r, t, \tau), \mathcal{U}(r, t, \tau), \) and \( \mathcal{L}^{ij}(r, t, \tau) \) the anomalous properties of random walks near the boundary \( \Upsilon \) are quantified by their singular components \( \mathcal{U}^{*}(\tau, x^M) \) and \( \mathcal{L}^{*ij}(\tau, x^M) \) scaling as \( \sqrt{\tau} \). The symbol \( * \) is not applied to \( \mathcal{R}(\tau, x^M) \) because it possesses no regular component at all. In other words the desired quantities are determined by the following means

\[
\int_{Q_\alpha} d\bar{r} \mathcal{G}(\bar{r}, x^M|\tau) = 1 - \mathcal{R}(\tau, x^M),
\]

(69)

\[
\int_{Q_\alpha} d\bar{r} \mathcal{L}^{*ij}(\bar{r}, x^M|\tau) = \mathcal{U}^{*}(\tau, x^M) + O(\tau),
\]

(70)

\[
\frac{1}{2} \int_{Q_\alpha} d\bar{r} \mathcal{L}^{*ij}(\bar{r}, x^M|\tau) = \mathcal{L}^{*ij}(\tau, x^M) + O(\tau),
\]

(71)

where \( \mathcal{L}^{*ij} = \tilde{x}^{\alpha} \) and \( \mathcal{L}^{*ij} = \tilde{x}^M - x^M \).

In order to calculate these boundary singularities we, first, fix the value \( \tau \) and introduce a new time scale \( \tau_0 \ll \tau \). Then the lattice constructed is Sec. IV and random walks on it are applied to calculate the desired quantities. The advantage of using these lattice random walks is due to two reasons. First, the choice of the basis \( b = b_\tau \oplus b_M \) enables us to simulate the continuous
Markovian process as independent random walks along the directions parallel to the hyperplane $\Upsilon$ and along the vector $b_M$. Second, it becomes possible to ascribe special features to the nodes of the boundary layer and in this way to simulate some physical properties of the medium boundary. In particular, it can either absorb a random walker or cause it to migrate extremely fast along the boundary within a thin layer. Finally, to restore the continuous description the limit $\tau_n \to 0$ is used.

The implementation of this approach again is based on just mathematical manipulations with the probability function for lattice random walks. So only the final results are stated here, referring a reader to Appendix for the proof.

**Proposition 2** Let us consider a Markovian system in a homogeneous half-space $\mathbb{R}^M+$ bounded by a hyperplane $\Upsilon$ and endowed with the basis $b = b_{\Upsilon} \oplus b_M$ described in Proposition. The hyperplane $\Upsilon$ treated as a physical boundary can absorb the system as well as force it to migrate fast along the boundary if it would be affected by the same forces.

The continuous motion of the Markovian system is simulated by random walks on the lattice constructed in Sec. with time step $\tau$. Finally the limit $\tau_n \to 0$ is applied.

Then, first, the boundary absorption and fast transport can be characterized by two kinetic coefficients called the surface absorption rate $\sigma$ and the surface diffusion length $l_\tau$, assumed to be determined in the basis $b$. It should be noted that the boundary drift velocity $v_\tau^b$ is the velocity at which the system had moved outside the boundary if it would have been affected by the same forces.

The hyperplane $\Upsilon$ imitated by random walks on the lattice constructed in Sec. with time step $\tau$. Finally the limit $\tau_n \to 0$ is applied.

Then, first, the boundary absorption and fast transport can be characterized by two kinetic coefficients called the surface absorption rate $\sigma$ and the surface diffusion length $l_\tau$ ascribed directly to the boundary $\Upsilon$ itself, meaning these quantities to be independent of the discretization time $\tau_n$.

Second, random walks near the hyperplane $\Upsilon$ exhibit anomalous properties reflected in the following singular means scaling with the time $\tau$ as $\sqrt{\tau}$:

$$ \mathcal{R}_b(\tau, \zeta^M) = D^{-1/2}_{MM} \sigma \cdot \mathcal{K}(\tau, \zeta^M), $$

$$ ^* \mathcal{U}_b^M(\tau, \zeta^M) = D^{-1/2}_{MM} \omega \cdot \mathcal{K}(\tau, \zeta^M), $$

$$ ^* \mathcal{U}_b^L(\tau, \zeta^M) = D^{-1/2}_{MM} l_\tau v_\tau^b \cdot \mathcal{K}(\tau, \zeta^M), $$

$$ ^* \mathcal{L}_b^{\alpha\beta}(\tau, \zeta^M) = D^{-1/2}_{MM} l_\tau D^{\alpha\beta} \cdot \mathcal{K}(\tau, \zeta^M). $$

Here the label $b$ notes the basis $b$ used, $\zeta^M$ is the distance between the point $r$ and the hyperplane $\Upsilon$, measured along the vector $b_M$, and the function $\mathcal{K}(\tau, \zeta^M)$ is specified by the integral

$$ \mathcal{K}(\tau, \zeta^M) = \frac{1}{\sqrt{\tau}} \int_0^1 dz \exp \left[-\frac{(\zeta^M)^2}{4D_M \tau} \frac{1}{z} \right]. $$

In order to represent these boundary singularities in the initial basis $e$ Proposition 1 is applied again. The initial basis has been assumed to be of the form $e = e_{\Upsilon} \oplus n$ with the unit normal $n$ to the boundary $\Upsilon$ directed towards the medium. Let $\vec{U}^{-1} = [\vec{w}_{\alpha\beta}]$ be operator mapping the boundary basis $e_{\Upsilon}$ onto the basis $e$. Then transition from the coordinates $\{\zeta^i\}, \zeta^M$ of a vector $r$ in the basis $b$ to its coordinates $\{x^\alpha\}, x^M$ in the basis $e$ is specified by expressions and using the tensor $\vec{w}_{\alpha\beta}$ and the diffusion tensor $D^{ij}$ determined in the initial basis $e$. In the vector form these coordinates are related by equality. The quantities $^* \mathcal{U}_b^L(\tau, \zeta^M)$ and $^* \mathcal{L}_b^{\alpha\beta}(\tau, \zeta^M)$ are obtained by averaging variations of the coordinates $\zeta^i$. Thereby, they are a contravariant vector and tensor, respectively, with the latter being proportional to the diffusion tensor written in the basis $b$ and reduced to the hyperplane $\Upsilon$, namely, the tensor $D_{\alpha\beta}$. The value $\mathcal{R}_b(\tau, \zeta^M)$ is naturally a scalar. Whence it follows directly that

$$ \mathcal{R}(\tau, x^M) = D^{-1/2}_{MM} \sigma \cdot \mathcal{K}(\tau, x^M), $$

$$ ^* \mathcal{U}(\tau, x^M) = D^{-1/2}_{MM} \left[ D^{M} + l_\tau v_\tau^L \right] \cdot \mathcal{K}(\tau, x^M), $$

$$ ^* \mathcal{L}^{\alpha\beta}(\tau, x^M) = D^{-1/2}_{MM} l_\tau D^{\alpha\beta} \cdot \mathcal{K}(\tau, x^M). $$

