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Outflow Probability for Drift–Diffusion Dynamics

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The proposed explanations are provided for the one–dimensional diffusion process with constant drift by using forward Fokker–Planck technique. We present the exact calculations and numerical evaluation to get the outflow probability in a finite interval, i.e. first passage time probability density distribution taking into account reflecting boundary on left hand side and absorbing border on right hand side. This quantity is calculated from balance equation which follows from conservation of probability. At first, the initial-boundary-value problem is solved analytically in terms of eigenfunction expansion which relates to Sturm–Liouville analysis. The results are obtained for all possible values of drift (positive, zero, negative). As application we get the cumulative breakdown probability which is used in theory of traffic flow.

KEY WORDS: boundary-value problem; stochastic analysis; Markov process.
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1. INTRODUCTION

Nowadays, the natural sciences deal with objects which have nondeterministic behaviour. Their descriptions can be found in theory of stochastic processes as a branch of probability theory (Gardiner, 2004). There are different theoretical approaches for similar investigations using language of stochastic trajectories as well as probability distributions. The fundamental equation which gives us the probabilistic description is the Fokker–Planck equation (Gardiner, 2004; Risken, 1996). Our motivations for theoretical investigations in this field are given by application of the models of many-particles system which are considered in theoretical physics, i.e. physics of traffic flow (Mahnke *et al.*, 2005). Here we would like to find an analytical solution for the special case when the stochastic variable belongs to a finite interval in terms of probability density distributions as well as cumulative probability (Redner, 2001). The interval is defined as closed on left hand side and opened on right hand side. Due to these properties we introduce boundary conditions which determine the behaviour of the solution. Another

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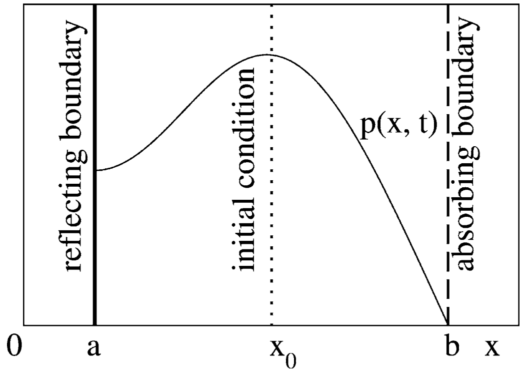


Fig. 1. Schematic picture of the boundary-value problem showing the probability density $p(x,t)$ in the interval $a \le x \le b$.

important analysed quantity is the outflow (or breakdown) probability at right border which is found from the solution of Fokker–Planck equation by using balance equation.

Let us consider the initial-boundary-value-problem (shown schematically in Fig. 1) with constant diffusion coefficient D and constant drift coefficient v. Our task is to calculate the probability density $p(x,t)$ to find the system in state x (exact in interval $[x; x+dx]$) at time moment t. The dynamics of $p(x,t)$ is given by the forward drift-diffusion-equation as well as initial and boundary conditions (Gardiner, 2004) by following dynamics

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

or

$$\frac{\partial p(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0 \tag{2}$$

with flux

$$j(x,t) = v\,p(x,t) - D\,\frac{\partial p(x,t)}{\partial x} \tag{3}$$

with the initial condition

$$p(x, t=0) = \delta(x - x_0), \tag{4}$$

and two boundary conditions (Gardiner, 2004), i.e. reflecting boundary at $x = a$

$$j(x=a,t) = v\,p(x=a,t) - D\,\left.\frac{\partial p(x,t)}{\partial x}\right|_{x=a} = 0, \tag{5}$$

and absorbing boundary at $x = b$

$$p(x = b, t) = 0. \tag{6}$$

It is convenient to formulate the drift-diffusion problem in dimensionless variables. For this purpose we define new variables y and T by

$$y = \frac{x - a}{b - a} \quad \text{and} \quad T = \frac{D}{(b - a)^2}\, t. \tag{7}$$

As a result, the system of partial differential equations (1)–(6) can be rewritten as

$$\frac{\partial P(y, T)}{\partial T} = -\Omega \frac{\partial P(y, T)}{\partial y} + \frac{\partial^2 P(y, T)}{\partial y^2}, \tag{8}$$

with initial condition

$$P(y, T = 0) = \delta(y - y_0), \tag{9}$$

reflecting boundary at $y = 0$

$$J(y = 0, T) = \Omega\, P(y = 0, T) - \left. \frac{\partial P(y, T)}{\partial y} \right|_{y=0} = 0, \tag{10}$$

and absorbing boundary at $y = 1$

$$P(y = 1, T) = 0. \tag{11}$$

Hence, our problem has only one dimensionless control parameter $\Omega = \frac{v}{D}\,(b - a)$ (scaled drift v which may have positive, zero, or negative values). The parameter Ω has the same meaning as Péclet number which has been used in Redner (2001).

The system of equations (8)–(11) will be solved exactly by applying the forward technique (Gardiner, 2004). The main idea is to obtain the solution of Fokker–Planck equation and after that the first passage time distribution in terms of probability density. Both quantities will be presented as eigenfunction expansions. The survival probability and moments of first passage time can be calculated differently by using backward drift-diffusion equation. These results shown in Choi and Fox (2002), Fox and Choi (2001), and Redner (2001) do not give the complete solution of the problem under consideration. Our presented analysis of the reference system (8)–(11) is the key result in order to study more complicated situations with nonlinear drift function $\Omega(y)$.

