THE FIRST-PASSAGE-TIME PROBLEMS WITH TIME-VARYING DRIVING FIELDS

BEZÁK V.,[1]) Bratislava

The first-passage-time problem is analysed for a diffusion process running on a line segment with absorbing ends. The process is assumed to be driven by a general time-varying field. Emphasis is put on the derivation of compact formal expressions in a "greenistic style". General formulae are derived for the probabilities of the survival on the segment, for the related probability densities of the first-passage times and for the statistical moments (including the mean) of the first-passage times (residence times).

I. INTRODUCTION

'he theory of the first-passage times is a classical part of the theory of :hastic processes that has been worked out in great detail for time-homogeus Markov processes [1]. If the Markov processes are inhomogeneous in e, the theory becomes much more complicated but we must well cope with fact when we want to understand results obtained by some up-to-date omatographic experiments or, say, by the pulsed-field gel electrophoresis. e latter is a relatively new technique which has evoked much interest among physicists, since it enables to separate effectively large DNA molecules -4].)Having in ming such applications, Fletcher, Havlin and Weiss IW) [5] have recently elaborated a first-passage-time theory with a time-endent drift. They have presented two versions of their theory: 1) a random-lker theory and 2) a diffusion theory. Here we will only comment on their usion theory.

Their basic equation was the forward Kolmogorov equation

$$\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2} - v(t) \frac{\partial p}{\partial x}, \qquad t > 0, \tag{1}$$

a diffusion process on a line segment with absorbing ends at $x = 0$ and

[1]) Department of Solid State Physics, Comenius University, 842 15 BRATISLAVA, Czecho-akia

$x = L > 0$. In particular, they have assumed the uniformity of the initial probability density p_0:

$$p(x, 0) = p_0(x) = \frac{1}{L} = \text{const.} \tag{2}$$

The probability density $p(x, t)$ has to fulfil the boundary conditions

$$p(0, t) = p(L, t) = 0. \tag{3}$$

In eq. (1), $D > 0$ is a constant diffusion coefficient and $v(t)$ an arbitrary function of the time variable t. In numerical calculations, however, FHW have used the drift velocity $v(t)$ in a special form,

$$v(t) = V \sin(\omega_0 t + \alpha), \tag{4}$$

under the assumption that the constant V is small. (In some calculations, they have chosen the phase α as zero; anyway, we will not specify the function $v(t)$.)

After having represented $p(x, t)$ as the Fourier series

$$p(x, t) = \sum_{n=1}^{\infty} a_n(t) \sin\left(\frac{\pi n x}{L}\right), \tag{5}$$

FHW have derived an infinite set of ordinary differential equations for $a_n(t)$ ($n = 1, 2, \ldots$) and shown that these equations can be solved in a perturbational way (with respect to the parameter V).

Nevertheless, such a scheme, as we will show in the present paper, is not the best from a modern theoretical viewpoint. Our scheme (Section II) — avoiding the equations for $a_n(t)$ at all — provides surely a more compact formulation being much nearer to the "greenistic ideology".

Our basic equation is not eq. (1) but rather the backward Kolomogorov equation for the fundamental solution $P(x, t; x_0, t_0)$. We rewrite this equation into an integral form. This idea will enable us to make formal developments of the survival distributions

$$S(t; x_0) = \int_0^L \mathrm{d}x P(x, t; x_0, 0), \tag{6}$$

$$s(t) = \int_0^L \mathrm{d}x p(x, t) \tag{7}$$

with respect to $v(t)$ in the most straightforward way. In (7), we have defined the probability density

$$p(x, t) = \int_0^L \mathrm{d}x_0 P(x, t; x_0, 0) p_0(x_0). \tag{8}$$

In Section III, we comment on some further notions (such as the probability density of the first-passage times and the mean residence time). It is not our aim to present new numerical calculations in this paper (since we take those published in Ref. [5] as sufficiently instructive).

II. GENERAL THEORY

We define the Green function $P(x, t; x_0, t_0)$ first:

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2} - v(t) \frac{\partial P}{\partial x}, \qquad t > t_0, \tag{9}$$

$$\lim_{t \to t_0} P(x, t; x_0, t_0) = \delta(x - x_0). \tag{10}$$

(Taking the initial distribution $p_0(x)$ for $t_0 = 0$ as an arbitrary function given in advance, we see that $p(x, t)$ given by formula (8) is the unique solution to the forward Kolomogorov eq. (1).) The function $P(x, t; x_0, t_0)$ is simultaneously the fundamental solution to the backward Kolomogorov equation:

$$-\frac{\partial P}{\partial t_0} = D \frac{\partial^2 P}{\partial x_0^2} + v(t_0) \frac{\partial P}{\partial x_0}, \qquad t_0 < t, \tag{11}$$

$$\lim_{t_0 \to t} P(x, t; x_0, t_0) = \delta(x_0 - x). \tag{12}$$

Clearly,

$$P(0, t; x_0, t_0) = P(L, t; x_0, t_0) = 0 \tag{13}$$

and

$$P(x, t; 0, t_0) = P(x, t; L, t_0) = 0. \tag{14}$$

We define the non-perturbed Green function $P_0(x, t; x_0, t_0)$:

$$-\frac{\partial P_0}{\partial t_0} = D \frac{\partial^2 P_0}{\partial x_0^2}, \qquad t_0 < t, \tag{15}$$

$$\lim_{t_0 \to t} P_0(x, t; x_0, t_0) = \delta(x_0 - x), \tag{16}$$

$$P_0(x, t; 0, t_0) = P_0(x, t; L, t_0) = 0. \tag{17}$$

Explicitly, we can apply the construction

$$P_0(x, t; x_0, t_0) = \frac{2}{L} \sum_{n=1}^{\infty} \exp\left[-\frac{\pi^2 n^2 D}{L^2}(t - t_0)\right] \sin\left(\frac{\pi n x_0}{L}\right) \sin\left(\frac{\pi n x}{L}\right). \tag{18}$$

(The sum converges rapidly if $t - t_0 \gtrsim L^2/(\pi^2 n^2 D)$; for small values of $t - t_0$, however, it is more advantageous to use another form $P_0(x, t; x_0, t_0)$, the so-called path representation — cf. [6] — which can be obtained from formula (18) if the Poisson summation procedure is applied.)

The integral form of equation (11) is

$$P(x, t; x_0, 0) = P_0(x, t; x_0, 0) + \\ + \sum_0^t dt' v(t') \sum_0^L dx' \frac{\partial P(x, t; x', t')}{\partial x'} P_0(x', t'; x_0, 0). \tag{19}$$

(We have chosen $t_0 = 0$.)
Hence we obtain directly the development

$$P(x, t; x_0, 0) = \sum_{j=0}^{\infty} P^{(j)}(x, t; x_0, 0), \tag{20}$$

where

$$P^{(0)}(x, t; x_0, 0) = P_0(x, t; x_0, 0), \tag{21}$$

$$P^{(1)}(x, t; x_0, 0) = \int_0^t dt' v(t') \int_0^L dx' \frac{\partial P_0(x, t; x', t')}{\partial x'} P_0(x', t'; x_0, 0), \tag{22}$$

$$P^{(2)}(x, t; x_0, 0) = \int_0^t \int_0^t dt' dt'' v(t') v(t'') \int_0^L \int_0^L dx' dx'' \times \\ \times \frac{\partial P_0(x, t; x'', t'')}{\partial x''} \frac{\partial P_0(x'', t''; x', t')}{\partial x'} P_0(x', t'; x_0, 0), \tag{23}$$

etc. When the sum (18) is inserted in formulae (22), (23), we can carry out the integration with respect to x' and x'' explicitly (Appendix).

The integral equation (19) implies directly the integral equation for the survival distribution $S(t; x_0)$ (cf. definition (6)):

$$S(t; x_0) = S_0(t; x_0) + \int_0^t dt' v(t') \int_0^L dx' \frac{\partial S(x, t; x', t')}{\partial x'} P_0(x', t'; x_0, 0), \tag{24}$$

where

$$S_0(t; x_0) = \int_0^L dx P_0(x, t; x_0, 0) = \\ = \frac{4}{\pi} \sum_{m=1}^{\infty} \exp\left[-\frac{\pi^2 (2m-1)^2 Dt}{L^2} \right] \sin\left[\frac{\pi(2m-1) x_0}{L} \right]. \tag{25}$$

Thus we can obtain the development

$$S(t; x_0) = \sum_{j=0}^{\infty} S^{(j)}(t; x_0) \tag{26}$$

for the survival distribution $S(t; x_0)$ when the diffusion starts from the point x_0; here

$$S^{(j)}(t; x_0) = \int_0^L dx P^{(j)}(x, t; x_0, 0); \tag{27}$$

or the development

$$s(t) = \sum_{j=0}^{\infty} s^{(j)}(t) \tag{28}$$

for the survival distribution $s(t)$ in the special case when the initial distribution $p_0(x)$ is uniform (cf. definition (2)); here

$$s^{(j)}(t) = \frac{1}{L} \int_0^L dx_0 S^{(j)}(t; x_0). \tag{29}$$

III. CONCLUDING REMARKS

The survival probabilities $S(t; x_0)$, $s(t)$ define, respectively, the probability densities $\Phi(t; x_0)$, $\varphi(t)$ for the first-passage times:

$$\Phi(t; x_0) = -\frac{\partial S(t; x_0)}{\partial t}, \tag{30}$$

$$\varphi(t) = -\frac{ds(t)}{dt}. \tag{31}$$

Indeed, the probability for the process under consideration to reach one of the end points ($x = 0$ or $x = L$) and to become thus "annihilated" is $1 - S(t; x_0)$ or $1 - s(t)$ if the initial distribution is $p_0(x) = \delta(x - x_0)$ or $p_0(x) = 1/L$, respectively. Then $-(\partial S/\partial t) . dt$ and $-(ds/dt) . dt$ are the corresponding probabilities that the exit through one of the end points (i.e. "absorption") takes place during the interval $(t, t + dt)$. The functions $\Phi(t; x_0)$, $\varphi(t)$ are (and must be) non-negative.