Here the coordinate $x^M$ and $\zeta^M$ are interrelated by formula and the boundary diffusion tensor $D^{\alpha\beta}$ is specified by expression. Formula can be also rewritten in the vector form

$$ ^* \mathcal{U}(\tau, x^M) = D^{-1/2}_{MM} \left[ b + l_\tau v_\tau^L \right] \mathcal{K}(\tau, x^M), $$

where the vector $b$ of boundary singularities is given by formula.

**VI. BOUNDARY SINGULARITIES AND THE BOUNDARY CONDITIONS**

The obtained expressions actually directly lead us to the final results. First, they relate the singular kinetic coefficients to the diffusion tensor and the physical characteristics of the medium boundary. Second, they reduce the problem of canceling the singularities inside a thin layer $\Upsilon$ adjacent the boundary $\Upsilon$ measured along the vector $b_M$, and the function $\mathcal{K}(\tau, \zeta^M)$ is specified by the integral

$$ \mathcal{K}(\tau, \zeta^M) = \frac{1}{\sqrt{\tau}} \int_0^1 dz \exp \left[-\frac{(\zeta^M)^2}{4D_M \tau} \frac{1}{z} \right]. $$

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$$ \mathcal{K}(\tau, \zeta^M) = \frac{1}{\sqrt{\tau}} \int_0^1 dz \exp \left[-\frac{(\zeta^M)^2}{4D_M \tau} \frac{1}{z} \right]. $$
A. Boundary condition for the backward Fokker-Planck equation

As shown in Sec. [13] the boundary singularities that appear in the expansion the Chapman-Kolmogorov equation leading to the backward Fokker-Planck equation will vanish if equality (15) holds. At first, in order to lighten the perception of results let us consider a rather small neighborhood of the point \( s \) belonging to the boundary \( \Upsilon \) wherein it is actually a hyperplane and chose the basis \( \epsilon_T \oplus n \) composed of its hyperplane basis \( \epsilon_T(s) \) and unit normal \( n(s) \) directed inward the domain \( \Omega \). Then substituting expressions (77)–(79) into formula (18), we immediately get the conclusion that at the boundary point \( s \in \Upsilon \) the Green function \( G(r, t|s_0, t_0) \) with respect to the latter pair of its arguments with \( s_0 \to s \) has to meet the condition

\[
\sum_{i=1}^{M} D^{iM}(s, t_0) \nabla_i^{s} G(r, t|s, t_0) = \sigma(s, t_0) G(r, t|s, t_0) \\
- l_T(s, t_0) \left[ \sum_{a=1}^{M-1} v^{(a)}_T(s, t_0) \nabla^{a}_s G(r, t|s, t_0) \\
+ \sum_{\alpha, \beta = 1}^{M-1} \mathcal{D}^{\alpha\beta}(s, t_0) \nabla^{\alpha}_s \nabla^{\beta}_s G(r, t|s, t_0) \right].
\]

(81)

We note that two last terms in expression (81) describe effective motion of the system inside the boundary \( \Upsilon \) and has the form of the backward Fokker-Planck operator \( \hat{\mathcal{L}}_{FPb} \) with the diffusion tensor \( \mathcal{D}^{\alpha\beta} \) and drift velocity \( v^{(a)}_T \) whose action is confined to the boundary \( \Upsilon \). In order to rewrite this expression for an orthonormal basis of general orientation we make use of the definition of the boundary singularity vector \( b(s, t) \), expression (10), and take into account expression (18) for the surface tensor diffusion. Then introducing the backward Fokker-Planck operator acting only within the hyperplane \( \Upsilon \)

\[
\hat{\mathcal{L}}_{FPb}(s, t_0) \{ \phi \} = l_T(s, t_0) \\
\times \left[ \sum_{i,j=1}^{M} \mathcal{D}^{ij}(s, t_0) \nabla^{i}_s \nabla^{j}_s \phi + \sum_{i=1}^{M} v^{i}_T(s, t_0) \nabla^{i}_s \phi \right],
\]

(82)

where as before the symbol \( \hat{\phi} \) stands for a function acted upon by this operator. Then in the vector invariant form the boundary condition for the backward Fokker-Planck equation is written as

\[
b(s, t_0) \cdot \nabla^{s} G(r, t|s, t_0) = \sigma(s, t_0) G(r, t|s, t_0) \\
- \hat{\mathcal{L}}_{FPb}(s, t_0) \{ G(r, t|s, t_0) \}
\]

(83)

which is desired formula.

In deriving expression (81) the boundary \( \Upsilon \) was treated as a hyperplane, i.e. the Euclidian space of dimension \( (M-1) \) and its local basis \( \epsilon_T \) was used. To write it again in the general form underlining the fact that the operator \( \hat{\mathcal{L}}_{FPb} \) acts in this hyperplane only the tensor notions of covariant derivatives are used (see, e.g., Ref. [23]). In these terms the action of the operator \( \hat{\mathcal{L}}_{FPb} \) on the Green function taken at the boundary \( \Upsilon \) can be rewritten as

\[
\hat{\mathcal{L}}_{FPb}(s, t_0) \{ G(r, t|s, t_0) \} = l_T(s, t_0) \\
\times \left[ \sum_{a=1}^{M-1} v^{(a)}_T(s, t_0) G(r, t|s, t_0) \\
+ \sum_{\alpha, \beta = 1}^{M-1} \mathcal{D}^{\alpha\beta}(s, t_0) G(r, t|s, t_0) \right].
\]

(84)

In the given case it is no more that another form of the corresponding term in expression (81). However, for a nonplanar boundary formula (81) holds allowing for the boundary curvature, where as expression (82) loses the curvature effect. Its analysis goes far beyond the scope of the present paper, so, here we will just ignore it.