2. SOLUTION IN TERMS OF ORTHOGONAL EIGENFUNCTIONS

To find the solution of the well–defined drift–diffusion problem, first we take the dimensionless form (8)–(11) and use a transformation to a new function Q by

$$Q(y, T) = e^{-\frac{\Omega}{2} y}\, P(y, T). \tag{12}$$

This results in a dynamics without first derivative called reduced Fokker–Planck-equation

$$\frac{\partial Q(y,T)}{\partial T} = -\frac{\Omega^2}{4}\, Q(y,T) + \frac{\partial^2 Q(y,T)}{\partial y^2}. \tag{13}$$

According to (12) the initial condition is transformed to

$$Q(y, T=0) = e^{-\frac{\Omega}{2} y_0}\, P(y, T=0), \tag{14}$$

whereas the reflecting boundary condition at $y = 0$ becomes

$$\frac{\Omega}{2}\, Q(y=0,T) - \left.\frac{\partial Q(y,T)}{\partial y}\right|_{y=0} = 0, \tag{15}$$

and the absorbing boundary condition at $y = 1$ now reads

$$Q(y=1, T) = 0. \tag{16}$$

The solution of reduced Eq. (13) can be found by the method of separation of variables (Selvadurai, 2000). Making a separation ansatz $Q(y,T) = \chi(T)\psi(y)$, we obtain

$$\frac{1}{\chi(T)}\frac{d\chi(T)}{dT} = -\frac{\Omega^2}{4} + \frac{1}{\psi(y)}\frac{d^2\psi(y)}{dy^2}. \tag{17}$$

Both sides should be equal to a constant. This constant is denoted by $-\lambda$, where λ has the meaning of an eigenvalue. The eigenvalue λ should be real and nonnegative.

Integration of the left hand side gives exponential decay

$$\chi(T) = \chi_0 \exp\{-\lambda T\} \tag{18}$$

with $\chi(T=0) = \chi_0$ and setting $\chi_0 = 1$.

Let us now define the dimensionless wave number k as $k^2 = \lambda$. The right-hand side of Eq. (17) then transforms into the following wave equation

$$\frac{d^2\psi(y)}{dy^2} + \left(k^2 - \frac{\Omega^2}{4}\right)\psi(y) = 0. \tag{19}$$

Further on, we introduce a modified wave number $\tilde{k}^2 = k^2 - \Omega^2/4$. Note that $\tilde{k} = +\sqrt{k^2 - \Omega^2/4}$ may be complex (either pure real or pure imaginary).

First we consider the case where $\tilde{k}$ is real. A suitable complex ansatz for the solution of the wave equation (19) reads

$$\psi(y) = C^* \exp\{+i\tilde{k}y\} + C\exp\{-i\tilde{k}y\} \tag{20}$$

with complex coefficients $C = A/2 + i\,B/2$ and $C^* = A/2 - i\,B/2$ chosen in such a way to ensure a real solution

$$\psi(y) = A\cos(\tilde{k}y) + B\sin(\tilde{k}y). \tag{21}$$

The two boundary conditions (15) and (16) can be used to determine the modified wave number $\tilde{k}$ and the ratio A/B. The particular solutions are eigenfunctions $\psi_m(y)$, which form a complete set of orthogonal functions. As the third condition, we require that these eigenfunctions are normalised

$$\int_0^1 \psi_m^2(y)\, dy = 1. \tag{22}$$

In this case all three parameters $\tilde{k}$, A, and B are defined.

The condition for the left boundary (15) reads

$$\frac{\Omega}{2}\psi(y=0) - \left.\frac{d\psi(y)}{dy}\right|_{y=0} = 0. \tag{23}$$

After a substitution by (20) it reduces to

$$\frac{\Omega}{2}(C^* + C) = i\tilde{k}\,(C^* - C) \tag{24}$$

or

$$\frac{\Omega}{2}A = \tilde{k}B. \tag{25}$$

The condition for the right boundary (16)

$$\psi(y=1) = 0 \tag{26}$$

gives us

$$C^* \exp\{+i\tilde{k}\} + C\exp\{-i\tilde{k}\} = 0 \tag{27}$$

or

$$A\cos(\tilde{k}) + B\sin(\tilde{k}) = 0. \tag{28}$$

By putting both equalities (25) and (28) together and looking for a nontrivial solution, we arrive at a transcendental equation

$$i\frac{\Omega}{2}(\exp\{+i\tilde{k}\} - \exp\{-i\tilde{k}\}) = \tilde{k}(\exp\{+i\tilde{k}\} + \exp\{-i\tilde{k}\}) \tag{29}$$

or

$$\frac{\Omega}{2}\sin(\tilde{k}) + \tilde{k}\cos(\tilde{k}) = 0, \tag{30}$$

respectively

$$\tan(\tilde{k}) = -\frac{2}{\Omega}\tilde{k}, \tag{31}$$

which gives the spectrum of values $\tilde{k}_m$ with $m = 0, 1, 2, \ldots$ (numbered in such a way that $0 < \tilde{k}_0 < \tilde{k}_1 < \tilde{k}_2 < \ldots$) and the discrete eigenvalues $\lambda_m > 0$.

Due to (21) and (28), the eigenfunctions can be written as

$$\psi_m(y) = R_m[\cos(\tilde{k}_m y)\sin(\tilde{k}_m) - \cos(\tilde{k}_m)\sin(\tilde{k}_m y)], \tag{32}$$

where $R_m = A_m/\sin(\tilde{k}_m) = -B_m/\cos(\tilde{k}_m)$. Taking into account the identity $\sin(\alpha - \beta) = \sin\alpha\cos\beta - \cos\alpha\sin\beta$, Eq. (32) reduces to

$$\psi_m(y) = R_m \sin[\tilde{k}_m(1 - y)]. \tag{33}$$

The normalisation constant R_m is found by inserting (33) into (22). Calculation of the normalisation integral by using the transcendental equation (30) gives us

$$R_m^2 \int_0^1 \sin^2[\tilde{k}_m(1 - y)]dy = R_m^2 \left[\frac{1}{2} - \frac{1}{4\tilde{k}_m}\sin(2\tilde{k}_m)\right]$$
$$= \frac{R_m^2}{2}\left(1 + \frac{\Omega}{2}\frac{1}{\tilde{k}_m^2 + \Omega^2/4}\right) = 1, \tag{34}$$

and hence (33) becomes

$$\psi_m(y) = \sqrt{\frac{2}{1 + \frac{\Omega}{2}\frac{1}{\tilde{k}_m^2 + \Omega^2/4}}}\sin[\tilde{k}_m(1 - y)] \tag{35}$$

or

$$\psi_m(y) = \sqrt{\frac{2}{1 + \frac{\Omega}{2}\frac{1}{k_m^2}}}\sin\left[\sqrt{k_m^2 - \Omega^2/4}\,(1 - y)\right]. \tag{36}$$

This calculation refers to the case $\Omega > -2$ where all wave numbers k_m or $\tilde{k}_m = \sqrt{k_m^2 - \Omega^2/4}$ are real and positive.