We denote by $T_r(x_0)$ and t_r the residence times (corresponding to the distributions $S(t; x_0)$ and $s(t)$); obviously, $T_r(x_0)$, t_r are stochastic variables. (Note that the residence time and the first-passage time are synonyms. For a specialist in chromatography, it is the same notion as the so-called elution time.)
Their statistical moments are defined by the expressions (for $p = 1, 2, \ldots$):

$$\langle [T_r(x_0)]^p \rangle = \int_0^{\infty} dt t^p \Phi(t; x_0), \tag{32}$$

$$\langle t_r^p \rangle = \int_0^\infty dt\, t^p \varphi(t). \tag{33}$$

Integrating them by parts, we can also write

$$\langle [T_r(x_0)]^p \rangle = p \int_0^\infty dt\, t^{p-1} S(t;\, x_0), \tag{34}$$

$$\langle t_r^p \rangle = p \int_0^\infty dt\, t^{p-1} s(t). \tag{35}$$

Particularly, taking $p = 1$, we can write for the mean residence time the formulae

$$\langle T_r(x_0) \rangle = \int_0^\infty dt S(t;\, x_0), \tag{36}$$

$$\langle t_r \rangle = \int_0^\infty dt s(t). \tag{37}$$

When using the developments (27), (29), we obtain easily the corresponding developments in $v(t)$ for $\Phi(t;\, x_0)$, $\varphi(t)$, as well as for the statistical moments $\langle [T_r(x_0)]^p \rangle$, $\langle t_r^p \rangle$.

Finally, let us note that the problem solved in the present paper is closely related to our statistical theory of wear (or reliability) that we have published recently in APS [7, 8]. Now, however, we do not consider an "annihilation rate" (or "killing rate") in our basic evolution equations (in eq. (9) or (11)). Instead, the annihilation is merely due to the exits through the end points of the segment. The reader who wishes to learn more about the reliability theory or about the so-called failure modelling should also consult the papers by Lemoine and Wenocur [9, 10].

APPENDIX

Our intent is to perform the x-integration in formulae (22) and (23). First of all, we note that the integrals

$$G_{kl} = \int_0^L dx' \frac{\partial \sin(\pi l x'/L)}{\partial x'} \sin(\pi k x'/L) \tag{A.1}$$

represent L-independent numbers:

$$G_{kl} = \begin{cases} \dfrac{2kl}{k^2 - l^2} & \text{if} \quad k + l \text{ is odd} \\ 0 & \text{if} \quad k + l \text{ is even} \end{cases} \tag{A.2}$$

(where k, l are two integers).

Utilizing the series (18) for $P_0(x, t;\, x_0, t_0)$, we obtain the expressions:

$$\int_0^L dx' \frac{\partial P_0(x, t;\, x', t')}{\partial x'} P_0(x', t';\, x_0, 0) =$$

$$= \frac{4}{L^2} \sum_{k,l=1}^\infty \exp\left[-\frac{\pi^2 l^2 D}{L^2}(t - t')\right] \exp\left[-\frac{\pi^2 k^2 D}{L^2} t'\right] G_{kl} \sin\left(\frac{\pi l x}{L}\right) \sin\left(\frac{\pi k x_0}{L}\right), \tag{A.3}$$

$$\int_0^L \int_0^L dx' dx'' \frac{\partial P_0(x, t;\, x'', t''}{\partial x''} \frac{\partial P_0(x'', t'';\, x', t')}{\partial x'} P_0(x', t';\, x_0, 0) =$$

$$= \frac{8}{L^3} \sum_{k,l,m=1}^\infty \exp\left[-\frac{\pi^2 m^2 D}{L^2}(t - t'')\right] \exp\left[-\frac{\pi^2 l^2 D}{L^2}(t'' - t')\right] \cdot$$

$$\cdot \exp\left[-\frac{\pi^2 k^2 D}{L^2} t'\right] \cdot G_{kl} G_{lm} \sin\left(\frac{\pi m x}{L}\right) \sin\left(\frac{\pi k x_0}{L}\right). \tag{A.4}$$

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ПРОБЛЕМЫ ВРЕМЕНИ ПЕРВОГО ВЫХОДА ЗА ГРАНИЦУ ПРИ ВРЕМЕННО-ПЕРЕМЕНЧИВЫХ ДРЕЙФУЮЩИХ ПОЛЯХ

В статье излагается проблема времени первого выхода за любую из границ линейного сегмента, вдоль которого происходит диффузия. Предполагается, что диффузионный процесс дрейфует в присутствии общего временно-переменчивого поля. Подчеркивается возможность получения компактных формальных выражений в «гринистическом стиле». Выведены общие формулы для вероятностей переживания на сегменте, для родственных вероятностей времени первого выхода за границу и для статистических моментов (включая среднее значение) времени первого выхода за границу (времени резиденции).