B. Boundary condition for the forward Fokker-Planck equation

The boundary conditions are obtained in a similar way. First, we note that the integrand of expression (29) is is similar to the boundary relation (13) within the replacement the test function \( \phi(r) \) by the Green function \( G(r, t|s_0, t_0) \) and action of the operators at the argument \( r \) in stead of \( r_0 \). This analogy and the boundary condition (83) for the backward Fokker-Planck equation enable us to reduce equality (29) to the following

\[
b(s, t) \cdot \nabla^{s} \phi(s) = \sigma(s, t_0) \phi(s) - \hat{\mathcal{L}}_{FPf}(s, t) \{ \phi(s) \}
\]

(85)

for an arbitrary boundary point \( s \in \Upsilon \). Since the boundary part of the backward Fokker-Planck equation acts only within the boundary \( \Upsilon \) only the left part of expression (85) contains the first derivative of the test function \( \phi(s) \) in the direction normal to the boundary \( \Upsilon \) at the point \( s \). All the other terms are either the boundary value of the function \( \phi(s) \) itself or its derivatives along the hyperplane \( \Upsilon \). It justifies the adopted previously statement that in the vicinity of \( \Upsilon \) the test function \( \phi(r) \) can have any boundary value \( \phi(s) \).

Then noting that the left-hand side of the condition (80) is just the combination

\[
b(s, t) \cdot \nabla^{s} G(s, t|s_0, t_0)
\]

the last equability converts expression (80) into

\[
\int_{\Upsilon} ds \phi(s) \sum_{i=1}^{M} v^{i}(s) J^{i} \{ G(s, t|s_0, t_0) \},
\]

\[
= - \int_{\Upsilon} ds \phi(s) \sigma(s, t) G(s, t|s_0, t_0) \\
+ \int_{\Upsilon} ds \hat{\mathcal{L}}_{FPf}(s, t) \{ \phi(s) \} G(s, t|s_0, t_0).
\]

(86)
The last term in (86) using the divergence integral theorem for the surfaces is reduced to the form

$$
\oint_{\Sigma} ds \hat{F}_{FP_0}(s, t) \{ \phi(s) \} G(s, t | r_0, t_0) = \oint_{\Sigma} ds \phi(s) \hat{F}_{FP_0}(s, t) \{ G(s, t | r_0, t_0) \}.
$$

Here the operator $\hat{F}_{FP_0}$ is the boundary forward Fokker-Planck equation

$$
\hat{F}_{FP_0}(s, t) \{ \phi \} = \sum_{i=1}^{M} \nabla_i^s \left[ \sum_{j=1}^{M} \nabla_j^s \left( t_T(s, t) D^{ij}(s, t) \phi \right) - t_T(s, t) v_i^s(s, t) \phi \right],
$$

(87)

where again the symbol $\phi$ stands for the acted function. Since the test function $\phi(s)$ takes any arbitrary values at the boundary $\Sigma$ equality (86) holds for any point on the boundary $\Sigma$, i.e.

$$
n(s) \cdot \vec{J} \{ G(s, t | r_0, t_0) \} = -\sigma(s, t) G(s, t | r_0, t_0) + \hat{F}_{FP_0}(s, t) \{ G(s, t | r_0, t_0) \}
$$

(88)

which is the desired boundary condition for the forwards Fokker-Planck equation. As it should be the boundary condition (88) can be interpreted in terms of mass conservation: the component of walker flux normal to the boundary $\Sigma$ is determined by the surface rate of walker absorption and the rate of fast surface transport withdrawing the walkers from the given boundary point.

VII. CONCLUSION

The present paper has developed a technique of deriving the boundary conditions for the Fokker-Planck equations based on the Chapman-Kolmogorov integral equation. The idea of the work is illustrated in Fig. VII.

The interest to this problem is partly due to the following. It is well known that the Fokker-Planck equations, forward and backward ones, stem directly from the Chapman-Kolmogorov equation under additional two assumptions, the short time confinement of the corresponding Markovian process and the local homogeneity of the medium. There are rather rigorous techniques of deriving them from the integral Chapman-Kolmogorov equation based on expanding the latter on short time scales in the possible limits. By contrast, the corresponding boundary conditions are typically postulated applying to the physical meaning of the probability flux and the analogy between the forward Fokker-Planck equation and the mass conservation law.

However such simple arguments can fail in dealing with more complex Markovian processes like sub- or super-diffusion, for which the Fokker-Planck equations with fractional derivatives form the governing equations. In this case it would be appropriate to have a formal technique giving rise to the boundary conditions starting from the general description. However, up to now constructing such a technique is a challenging problem. It was the case also with respect to the normal Markovian processes in continua.

This paper actually has demonstrated how to do this dealing with the normal Markovian processes. The key point is the fact that the medium boundary breaks down the symmetry of random walks near it. As result, the coefficients in the corresponding expansion series of the Chapman-Kolmogorov equation are endowed with anomalous features called the boundary singularities. Namely, they scale on short time scales as $\delta t^{-1/2}$. Since the probability distribution on macroscopic scales cannot contain such singularities the corresponding co-factors in the expressions for the boundary singularities should be set equal to zero, leading one to the required boundary conditions. In this way we have shown that the boundary conditions of the Fokker-Planck equations are also the direct consequence of the Chapman-Kolmogorov equation supplemented with some rather general assumptions about the properties of the medium boundary. As it must the boundary conditions obtained in this way match mass conservation.

APPENDIX A: PROOF OF PROPOSITION II

At the first step the initial basis $e$ of the half-space $\mathbb{R}^{M+}$ is assumed to comprise a certain basis

$$
e_T = \{ e_1, e_2, \ldots e_{M-1} \}.$$

FIG. VII: Illustration of the main purpose of the present work represented by grey directed line.
Here the tensor $x$ Correspondingly, an arbitrary vector $b \in \mathbb{R}^M$ of the space $\mathbb{R}^M$ mapping, in particular, the hyperplane $\mathcal{Y}$ to itself. This transformation $\tilde{\mathcal{U}} = \|U_j\|$ is specified by the relationship between the basis vectors

$$e_\alpha = \sum_{\beta=1}^{M-1} b_\alpha u_\beta^\alpha \quad n = \sum_{\alpha=1}^{M-1} b_\alpha \omega^\alpha + b_M \omega^M. \quad (A1)$$