However the smallest or ground–state wave vector $\tilde{k}_0$ vanishes when Ω tends to -2 from above, and no continuation of this solution exists on the real axis for $\Omega < -2$. A purely imaginary solution $\tilde{k}_0 = i\kappa_0$ appears instead, where κ_0 is real, see Fig. 2. In this case (for $\Omega < -2$) a real ground-state eigenfunction $\psi_0(y)$ can be found in the form (20) where $C = A/2 + B/2$ and $C^* = A/2 - B/2$, i.e.,

$$\psi_0(y) = A\cosh(\kappa_0 y) + B\sinh(\kappa_0 y). \tag{37}$$

The transcendental equation for the wave number $\tilde{k}_0 = i\kappa_0$ can be written as the following equation for κ_0

$$\frac{\Omega}{2}\sinh(\kappa_0) + \kappa_0\cosh(\kappa_0) = 0. \tag{38}$$

As compared to the previous case $\Omega > -2$, trigonometric functions are replaced by the corresponding hyperbolic ones. Similar calculations as before yield

$$\psi_0(y) = \sqrt{-\frac{2}{1 + \frac{\Omega}{2}\frac{1}{-\kappa_0^2 + \Omega^2/4}}}\sinh[\kappa_0(1 - y)]. \tag{39}$$

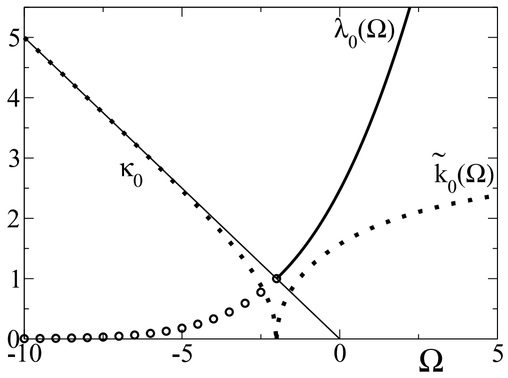


Fig. 2. The wave number $\tilde{k}_0$ ($\Omega - 2$) respectively κ_0 ($\Omega \leq -2$) and eigenvalue λ_0 for ground state $m = 0$. The thin straight line shows the approximation $\kappa_0 \approx -\Omega/2$ valid for large negative $\Omega < -5$.

Note that $\kappa_0 = -i\tilde{k}_0$ is the imaginary part of $\tilde{k}_0$ and $\kappa_0^2 = -\tilde{k}_0^2$. As regards other solutions of (30) called excited states, i.e., those for $\tilde{k}_m$ with $m > 0$, nothing special happens at $\Omega = -2$, so that these wave numbers are always real. The situation for ground state $m = 0$ at different values of dimensionless drift parameter Ω is summerized in Table 1 which presents the solutions κ_0 from transcendental equation (38) together with $\lambda_0 = -\kappa_0^2 + \Omega^2/4$ and $\tilde{k}_0$ from transcendental equation (30) together with eigenvalues $\lambda_0 = \tilde{k}_0^2 + \Omega^2/4$. Table 2. shows the behaviour of lowest wave numbers $\tilde{k}_m$ with $m = 0, 1, \ldots, 5$. The results are plotted in Fig. 3.

In general (for arbitrary Ω), the eigenfunctions are orthogonal and normalised, i.e.,

$$\int_0^1 \psi_l(y)\psi_m(y)\, dy = \delta_{ml}. \tag{40}$$

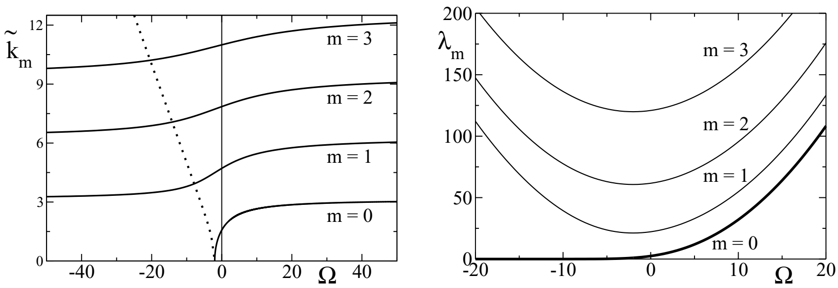


Fig. 3. The parameter dependence of wave numbers $\tilde{k}_m(\Omega)$ and eigenvalues $\lambda_m(\Omega)$ for ground state $m = 0$ and excited states $m = 1, 2, 3$.

Table I. The Ground-State Wave Number κ_0 (for $\Omega \leq -2$) and $\tilde{k}_0$ (for $\Omega -$ 2) and Eigenvalue λ_0 Depending on the Dimensionless Drift Parameter Ω

Ω	κ_0	λ_0	Ω	$\tilde{k}_0$	λ_0
−9.00	4.499	0.010	−2.00	0.000	1.000
−8.50	4.248	0.015	−1.50	0.845	1.276
−8.00	3.997	0.021	−1.00	1.165	1.608
−7.50	3.745	0.031	−0.50	1.393	2.004
−7.00	3.493	0.045	0.00	1.571	2.468
−6.50	3.240	0.064	0.50	1.715	3.005
−6.00	2.984	0.091	1.00	1.836	3.623
−5.50	2.726	0.128	1.50	1.939	4.325
−5.00	2.464	0.178	2.00	2.028	5.116
−4.50	2.195	0.245	2.50	2.106	5.999
−4.00	1.915	0.333	3.00	2.174	6.979
−3.50	1.617	0.446	3.50	2.235	8.058
−3.00	1.288	0.591	4.00	2.288	9.239
−2.50	0.888	0.774	4.50	2.337	10.525
−2.00	0.000	1.000	5.00	2.381	11.917

Figure 4 shows the ground eigenstate ($m = 0$) for different parameter values Ω, whereas Fig. 5 gives a collection of eigenstate functions ($m = 0, 1, \ldots, 5$) for $\Omega = -5.0$ and $\Omega = 3.0$.

In the following, explicit formulae (where $\psi_m(y)$ is specified) are written for the case $\Omega > -2$.

In order to construct the time-dependent solution for $Q(y, t)$, which fulfills the initial condition, we consider the superposition of all particular solutions with different eigenvalues λ_m

$$Q(y, T) = \sum_{m=0}^{\infty} C_m e^{-\lambda_m T} \psi_m(y). \tag{41}$$

Table II. The Wave Numbers $\tilde{k}_m$ ($m = 0, 1, \ldots, 5$) Depending on the Dimensionless Drift Parameter Ω

Ω	−10.0	−5.0	−2.0	−1.0	0.0	1.0	2.0	5.0	10.0
$m = 0$	4.999	2.464	0.000	1.165	1.571	1.836	2.028	2.381	2.653
$m = 1$	3.790	4.172	4.493	4.604	4.712	4.816	4.913	5.163	5.454
$m = 2$	7.250	7.533	7.725	7.789	7.854	7.917	7.979	8.151	8.391
$m = 3$	10.553	10.767	10.904	10.949	10.995	11.040	11.085	11.214	11.408
$m = 4$	13.789	13.959	14.066	14.101	14.137	14.172	14.207	14.310	14.469
$m = 5$	16.992	17.133	17.220	17.249	17.279	17.308	17.336	17.421	17.556

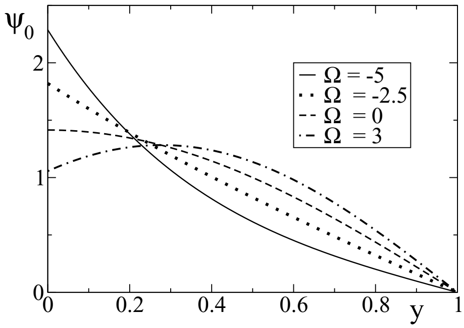


Fig. 4. The eigenfunction $\psi_0(y)$ for different values of control parameter Ω.

By inserting the initial condition

$$P(y, T = 0) = e^{\frac{\Omega}{2}y} Q(y, T = 0) = \delta(y - y_0) \tag{42}$$

into (41) we obtain

$$\sum_{m=0}^{\infty} C_m \psi_m(y) = e^{-\frac{\Omega}{2}y} \delta(y - y_0). \tag{43}$$

Now we expand the right hand side of this equation by using the basis of orthonormalised eigenfunctions (35) and identify C_m with the corresponding coefficient at ψ_m, i.e.,

$$C_m = \int e^{\frac{\Omega}{2}y} \delta(y - y_0) \psi_m dy = e^{-\frac{\Omega}{2}y_0} \psi_m(y_0). \tag{44}$$

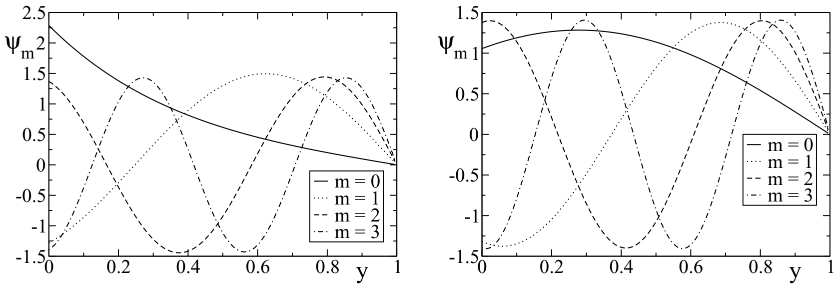


Fig. 5. The eigenfunctions $\psi_m(y)$ for $m = 0, 1, 2, 3$ and for $\Omega = -5.0$ (*left*) and $\Omega = 3.0$ (*right*).

This allows us to write the solution for $P(y,T)$ as

$$P(y,T) = e^{\frac{\Omega}{2}(y-y_0)} \sum_{m=0}^{\infty} e^{-\lambda_m T} \psi_m(y_0)\psi_m(y), \tag{45}$$

with eigenfunctions (35) and (39) of ground state ($m = 0$)

$$\psi_0(y) = \begin{cases} \sqrt{\dfrac{2}{1+\frac{\Omega}{2}\frac{1}{\tilde{k}_0^2+\Omega^2/4}}}\, \sin[\tilde{k}_0(1-y)], & \Omega > -2 \\ \sqrt{3}\,(1-y)\,, & \Omega = -2 \\ \sqrt{-\dfrac{2}{1+\frac{\Omega}{2}\frac{1}{-\kappa_0^2+\Omega^2/4}}}\, \sinh[\kappa_0(1-y)]\,, & \Omega < -2 \end{cases} \tag{46}$$

and all other eigenfunctions (35)

$$\psi_m(y) = \sqrt{\frac{2}{1+\frac{\Omega}{2}\frac{1}{\tilde{k}_m^2+\Omega^2/4}}}\, \sin[\tilde{k}_m(1-y)] \quad m = 1, 2, \ldots. \tag{47}$$

The eigenvalue of ground state ($m = 0$) is given by

$$\lambda_0 = \begin{cases} \tilde{k}_0^2 + \Omega^2/4\,, & \Omega > -2 \\ 1\,, & \Omega = -2 \\ -\kappa_0^2 + \Omega^2/4\,, & \Omega < -2 \end{cases} \tag{48}$$

and all others are

$$\lambda_m = \tilde{k}_m^2 + \Omega^2/4 \qquad m = 1, 2, \ldots, \tag{49}$$

where the wave numbers are calculated from transcendental Eq. (31)

$$\tilde{k}_0 : \quad \tan\tilde{k}_0 = -\frac{2}{\Omega}\tilde{k}_0 \qquad \Omega > -2 \tag{50}$$

$$\kappa_0 : \quad \tanh\kappa_0 = -\frac{2}{\Omega}\kappa_0 \qquad \Omega < -2 \tag{51}$$

$$\tilde{k}_m : \quad \tan\tilde{k}_m = -\frac{2}{\Omega}\tilde{k}_m \qquad m = 1, 2, \ldots. \tag{52}$$

The set of Fig. 6 illustrates the time evolution of probability density (45) choosing different parameter values Ω.