Here the tensor $u^\alpha_\beta$ represents an operator $\tilde{\mathcal{U}}_\alpha$ acting on the hyperplane $\mathcal{Y}$ whereas the tensor $\omega^\alpha$ (in $\mathcal{Y}$) and the coefficient $\omega^M \neq 0$ complement it to the operator $\tilde{\mathcal{U}}$, namely,

$$U^\alpha_\beta = u^\alpha_\beta, \quad U^\alpha_M = \omega^\alpha, \quad (A2a)$$

$$U^M_\beta = 0, \quad U^M_M = \omega^M. \quad (A2b)$$

According to the rule of tensor transformations (see, e.g., Ref. [23]) in the basis $b$ the diffusion matrix has the components

$$\tilde{D}^{\alpha\beta} = \sum_{\gamma,\gamma'=1}^{M-1} u^\alpha_\gamma u^\beta_\gamma D^{\gamma\gamma'} + \omega^\alpha \omega^\beta D^{MM}$$

$$+ \sum_{\gamma=1}^{M-1} (\omega^\alpha u^\beta_\gamma + \omega^\beta u^\alpha_\gamma) D^{\gamma M}, \quad (A3a)$$

$$\tilde{D}^{M\alpha} = \omega^M \left( \sum_{\gamma=1}^{M-1} u^\alpha_\gamma D^{\gamma M} + \omega^\alpha D^{MM} \right), \quad (A3b)$$

$$\tilde{D}^{M\gamma} = (\omega^M)^2 D^{MM}. \quad (A3c)$$

Correspondingly, an arbitrary vector $x^i = \{x^\alpha, x^M\}$ is converted as

$$\bar{x}^\alpha = \sum_{\gamma=1}^{M-1} u^\alpha_\gamma x^\gamma + \omega^\alpha x^M, \quad \quad (A4a)$$

$$\bar{x}^M = \omega^M x^M. \quad \quad (A4b)$$

Currently there is no restrictions imposed on the basis $b$ (except for its general structure). Now let us choose a specific version of the tensor $\omega^\alpha$ that eliminates the off-diagonal elements of the diffusion tensor in the basis $b$. By virtue of $\omega^M = \sum_{\gamma=1}^{M-1} u^\alpha_\gamma D^{\gamma M}$,

$$\omega^\alpha = -\frac{1}{D^{MM}} \sum_{\gamma=1}^{M-1} u^\alpha_\gamma D^{\gamma M}. \quad (A5)$$

Here the division by $D^{MM}$ is possible because according to definition $D^{MM}$ the diagonal elements of diffusion tensor are positive, in particular, $D^{MM} > 0$ except for the case where the system motion along the direction $n$ is rigorously deterministic. However, setting further $D^{MM} \to +0$ the latter case can be also allowed for. The substitution of $[A5]$ into $[A3a]$ yields

$$\tilde{D}^{\alpha\beta} = \sum_{\gamma,\gamma'=1}^{M-1} u^\alpha_\gamma u^\beta_\gamma D^{\gamma\gamma'}, \quad (A6)$$

where the object

$$D^{\alpha\beta} = D^{\alpha\beta} - \frac{1}{D^{MM}} D^{\alpha M} D^{\beta M} \quad \quad (A7)$$

is a tensor within the hyperplane $\mathcal{Y}$ because, up to now, the collections of vectors $\mathbf{e}_\alpha$ and $\mathbf{b}_\gamma$ are general bases of this hyperplane.

The tensor $D^{\alpha\beta}$ is symmetric and positive definite. The latter property stems directly from inequality $\lVert D^{\beta\gamma} \rVert$ written for an arbitrary covector $l_\alpha$ of the hyperplane $\mathcal{Y}$ with the component

$$l_M = -\frac{1}{D^{MM}} \sum_{\gamma=1}^{M-1} D^{\gamma M} l_\gamma, \quad \quad (A8)$$

namely,

$$\sum_{i,j=1}^{M} D^{ij} l_i l_j = \sum_{\alpha,\beta=1}^{M-1} D^{\alpha\beta} l_\alpha l_\beta > 0. \quad (A9)$$

Therefore the basis $b_\gamma$ of the hyperplane $\mathcal{Y}$ can be chosen to be orthonormal one wherein the tensor $D^{\alpha\beta}$ takes the diagonal form with the diagonal components being positive values, i.e. $D^{\alpha\beta} = D^{\alpha\gamma} = D_{\alpha\gamma} = D_{\alpha\beta}[24]$. This basis $b_\gamma$ is made up of the eigenvectors of the operator $\mathcal{D} := \lVert D^{\beta\gamma} \rVert$ whose eigenvalues are $\{D_{\alpha\gamma}\}$. For example, in the initial basis $\mathbf{e}_\alpha$ the tensor $D^{\alpha\beta}$ is related to the tensor $D^{\alpha\beta}$ by the expression

$$D^{\alpha\gamma} = \sum_{\gamma=1}^{M-1} g_{\alpha\gamma} D^{\beta\gamma}, \quad \text{where} \quad g_{\alpha\beta} := (\mathbf{e}_\alpha \cdot \mathbf{e}_\beta)$$

is the matric tensor of the hyperplane $\mathcal{Y}$.

The choice of the given basis $b_\gamma$ specifies the transformation matrix $\lVert u^\alpha_\gamma \rVert$ which together with expression $[A5]$ gives us the vector $b_M$ and the corresponding component $D_M$ of the diffusion tensor. Namely, first, substituting $[A5]$ into the latter equality of $[A1]$ and taking into account the former one we write

$$b_M \omega^M = n + \frac{1}{D^{MM}} \sum_{\alpha,\gamma=1}^{M-1} b_\alpha u^\alpha_\gamma D^{\gamma M}$$

$$= n + \frac{1}{D^{MM}} \sum_{\gamma=1}^{M-1} \mathbf{e}_\gamma D^{\gamma M}. \quad (A10)$$
In the invariant form this expression can be rewritten as
\[ b_M = \frac{1}{\omega} \sum_{i,j=1}^{M} e_i D^{ij} (e_j \cdot n), \]
(A11)
where the normalization factor \( \omega \)
\[ \omega = \left[ \sum_{i,j,k,p=1}^{M} D^{ik} D^{jp} (e_i \cdot e_j) (e_k \cdot e_p) \right]^{1/2} \]
(A12)
is due to the vector \( b_M \) being of unit length. Since the obtained expressions (A11) and (A12) are of the tensor form and are scaler in this meaning they hold within any basis, proving formulae (41) and (42).

Second, according to (A10) and (A11), the coefficient \( \omega_M = \omega / D^{MM} \). Thereby expressions (A3a) and (A12) give us the diffusion tensor component \( D_M \) related to the vector \( b_M \) in the basis \( b \)
\[ D_M = \omega^2 \left[ \sum_{i,j=1}^{M-1} D^{ij} (e_i \cdot n) (e_j \cdot n) \right]^{-1} \]
(A13)
and written in the invariant form. Formula (44) is proved. In addition, expressions (A4) and (A5) together with the equality \( \omega = \omega_M D^{MM} \) immediately lead to formulae (46a) and (46b).

Finally, we need the transformation \( \hat{U}_T^{-1} = \| \hat{u}^\alpha \| \) of the hyperplane \( \Upsilon \) that is inverse to the transformation \( \hat{U}_T = \| u^\alpha \| \); its components obey the equality
\[ \sum_{\gamma=1}^{M-1} \hat{u}^\alpha \gamma \hat{u}^\gamma = \delta^\alpha \beta. \]
(A14)
It exists due to the transformation \( \hat{U}_T \) being one-to-one map of the bases \( c \) and \( b \). Then the inversion of equalities (A4) with \( \omega^\alpha \) given by expression (A5) yields formulae (46c) and (46d). Inverting now relationship (A6) and taking into account the tensor \( \hat{D}^{\alpha \beta} \) to have the diagonal form \( D_\alpha \delta_{\alpha \beta} \) in the orthonormal basis \( b \) we directly get
\[ \sum_{\gamma=1}^{M-1} \hat{u}^\alpha \gamma \hat{u}^\gamma D_\gamma = \hat{D}^{\alpha \beta}. \]
which together with expressions (A7) gives rise to formula (47). The Proposition is proved.

**APPENDIX B: PROOF OF PROPOSITION 2**

The homogeneous half-space \( \mathbb{R}^{M+} \) bounded by the hyperplane \( \Upsilon \) is under consideration and a lattice described in Sec. [IV] is constructed. It is made up of the node layers \( \{ \Upsilon \} \) parallel to the hyperplane \( \Upsilon \) with the interplane spacing vector \( a_M b_M \). The individual node arrangement of the layers \( \Upsilon \) is determined by the vectors of the hyperplane basis \( b_\Upsilon \) with spacings \( \{ a_\alpha \} \). In other words, the nodes of this lattice are the points
\[ r_n = \sum_{\alpha=1}^{M-1} n^\alpha (a_\alpha b_\alpha) + n a_M b_M, \]
where \( n \) is the collection of numbers \( \{ n_\Upsilon, n \} = \{ n^\alpha \}, n \) taking any integer value, \( n^\alpha |_{1}^{M-1} = 0, \pm 1, \pm 2, \ldots \), except for the last one; it takes only nonnegative values \( n = 0, 1, 2, \ldots \). In particular, the points \( \{ r_n \}_\Upsilon \) with \( n = 0 \) form the boundary layer \( \Upsilon_0 \).

The Markovian process in the half-space \( \mathbb{R}^{M+} \) is simulated by random walks on this lattice with hop probabilities given in Sec. [IV]. To find the desired boundary singularities we will analyze evolution of the walker distribution over the given lattice, i.e. the dynamics of the probability \( P_{t,n} \) to find the walker at node \( n \) after hop \( t \). Here \( t \) is the time measured in jump numbers, i.e. in units of the hop duration \( \tau_\alpha \). At the initial time \( t = 0 \) the walker is assumed to be located at a certain internal node \( n_0 \). Without lost of generality all the components of the index \( n_0 \) can be set equal to zero except for the last one, i.e. \( n_0 = \{ 0, 0, \ldots, 0, n_0 \} \).

1. **Moments of the walker distribution and the generation function**

Actually the main purpose of the present appendix is to find the zero-th, first, and second order moments of the distribution function \( P_{t,m} \). The zero-th moment quantifies the trapping effect, whereas the first and second ones characterize the walker propagation in space. Namely, the following quantities
\[ \mathcal{R}_i(t, n_0) = 1 - \sum_{n=0}^{\infty} \sum_{n_\Upsilon} P_{t,(n_\Upsilon,n)}, \]
(B1)
\[ \mathcal{L}_i(t, n_0) = \sum_{n=0}^{\infty} \sum_{n_\Upsilon} \left( n^i - n^i_0 \right) P_{t,(n_\Upsilon,n)}, \]
(B2)
\[ \mathcal{D}_i(t, n_0) = \frac{1}{2} \sum_{n=0}^{\infty} \sum_{n_\Upsilon} \left( n^i - n^i_0 \right) \left( n^j - n^j_0 \right) P_{t,(n_\Upsilon,n)} \]
(B3)
have to be calculated. Here the index \( i \) is used as a general symbol for one of the indices \( \{ \alpha \} \). In order to do this the generation function and its analogy written
for the boundary nodes only

\[ G(s, p, k_T) = \sum_{t=0}^{\infty} \sum_{n=0}^{n_T} e^{-st-p(n-n_0)+i(k_T \cdot n_T)} P_{t,(n_T,n)}, \]  
(B4)

\[ g(s, k_T) = \sum_{t=0}^{\infty} \sum_{n=0}^{n_T} e^{-st+i(k_T \cdot n_T)} P_{t,(n_T,0)} = \lim_{p \to \infty} \left[ e^{-p\eta_0} G(s, p, k_T) \right] \]  
(B5)

are introduced, where the complex arguments \( s \), \( p \) have the positive real parts, \( \text{Re} \, s, \text{Re} \, p \geq 0 \). It should be noted that the traps are not included into these sums. The discrete Laplace transforms of the desired functions [B11]--[B13] are directly related to the generation function. Indeed

\[ \mathcal{R}_0(s, n_0) = \sum_{t=0}^{\infty} e^{-st} \mathcal{R}_0(t, n_0) = \frac{1}{1-e^{-s}} - G(s, 0, 0), \]  
(B6)

\[ \mathcal{U}_0^i(s, n_0) = \sum_{t=0}^{\infty} e^{-st} \mathcal{U}_0^i(t, n_0) = \nabla_i G(s, p, k_T)|_{p, k_T = 0}, \]  
(B7)

\[ \mathcal{L}_{0}^ij(s, n_0) = \sum_{t=0}^{\infty} e^{-st} \mathcal{L}_{0}^ij(t, n_0) = \frac{1}{2} \nabla_i \nabla_j G(s, p, k_T)|_{p, k_T = 0}, \]  
(B8)

where the operator \( \nabla_i \) is \( \nabla_\alpha = -i \partial_\alpha \) if the index \( i = \alpha \) is one of the indices of the hyperplane \( \Upsilon \) and \( \nabla_M = -\partial_p \) for the index \( i = M \).