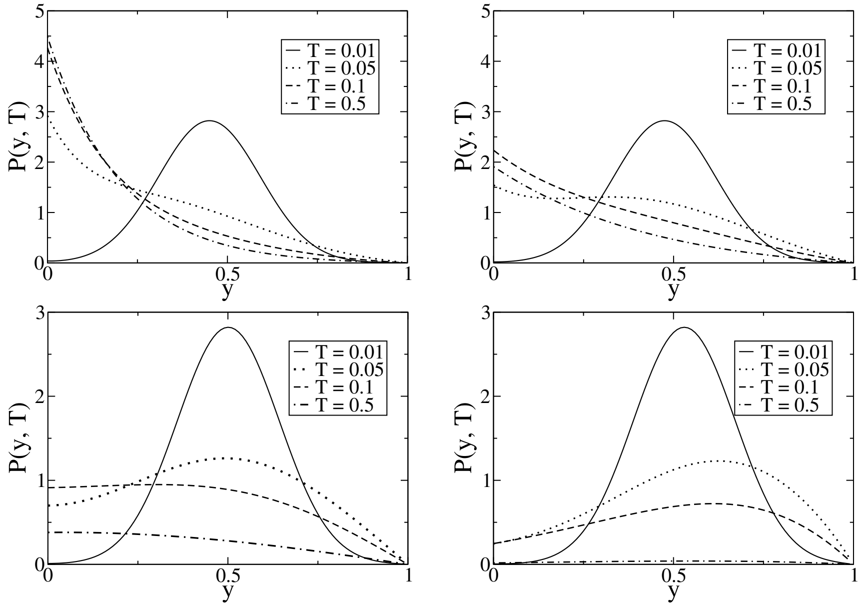


Fig. 6. The solution of drift-diffusion Fokker–Planck equation with initial condition $y_0 = 0.5$ for different values of the control parameter Ω, i.e. $\Omega = -5.0$ (*top left*), $\Omega = -2.5$ (*top right*), $\Omega = 0.1$ (*bottom left*), $\Omega = 3.0$ (*bottom right*).

3. FIRST PASSAGE TIME PROBABILITY DENSITY

It has been shown in previous sections that the probability density $P(y, T)$ is not normalized under given restrictions, i.e. reflected at $y = 0$ and absorbed at $y = 1$. Due to that fact, let us apply here the balance equation in the open system given in dimensionless variables by

$$\overline{\mathcal{P}}(T, y = 1) = -\frac{\partial}{\partial T} \int_0^1 P(y, T)\, dy \qquad (53)$$

which relates the probability $P(y, T)$ that the system is still in a state $y \in [0, 1]$ with the probability flux $\overline{\mathcal{P}}(T, y = 1)$ out of this interval at the right absorbing boundary $y = 1$ at time moment T. Hence, $\overline{\mathcal{P}}(T, y = 1)$ is the first passage time probability density (Choi and Fox, 2002; Fox and Choi, 2001; Redner, 2001). It can be calculated by using obtained results of previous section. The first passage time probability density distribution $\overline{\mathcal{P}}$ (breakdown probability density) depending on Ω reads as follows

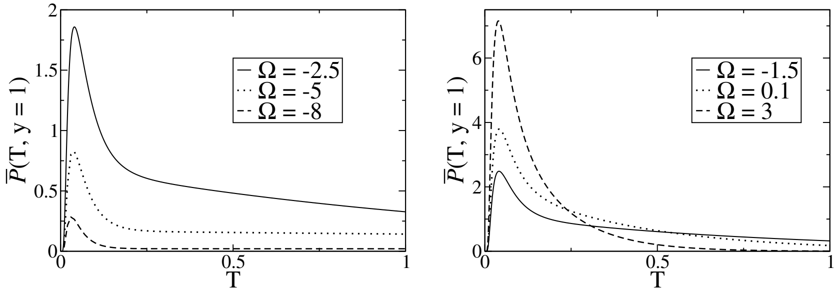


Fig. 7. The first passage time probability density distribution $\overline{\mathcal{P}}(T, y = 1)$ for $\Omega < -2$ (*left*) and $\Omega > -2$ (*right*).

1. $\Omega > -2$

$$\overline{\mathcal{P}}(T, y = 1) = 2e^{\frac{\Omega}{2}(1-y_0)} \sum_{m=0}^{\infty} \frac{e^{-(\tilde{k}_m^2+\Omega^2/4)T}}{1 + \frac{\Omega}{2}\frac{1}{\tilde{k}_m^2+\Omega^2/4}} \tilde{k}_m \sin[\tilde{k}_m(1 - y_0)] \tag{54}$$

2. $\Omega = -2$

$$\overline{\mathcal{P}}(T, y = 1) = e^{-(1-y_0)} \Bigg[3\,(1 - y_0)\, e^{-T} + 2 \sum_{m=1}^{\infty} \frac{e^{-\left(\tilde{k}_m^2+1\right)T}}{1 - \frac{1}{\tilde{k}_m^2+1}} \tilde{k}_m \sin[\tilde{k}_m(1 - y_0)] \Bigg] \tag{55}$$

3. $\Omega < -2$

$$\overline{\mathcal{P}}(T, y = 1) = 2e^{\frac{\Omega}{2}(1-y_0)} \times \Bigg[- \frac{e^{-\left(-\kappa_0^2+\Omega^2/4\right)T}}{1 + \frac{\Omega}{2}\frac{1}{-\kappa_0^2+\Omega^2/4}} \kappa_0 \sinh[\kappa_0(1 - y_0)] + \sum_{m=1}^{\infty} \frac{e^{-\left(\tilde{k}_m^2+\Omega^2/4\right)T}}{1 + \frac{\Omega}{2}\frac{1}{\tilde{k}_m^2+\Omega^2/4}} \tilde{k}_m \sin[\tilde{k}_m(1 - y_0)] \Bigg] \tag{56}$$

The outflow distribution $\overline{\mathcal{P}}(T, y = 1)$ is shown in Fig. 7 (with different values of dimensionless drift Ω) as well as in Fig. 8 (with different values of initial condition y_0).