Master equation for lattice random walks and its general solution

To find the generation function for the discrete random walks under consideration the corresponding master equation is applied. For an internal node \( n = \{n_T, n\} \) with \( n \geq 2 \) it takes the form

\[ \mathcal{P}_{t+1,n} = \sum_m' \mathcal{P}_{t,m} \mathcal{P}_{mn}, \]  
(B9)

Here prime at the sum denotes the index \( m \) running over all the nearest neighbors of the given node \( n \) and according to expression [B11] the corresponding hop probabilities can be represented as

\[ \mathcal{P}_{mn} = \frac{1 + \epsilon_i \chi_i}{2M}, \]  
(B10)

where \( \epsilon_i = \tau_a v_i M/\alpha_i \) are some small quantities scaling with \( \tau_a \) as \( \epsilon_i \propto \tau_a^{1/2} \) and the value \( \chi_i = \pm 1 \) stands for hops along the basis vector \( b_i \) or in the opposite direction, i.e. the hop to the node with \( m^i = n^i \pm 1 \) and \( m^j = n^j \) for \( j \neq i \). For the nodes of the layer \( \Upsilon_1 \) the master equation becomes

\[ \mathcal{P}_{t+1,n} = \sum_m' \mathcal{P}_{t,m} \mathcal{P}_{mn} + \mathcal{P}_{t,n} \mathcal{P}_{t\Gamma}. \]  
(B11)

Here again prime at the sum has the same meaning except for only internal neighboring nodes being taken into account, \( \{n_0, n\} \) is the pair of nodes belonging to the boundary layer \( \Upsilon_0 \) and the adjacent internal layer \( \Upsilon_1 \) that are related to each other via walker hops, and the hop probability \( \mathcal{P}_{t\Gamma} \) is determined by expression [B6]. The walker distribution function \( \mathcal{P}_{n,\Gamma} \) in the boundary layer obeys the equation

\[ \mathcal{P}_{t+1,n} = \sum_{m_0 \in \Upsilon_0} \mathcal{P}_{t,m_0} \mathcal{P}_{T} \mathcal{P}_{m_0 n_0} + \mathcal{P}_{t,n} \mathcal{P}_{nn_0}. \]  
(B12)

We remind that the jumps inside the boundary layer can be complex and comprise individually \( g \) elementary hops. In this case the multihop probability \( \mathcal{P}_{m_0 n_0}^{(g)} \) is determined by formula [B6]. The one-hop probability along the basis vector \( b_0 \) provided the walker remains in the boundary layer \( \Upsilon_0 \) is

\[ \mathcal{P}_{m_0 n_0}^{(1)} = \frac{1 + \epsilon_\Upsilon \chi_\alpha}{2(M - 1)}, \]  
(B13)

where \( \epsilon_\Upsilon = \tau_a v_\Upsilon^2 M/\alpha_\Upsilon \) is again a small parameter scaling as \( \epsilon_\Upsilon \propto \tau_a^{1/2} \). The values \( \epsilon_\Upsilon \) quantify the asymmetry of hops in the boundary layer \( \Upsilon_0 \). In particular, these complex jumps are characterized by the means

\[ \langle n^\alpha \rangle_\Upsilon = \sum_{n_0 \in \Upsilon_0} n^\alpha \mathcal{P}_{0n_0}^{(g)} = \frac{g}{M - 1} \epsilon_\Upsilon \chi_\alpha, \]  
(B14)

\[ \langle n^\alpha n^\beta \rangle_\Upsilon = \sum_{n_0 \in \Upsilon_0} n^\alpha n^\beta \mathcal{P}_{0n_0}^{(g)} = \frac{g}{M - 1} \delta_\alpha\beta + \frac{g(g - 1)}{(M - 1)^2} \epsilon_\Upsilon^2 \epsilon_\beta. \]  
(B15)

Finally, the master equation for the traps is

\[ \mathcal{P}_{t+1,n_0}^{(r)} = \mathcal{P}_{t,n_0}^{(r)} + \mathcal{P}_{t,n_0} \mathcal{P}_{tr}. \]  
(B16)

The hop probabilities \( \mathcal{P}_{t}, \mathcal{P}_{tr} \), are given by expressions [B6] and the kinetic coefficients of walker jumps inside the boundary layer \( \Upsilon_0 \) are specified by expressions [B11], [B12], and [B24]. At the initial time the walker distribution meets the condition

\[ \mathcal{P}_{t=0,n} = \delta_{mn_0}. \]  
(B17)

To solve this system of equations we substitute [B9], [B11], and [B12] into definition [B4] of the generation function \( G(s, p, k_T) \) and after succeeding mathematical manipulations get the following equation (see comments about its derivation just after formula [B20])

\[ e^s - \Phi(p, k_T) \big( e^s - e^{p\eta_0} [\Phi(p, k_T) - \Phi(p, k_T)] \big) G(s, p, k_T) \]  
(B18)
resolving the given generation functions \( G(s, p, k_T) \) and \( g(s, k_T) \) to each other. Here the following functions

\[
\begin{align*}
\Phi(p, k_T) &= \frac{1}{M} (\cosh p - e_M \sinh p) \\
&+ \frac{1}{M} \sum_{\alpha=1}^{M-1} \left( \cos k_\alpha + i \alpha \sin k_\alpha \right), \\
\phi(p, k_T) &= \frac{(1 - \sigma_\alpha)}{M} e^{-p} \\
&+ \frac{(M - 1)}{M} \sum_{\alpha=1}^{M-1} \exp \left[ i (k_T \cdot n_T) \right] \rho_{\alpha}^{(g)} \quad (B19)
\end{align*}
\]

have been constructed in deriving equation \( B18 \). 