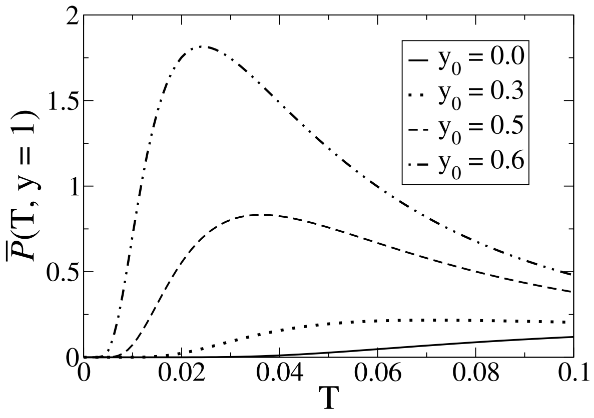


Fig. 8. Short time behaviour of first passage time probability density distribution $\overline{\mathcal{P}}(T, y = 1)$ for different initial conditions $0 \leq y_0 \leq 1$ showing time lag.

4. CUMULATIVE BREAKDOWN PROBABILITY

The probability that the absorbing boundary $y = 1$ is reached within certain observation time interval $0 \leq T \leq T_{\text{obs}}$ is given by the cumulative (breakdown) probability

$$W(\Omega, T = T_{\text{obs}}) = \int_0^{T_{\text{obs}}} \overline{\mathcal{P}}(T, y = 1)\, dT \tag{57}$$

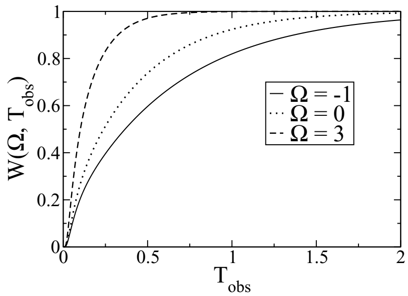
with $\overline{\mathcal{P}}(T, y = 1)$ from (53). For $T_{\text{obs}} \to \infty$ we have $W \to 1$. Generally, we obtain

1. $\Omega > -2$

$$W(\Omega, T_{\text{obs}}) = 2e^{\frac{\Omega}{2}(1-y_0)} \sum_{m=0}^{\infty} \frac{1 - e^{-\left(\tilde{k}_m^2 + \Omega^2/4\right) T_{\text{obs}}}}{\tilde{k}_m^2 + \Omega^2/4 + \Omega/2} \tilde{k}_m \sin[\tilde{k}_m(1 - y_0)] \tag{58}$$

2. $\Omega = -2$

$$W(\Omega, T_{\text{obs}}) = e^{-(1-y_0)} \Bigg[3\,(1 - e^{-T_{\text{obs}}})(1 - y_0) + 2 \sum_{m=1}^{\infty} \frac{1 - e^{-\left(\tilde{k}_m^2 + 1\right) T_{\text{obs}}}}{\tilde{k}_m} \sin[\tilde{k}_m(1 - y_0)] \Bigg]. \tag{59}$$



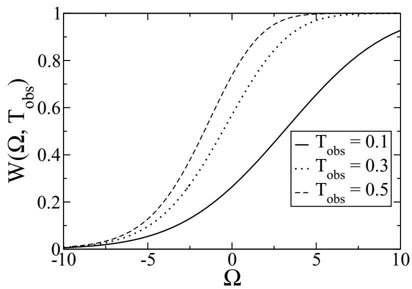


Fig. 9. The probability $W(\Omega, T_{\rm obs})$ (57) as function of observation time $T_{\rm obs}$ with fixed Ω (*left*) and vice versa (*right*).

3. $\Omega < -2$

$$W(\Omega, T_{\rm obs}) = 2\, e^{\frac{\Omega}{2}(1-y_0)} \times \left[- \frac{1 - e^{-\left(-\kappa_0^2+\Omega^2/4\right)T_{\rm obs}}}{-\kappa_0^2 + \Omega^2/4 + \Omega/2} \kappa_0 \sinh\left[\kappa_0(1-y_0)\right] + \sum_{m=1}^{\infty} \frac{1 - e^{-\left(\tilde{k}_m^2+\Omega^2/4\right)T_{\rm obs}}}{\tilde{k}_m^2 + \Omega^2/4 + \Omega/2} \tilde{k}_m \sin[\tilde{k}_m(1-y_0)] \right] \quad (60)$$

Figure 9 shows $W(\Omega, T_{\rm obs})$ as a function of observation time $T_{\rm obs}$ (*left*) as well as parameter dependence Ω (*right*).

5. LIMIT CASE FOR LARGE POSITIVE VALUES OF THE CONTROL PARAMETER

Consider parameter limit $\Omega \to +\infty$ which corresponds either to large positive drift v and/or large interval $b - a$, or to a small diffusion coefficient D. In this case, for a given m, the solution of the transcendental equation can be found in the form $\tilde{k}_m = \pi(m+1) - \varepsilon_m$, where ε_m is small and positive. From the periodicity property we obtain

$$\cos\tilde{k}_m = \cos(\pi(m+1) - \varepsilon_m) = -(-1)^m \cos(\varepsilon_m) = -(-1)^m + \mathcal{O}\left(\varepsilon_m^2\right)$$

$$\sin\tilde{k}_m = \sin(\pi(m+1) - \varepsilon_m) = (-1)^m \sin(\varepsilon_m) = (-1)^m \varepsilon_m + \mathcal{O}\left(\varepsilon_m^3\right).$$

By inserting this into the transcendental Eq. (30), we obtain

$$\varepsilon_m = \frac{2}{\Omega}\pi(m+1) + \mathcal{O}(\Omega^{-2}), \tag{61}$$

$$\sin(\tilde{k}_m) = \frac{2}{\Omega}(-1)^m \pi(m+1) + \mathcal{O}(\Omega^{-2}). \tag{62}$$

In this approximation the normalisation integral for large Ω and the initial condition $y_0 \to 0$ can be written as

$$\begin{aligned} I &= \int_0^\infty \overline{\mathcal{P}}(T, y=1)\, dT = 2e^{\Omega/2} \sum_{m=0}^{\infty} \frac{\tilde{k}_m \sin(\tilde{k}_m)}{\lambda_m + \Omega/2} \\ &\simeq e^{\Omega/2} \sum_{m=1}^{\infty} \frac{-4}{\Omega} \frac{(-1)^m (\pi m)^2}{\pi^2 m^2 + \Omega^2/4} = e^{\Omega/2} \sum_{m=-\infty}^{\infty} \frac{-2}{\Omega} \frac{(-1)^m (\pi m)^2}{\pi^2 m^2 + \Omega^2/4}. \end{aligned} \tag{63}$$

Further on we set $(-1)^m = e^{i\pi m}$ and, in a continuum approximation, replace the sum by the integral

$$I \simeq e^{\Omega/2} \int_{-\infty}^{\infty} \frac{-2}{\Omega} \frac{e^{i\pi m} (\pi m)^2}{\pi^2 m^2 + \Omega^2/4} dm. \tag{64}$$

Now we make an integration contour in the complex plane, closing it in the upper plane ($\mathrm{Im\, m} > 0$) at infinity where $|e^{i\pi m}|$ is exponentially small. According to the residue theorem, it yields

$$I = 2\pi i \sum_i \mathrm{Res(m_i)} = 2\pi \mathrm{iRes(m_0)}, \tag{65}$$

where $m_0 = \frac{i\Omega}{2\pi}$ is the location of the pole in the upper plane, found as a root of the equation $\pi^2 m^2 + \Omega^2/4 = 0$. According to the well-known rule, the residue is calculated by setting $m = m_0$ in the enumerator of (64) and replacing the denominator with its derivative at $m = m_0$. It gives the desired result $I = 1$, i.e., the considered approximation gives correct normalisation of outflow probability density $\overline{\mathcal{P}}(T, y = 1)$ at the right boundary.

The probability distribution function $P(y, T)$ given by (45) can also be calculated in such a continuum approximation. In this case the increment of wave numbers is

$$\Delta\tilde{k}_m = \tilde{k}_{m+1} - \tilde{k}_m = \pi + \varepsilon_m - \varepsilon_{m+1} \simeq \pi\left(1 - \frac{2}{\Omega}\right) \simeq \frac{\pi}{1 + 2/\Omega}. \tag{66}$$

Note that in this approximation for $\Omega \to \infty$ the normalisation constant R_m in (34) is related to the increment $\Delta\tilde{k}$ via

$$R_m^2 = \frac{2}{1 + \frac{\Omega}{2}\frac{1}{\tilde{k}_m^2 + \Omega^2/4}} \simeq \frac{2}{1 + 2/\Omega} \simeq \frac{2}{\pi}\Delta\tilde{k}_m. \tag{67}$$

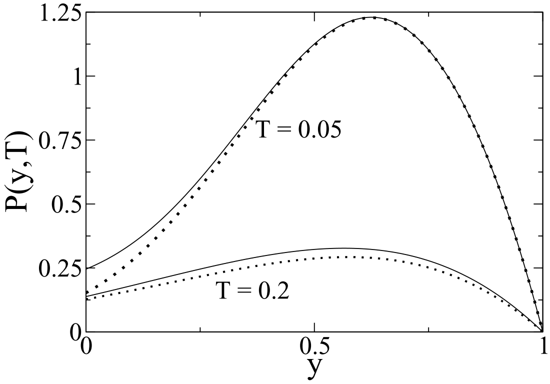


Fig. 10. Comparison of probability density $P(y, T)$ in drift–diffusion-dynamics with finite boundaries for two time moments. Parameter value is $\Omega = 3.0$; initial condition is $y_0 = 0.5$. The solid lines represent the exact result (45); dotted lines display the approximation (70).

Hence, the Eq. (45) for the probability density can be written as

$$\begin{aligned} P(y,T) &= 2e^{\frac{\Omega}{2}(y-y_0)} \sum_{m=0}^{\infty} R_m^2 e^{-\lambda_m T} \sin[\tilde{k}_m(1-y_0)] \sin[\tilde{k}_m(1-y)] \\ &\simeq \frac{2}{\pi} e^{\frac{\Omega}{2}(y-y_0)} \sum_{m=0}^{\infty} e^{-\left(\tilde{k}_m^2+\Omega^2/4\right)T} \sin[\tilde{k}_m(1-y_0)] \sin[\tilde{k}_m(1-y)] \Delta\tilde{k}_m \\ & . \end{aligned} \tag{68}$$

In the continuum approximation we replace the sum by the integral

$$\begin{aligned} P(y,T) &\simeq \frac{2}{\pi} e^{\frac{\Omega}{2}(y-y_0)} \int_0^\infty e^{-(\tilde{k}^2+\Omega^2/4)T} \sin[\tilde{k}(1-y_0)] \sin[\tilde{k}(1-y)]\, d\tilde{k} \\ &= \frac{1}{\pi} e^{\frac{\Omega}{2}(y-y_0)} \int_0^\infty e^{-(\tilde{k}^2+\Omega^2/4)T} (\cos[\tilde{k}(y-y_0)] - \cos[\tilde{k}(2-y-y_0)]) d\tilde{k} \\ & . \end{aligned} \tag{69}$$

In the latter transformation we have used the identity $\sin\alpha \sin\beta = \frac{1}{2}(\cos(\alpha-\beta) - \cos(\alpha+\beta))$. The resulting known integrals yield

$$P(y,T) \simeq \frac{1}{\sqrt{4\pi T}} e^{\frac{\Omega}{2}\left(y-y_0-\frac{\Omega}{2}T\right)} \left[e^{-\frac{(y-y_0)^2}{4T}} - e^{-\frac{(2-y-y_0)^2}{4T}} \right]. \tag{70}$$

The approximation (70) is shown in Fig. 10. For short enough times $4T \ll (2-y-y_0)^2$ the second term is very small. Neglecting this term, Eq. (70) reduces to the known exact solution for natural boundary conditions.

Based on (70), it is easy to calculate the probability flux

$$J(y, T) = \Omega P(y, T) - \frac{\partial}{\partial y} P(y, T) \tag{71}$$

and the first passage time distribution $\overline{\mathcal{P}}(T) = J(y = 1, T)$ which takes a particularly simple form

$$\overline{\mathcal{P}}(T) = \frac{1 - y_0}{\sqrt{4\pi T^3}} e^{-\frac{(1-y_0-\Omega T)^2}{4T}}. \tag{72}$$

The cumulative breakdown probability (57) is then

$$W(\Omega, T = T_{\text{obs}}) = \int_0^{T_{\text{obs}}} \frac{1 - y_0}{\sqrt{4\pi T^3}} e^{-\frac{(1-y_0-\Omega T)^2}{4T}} dT. \tag{73}$$

6. RELATIONSHIP TO STURM-LIOUVILLE THEORY

The particular drift-diffusion-problem over a finite interval with reflecting (*left*) and absorbing (*right*) boundaries belongs to the following general mathematical theory named after Jacques Charles Francois Sturm (1803–1855) and Joseph Liouville (1809–1882).