**Comments on deriving equation \( B18 \)**: The key fragments of deriving equation \( B18 \) are outlined below. The conversion in \( B17 \) from \( t \to t + 1 \) leads to the line

\[
G(s, p, k_T) = e^{-s} G(s, p, k_T) + 1,
\]

where

\[
G(s, p, k_T) = \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} e^{-\tau T} p^{(n-n_0)} + (i k_T \cdot n_T) \rho_{t+1}(n_T, n)
\]

and the initial condition \( B17 \) has been taken into account. Equations \( B19 \), \( B11 \), and \( B12 \) relating two succeeding steps of random walks are substituted into the latter expression. As a result the terms in sums \( B19 \)–\( B17 \) matching the interlayer hops split it into two parts

\[
G(s, p, k_T) = \Phi_1(p) G(s, p, k_T) + e^{\rho_{00}} [\phi_1(p) - \Phi_1(p)] g(s, k_T)
\]

with the latter summand caused by that the boundary nodes differ from the internal ones in properties. In their turn the components of sums \( B19 \)–\( B17 \) describing transitions between a given node \( n \) and the nodes of the same layer also split the term \( G(s, p, k_T) \) into two parts

\[
G(s, p, k_T) = \Phi_2(k_T) G(s, p, k_T) + e^{\rho_{00}} [\phi_2(k_T) - \Phi_2(k_T)] g(s, k_T),
\]

where the latter summand is due to fast diffusion in the boundary layer. The combination of the two last lines gives equation \( B18 \) with \( \Phi(p, k_T) = \Phi_1(p) + \Phi_2(k_T) \) and \( \phi(p, k_T) = \phi_1(p) + \phi_2(k_T) \). \( \Box \)

The generation function \( G(s, p, k_T) \) has no singularities in the region \( \text{Re } s, \text{Re } p > 0 \). Thereby the left hand-side of \( B18 \) is equal to zero when \( e^s - \Phi(p, k_T) = 0 \). Resolving the latter equality with respect to the variable \( p \) we obtain a function \( p = \varphi(s, k_T) \) defined by the equation

\[
\Phi[\varphi(s, k_T), k_T] = e^s \quad (B21)
\]

which specifies the locus in the space \( \{s, p, k_T\} \) where also the right hand-side of equation \( B18 \) has to be equal to zero. The latter enables us to write immediately the boundary generation function in the form

\[
g(s, k_T) = \frac{\exp [-\varphi(s, k_T)]}{1 - e^{-s}}. \quad (B22)
\]

Expressions \( B18 \) and \( B22 \) actually solve the problem giving us the following expression for the generation function

\[
G(s, p, k_T) = \frac{1}{1 - e^{-s}} \left[ \frac{\Phi(p, k_T) - 1}{1 - e^{-s}} \right] + e^{-[\varphi(s, k_T) - p] \rho_{00}} \left[ \Phi(p, k_T) - \Phi(p, k_T) \right] \left[ 1 - e^{-s} \right] \phi(s, k_T, k_T) \right] \quad (B23)
\]

where the first summand is the image of the delta function \( \rho_{t, n} = \delta_{nn_0} \), not contributing into one of the quantities \( B19 \)–\( B13 \), the second term is due to random walks over the internal nodes, and the last one is caused by the boundary effects. Formula \( B23 \) specifies the desired generation function in the general form.

### 2. Limit of multiple-step random walks on small time scales

In order to find the Laplace transforms \( B6 \)–\( B8 \) it suffices to expand the generation function \( G(s, p, k_T) \) into the Taylor series with respect to the arguments \( p \) and \( k_T \) with cutting off the series at the second order terms. However, in the case under consideration there are additional assumptions simplifying essentially obtaining the desired results. First, only random walks with many steps are of interest because the hop duration \( \tau_\alpha \) has been chosen to be much less than the observation time interval \( \tau \) of the analyzed Markovian process, \( \tau_\alpha \ll \tau \). It means the inequality \( s \ll 1 \) to hold. Second, the time interval \( \tau \) is regarded as any small value. So only the components of moments \( B11 \)–\( B3 \) that are characterized by scaling \( \tau^d \) with the exponent \( d \) not exceeding unity, \( d \leq 1 \), are to be taken into account. With respect to the generation function \( G(s, p, k_T) \) the latter assumption is converted to the statement that all the components of itself and its derivatives calculated at the point \( \{k_T = 0, p = 0\} \) that scale with the argument \( s \) as \( s^{-d} \) and have the exponent \( d \) exceeding two, \( d > 2 \), can be ignored.

At the point \( \{k_T = 0, p = 0\} \) according to their definition \( B19 \), \( B20 \) the function \( \Phi(0, 0) = 1 \) and the function

\[
\phi(0, 0) = 1 - \frac{\sigma_\alpha}{M},
\]

where the coefficient \( \sigma_\alpha \) is considered to be a small parameter, which is justified in the limit \( \tau_\alpha \to 0 \) as will be
The expansion of the functions $\Phi(p, k_T)$ for the generation function can be rewritten as

$$G(s, p, k_T) = \frac{1}{s} + \frac{\Phi(p, k_T) - 1}{s^2} + e^{-\varpi(s, 0)_{n_0}} \left[ \frac{\phi(p, k_T) - \Phi(p, k_T)}{s [s + 1 - \phi(\varpi(s, 0), 0)]} \right].$$  \hspace{1cm} (B24)

The expansion of the functions $\Phi(p, k_T)$, $\phi(p, k_T)$ with respect to $p$ and $k_T$ at the required order is

$$\Phi(p, k_T) = 1 - \frac{\epsilon_M p}{2M} + \frac{p^2}{2M} + \frac{1}{M} \sum_{\alpha=1}^{M-1} \left( i \epsilon_\alpha k_\alpha - \frac{1}{2} k_\alpha^2 \right).$$  \hspace{1cm} (B25)

and

$$\phi(p, k_T) = 1 - \frac{\sigma_a}{M} - \frac{p}{M} + \frac{p^2}{2M} + \frac{i g}{M} \sum_{\alpha=1}^{M-1} \zeta,T k_\alpha - \frac{g}{2M} \sum_{\alpha, \beta=1}^{M-1} k_\alpha k_\beta \left( \delta_{\alpha\beta} + \frac{g-1}{M} \epsilon_\alpha \epsilon_\beta \right).$$  \hspace{1cm} (B26)

In deriving expression (B26) formulae (B14), (B15) have been used. The substitution of the generation function written in form (B24) with approximations (B25), (B26) has been used obliquely. Third, for further converting the discrete Laplace transformation into continuous one within the replacement

$$\varpi(s\tau_a, 0) \rightarrow \int_0^\infty dt(\ldots)$$

all the functions (B27)–(B31) must be multiplied by the time scale $\tau_a$.

Leaping ahead we note that the absorption coefficient $\sigma_a$ has to scale with $\tau_a$ as $\sigma_a \propto \sqrt{s\tau_a}$. As before noted the coefficients $\{\epsilon_\alpha\}$ also behave in this way. Therefore the observation time interval $\tau$ can be chosen to be so small that the solution of equation (B21) become

$$\varpi(s\tau_a, 0) = 2M s\tau_a$$  \hspace{1cm} (B33)

and function (B32) matches a continuous Laplace transform

$$\tau_a K_a(s\tau_a, n_0) = \sqrt{\frac{M}{2\tau_a}} K(s, \zeta_0)$$  \hspace{1cm} (B34)

given by the expression

$$K(s, \zeta_0^M) = s^{-3/2} \exp \left( - \zeta_0 \sqrt{s/D_M} \right).$$  \hspace{1cm} (B35)

the mean $\zeta_0^M$ is equal to zero. Here the function $K_a(s, n_0)$ is defined by the expression

$$K_a(s, n_0) = \exp \left[ -\varpi(s, 0)_{n_0} \right] s \varpi(s, 0)_{n_0}$$  \hspace{1cm} (B32)

and we have ignored some insignificant terms where appropriate.

Previously in the given appendix we measured time $t$ in units of the hop duration $\tau_a$ and spatial coordinates $\{\zeta_i\}$ in units of the lattice spacings $\{a_i\}$ within the frame $b$. Now let us return to the initial units and deal with the corresponding spatial correlations. To do this, first, functions (B28)–(B31) should be multiplied by the spacings $a_M$ and $a_a$, or their products $a_a a_M$ and $\sigma_a^2$, respectively. Second, the dimensionless Laplace argument $s$ has to be replaced by the product $s\tau_a$, because previously when applying to the discrete Laplace transformation the replacement

$$st \rightarrow s\tau_a \cdot \frac{t}{\tau_a}$$

has been used obliquely. Third, for further converting the discrete Laplace transformation into continuous one within the replacement

$$\tau_a \sum_{t/t_a=0}^{\infty} \rightarrow \int_0^\infty dt(\ldots)$$

provided $\varpi(s\tau_a, 0) \gg \sigma_a$. Because $\sigma_a \sim \sqrt{\varepsilon \tau_a}$, where $\varepsilon$ is some constant, the latter inequality is reduced to the following $s \gg \varepsilon$ and $\tau \ll \varepsilon$. Since the time interval is an arbitrary small value the two inequalities can be adopted beforehand. Whence formulae (B33) and (B34) follows immediately for the spacing $a_M$ given by expression (501).
3. Continuum limit and a $\delta$-boundary model

To get the final results we analyze the obtained expression in the limit $\tau_a \to 0$. The probability distribution $\mathcal{P}_{1,m}$ of the lattice random walks can be treated as the discrete implementation of the Green function $G(r, r_0, t)$ giving the probability density to find a walker at the point $r$ at time $t$ provided it was initially at the point $r_0$. Using the Green function $G(r, r_0, t)$ the means under consideration are written as the following moments

$$\mathcal{R}(t, \zeta_0) = 1 - \int_{\mathbb{R}^3} dr G(r, r_0, t),$$  \hspace{1cm} (B36)

$$\mathcal{U}_b(t, \zeta_0) = \int_{\mathbb{R}^3} dr (\zeta^i - \zeta_0^i)G(r, r_0, t),$$  \hspace{1cm} (B37)

$$\mathcal{L}_{b}^{ij}(t, \zeta_0) = \frac{1}{2} \int_{\mathbb{R}^3} dr (\zeta^i - \zeta_0^i)(\zeta^j - \zeta_0^j)G(r, r_0, t),$$  \hspace{1cm} (B38)

and their Laplace transforms can be obtained from the quantities $\{B27\} - \{B31\}$ in the manner described in the previous subsection. As the result we have

$$\mathcal{R}(s, \zeta_0) = D_{MM}^{-1/2} s \mathcal{K}(s, \zeta_0),$$  \hspace{1cm} (B39)

$$\mathcal{U}_b^{M}(s, \zeta_0) = D_{MM}^{-1/2} \zeta \mathcal{K}(s, \zeta_0) + \frac{\zeta^M}{s^2},$$  \hspace{1cm} (B40)

$$\mathcal{U}_b^{P}(s, \zeta_0) = D_{MM}^{-1/2} l_T \mathcal{K}(s, \zeta_0) + \frac{\zeta^P}{s^2},$$  \hspace{1cm} (B41)

$$\mathcal{L}_{b}^{a\beta}(s, \zeta_0) = \left[ D_{MM}^{-1/2} l_T D_\alpha \mathcal{K}(s, \zeta_0) + \frac{D_\alpha}{s^2} \right] \delta_{a\beta},$$  \hspace{1cm} (B42)

$$\mathcal{L}_{b}^{MM}(s, \zeta_0) = \frac{D_M}{s^2},$$  \hspace{1cm} (B43)

the component $\mathcal{L}_{b}^{MM}(s, \zeta_0)$ is equal to zero. Here the following characteristics of the medium boundary treated as an infinitely thin layer $\Upsilon$

$$\sigma := \sigma_a \sqrt{\frac{D_{MM}}{2M\tau_a}}, \hspace{1cm} l_T := \sqrt[2]{\frac{MD_{MM}\tau_a}{2}}$$  \hspace{1cm} (B44)

have been introduced and expression $\{B14\}$ have been used. It should be noted that according to $\{B14\}$ the number $g$ of elementary hops forming the long distant jumps of wallers in the boundary layer $\Upsilon_0$ has to grow with $\tau_a$ as $\tau_a^{-1/2}$ in order to retain the effect of boundary fast transport in the limit $\tau_a \to 0$. As a result, the second term in the square brackets of expression $\{B14\}$ scales as $\sqrt{\tau_a}$ because, in turn, the coefficients $\{\zeta_a\}$ vary with $\tau_a$ as $\sqrt{\tau_a}$. Therfore it vanishes in the limit $\tau_a \to 0$ and the symmetry of the second moments caused by the boundary fast diffusion is restored.

The equality (see, e.g., Ref. \[20\])

$$\int_0^\infty \frac{dt}{\sqrt{\pi t}} \exp\left(-\frac{\zeta_0^2}{4D_M t} - st\right) = \frac{1}{\sqrt{s}} \exp\left(-\zeta_0 \sqrt{s/D_M}\right)$$

and the Laplace transform of integrals enable us represent the inverse Laplace transform $\mathcal{K}(t, \zeta_0)$ of function $\{B35\}$ in the integral form

$$\mathcal{K}(t, \zeta_0) = \sqrt{\frac{t}{\pi}} \int_0^1 \frac{dz}{\sqrt{z}} \exp\left(-\frac{\zeta_0^2}{4D_M t} z\right).$$ \hspace{1cm} (B45)

Expression $\{B45\}$ together with formulae $\{B39\} - \{B43\}$ proves Proposition 2.

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