The classical Sturm–Liouville theory considers a real second-order linear differential equation of the form (Zettl, 2005)

$$-\frac{d}{dx}\left[p(x)\frac{d\psi}{dx}\right] + q(x)\psi = \lambda\, w(x)\psi \tag{74}$$

together with boundary conditions at the ends of interval $[a, b]$ given by

$$\alpha_1 \psi(x = a) + \alpha_2 \left.\frac{d\psi}{dx}\right|_{x=a} = 0, \tag{75}$$

$$\beta_1 \psi(x = b) + \beta_2 \left.\frac{d\psi}{dx}\right|_{x=b} = 0. \tag{76}$$

The particular functions $p(x), q(x), w(x)$ are real and continuous on the finite interval $[a, b]$ together with specified values at the boundaries. The aim of the Sturm–Liouville problem is to find the values of λ (called eigenvalues λ_n) for which there exist non-trivial solutions of the differential Eq. (74) satisfying the boundary conditions (75) and (76). The corresponding solutions (for such λ_n) are called eigenfunctions $\psi_n(x)$ of the problem.

Defining the Sturm–Liouville differential operator over the unit interval [0, 1] by

$$\mathcal{L}\psi = -\frac{d}{dx}\left[p(x)\frac{d\psi}{dx}\right] + q(x)\psi \tag{77}$$

and putting the weight $w(x)$ to unity ($w = 1$) the general equation (74) can precisely be written as eigenvalue problem

$$\mathcal{L}\psi = \lambda\psi \tag{78}$$

with boundary conditions (75)($a = 0$) and (76) ($b = 1$) written as

$$\mathcal{B}_0\psi = 0 \qquad \mathcal{B}_1\psi = 0. \tag{79}$$

Assuming a differentiable positive function $p(x) > 0$ the Sturm–Liouville operator is called regular and it is self-adjoint to fulfil

$$\int_0^1 \mathcal{L}\psi_1 \cdot \psi_2 = \int_0^1 \psi_1 \cdot \mathcal{L}\psi_2. \tag{80}$$

Any self–adjoint operator has real nonnegative eigenvalues $\lambda_0 < \lambda_1 < \cdots < \lambda_n < \cdots \to \infty$. The corresponding eigenfunctions $\psi_n(x)$ have exact n zeros in (0, 1) and form an orthogonal set

$$\int_0^1 \psi_n(x)\psi_m(x)\,dx = \delta_{mn}. \tag{81}$$

The eigenvalues λ_n of the classical Sturm–Liouville problem (74) with positive function $p(x) > 0$ as well as positive weight function $w(x) > 0$ together with separated boundary conditions (75) and (76) can be calculated by the following expression

$$\lambda_n \int_a^b \psi_n(x)^2 w(x)dx = \int_a^b [p(x)\,(d\psi_n(x)/dx)^2 + q(x)\psi_n(x)^2]dx \\ - \left|p(x)\psi_n(x)\,(d\psi_n(x)/dx)\right|_a^b. \tag{82}$$

The eigenfunctions are mutually orthogonal ($m \neq n$) and usually normalized ($m = n$)

$$\int_a^b \psi_n(x)\psi_m(x)w(x)\,dx = \delta_{mn} \tag{83}$$

known as orthogonality relation (similar to (81).

Comming back to the original drift-diffusion problem written in dimensionless variables over unit interval $0 \leq y \leq 1$ and recalling (17 the separation constant λ appears in the following differential equation

$$-\frac{d^2\psi(y)}{dy^2} + \frac{\Omega^2}{4}\psi(y) = \lambda\psi(y) \tag{84}$$

which can be related to the regular Sturm–Liouville eigenvalue problem via $p(y) = 1 > 0$; $w(y) = 1 > 0$ and $q(y) = \Omega^2/4$.

The boundary conditions given by (23) and (26) can be expressed as

$$\frac{\Omega}{2} \cdot \psi(y=0) + (-1) \cdot \left.\frac{d\psi}{dy}\right|_{y=0} = 0, \tag{85}$$

$$1 \cdot \psi(y=1) + 0 \cdot \left.\frac{d\psi}{dy}\right|_{y=1} = 0 \tag{86}$$

in agreement with (75) and (76).

The up-to-now unknown separation constant λ has a spectrum of real positive eigenvalues which can be calculated using (82) from

$$\lambda_n = \int_0^1 \left[\left(\frac{d\psi_n(y)}{dy} \right)^2 + \frac{\Omega^2}{4} \psi_n(y)^2 \right] dx \; - \; \left| \psi_n(y) \frac{d\psi_n(y)}{dy} \right|_0^1 \tag{87}$$

taking into account normalized orthogonal eigenfunction (83)

$$\int_0^1 \psi_n(y)\psi_m(y)\, dy = \delta_{mn}. \tag{88}$$

7. CONCLUSIONS

The presented paper shows the analytical method how to solve drift-diffusion initial-boundary-value problem for the case of reflecting and absorbing boundaries (Choi and Fox, 2002; Fox and Choi, 2001; Linetsky, 2004; Redner, 2001; Linetsky, 2005). On the basis of Sturm–Liouville theory, the set of eigenvalues with corresponding eigenfunctions has been found. Here we have paid our attention to wave number calculations from transcendental equations. The equations have been solved numerically by Newton method. The main problem which has been solved was the dependence of obtained results on drift value, i.e. different cases of control parameter $\Omega < -2$, $\Omega = -2$ and $\Omega > -2$. First case of $\Omega < -2$ corresponds to the situation when it is difficult and probably impossible, with significant small probability and for long times only, to leave the interval due to the large negative value of drift. The case of $\Omega = -2$ has been considered as limit case and the corresponding solution has been found. The opposite case of $\Omega > -2$ shows the usual situation when the system reaches the right border relatively fast. As application, the first passage time distribution as well as the cumulative probability have been calculated. The case of large positive values of Ω has been investigated in detail and has been obtained as approximation.

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