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L.N. CHRISTOPHOROV

Bogolyubov Institute for Theoretical Physics, Natl. Acad. Sci. Ukraine
(14b, Metrologichna Str., Kyiv 03143, Ukraine; e-mail: lchrist@bitp.kyiv.ua)

CONTINUOUS TIME RANDOM WALKS WITH RESETTING IN A BOUNDED CHAIN

The model of classical random walks with Poissonian resetting in a one-dimensional lattice is analyzed in detail in its general version. A special emphasis is made on the resetting effects that emerge due to the variety of arbitrary initial and boundary conditions. A quantum analog of the model is also discussed.

Keywords: random walk, low-dimensional lattices, stochastic resetting, resetting expediency, quantum walks.

1. Introduction

If there is a lack of information about the location of the target, the search is usually carried out randomly. If the search area is large (unlimited), there are many trajectories that make the search ineffective or unsuccessful at all. The idea of increasing the efficiency of search by resetting (regular or random interruption of the search by returning to a certain state from which a new random search starts) is aimed at eliminating such detrimental trajectories. In fact, this way of optimizing the search is widespread, from the behavior of living organisms to the functioning of (bio)molecules, enzymes, in particular.

Although the systematic study of the effects of resetting began quite recently, it quickly turned into a flourishing branch of the theory of stochastic processes. After the cornerstone work [1], where the Poisson resetting was studied in the basic stochastic model – diffusion along an infinite line – numerous works (still mostly theoretical) on the effects of various resetting types in different dimensions and geometries, in the presence of different potentials, *etc.*, have appeared, see recent reviews [2–5]. The vast majority of these works concerns spatially continuous models, although their discrete analogs (random walks in lattices or networks) are no less important. For the latter, there were practically no exact results even in one dimension [6]. Even the direct discrete analog of the model in [1] – resetting random walks in a one-dimensional lattice – has been considered quite recently [7–9]. Apart from exact expressions for the characteristics of the main resetting effects (the emergence of a nonequilibrium stationary state, the possibility of minimizing the mean first passage time, MFPT), the influence of the chain finiteness and of various boundary conditions on some observables (unconditional and conditional MFPTs, splitting probabilities) was described.

The present paper summarizes the results obtained in [7–9], supplementing them with the study of the coefficient of variation (CV) of the first passage time. Except its general importance, the CV value for the underlying (i.e., without resetting) process allows one to judge the expediency of introducing the resetting. The obtained conditions of beneficial resetting differ from the known "universal" criterion in the general case. Finally, resetting in quantum walks is briefly discussed.

2. Theoretical Framework

2.1. Solution to the evolution equation

Classical symmetrical random walks on the nodes n ($0 \le n \le N$) of a regular chain with sinks on its edges and the stochastic Poissonian resetting to node n_r is described by the following evolution equation for node occupation probabilities $\rho_n(t)$'s:

$$\frac{\mathrm{d}\rho_n}{\mathrm{d}t} = k\,(\rho_{n-1} - 2\rho_n + \rho_{n+1}) - r\rho_n + \delta_{n_r n} r \sum_{m=0}^{N} \rho_m + k\rho_0\delta_{0n} + k\rho_N\delta_{Nn} - q_0\rho_0\delta_{0n} - q_N\rho_N\delta_{Nn}, \quad (1)$$

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with the initial condition $\rho_n(0) = \delta_{n_0 n}$. Here, k is the rate of jumps between adjacent nodes and r is that of Poisson resetting; q_0 and q_N are the corresponding sink intensities. It is implicitly assumed that the targets are situated at the nodes $n = -1,\ N+1$. The solution to Eq. (1) in Laplace transforms $\tilde{\rho}_n(p) = \int_0^\infty e^{-p\,t}\rho_n(t)\mathrm{d}\,t$ is found in [9]. In particular, for the terminal nodes, it reads:

$$\begin{aligned}\tilde{\rho}_0(p|n_0,n_r) &= B_0(p)/2kp\Delta(p),\\ \tilde{\rho}_N(p|n_0,n_r) &= B_N(p)/2kp\Delta(p),\end{aligned} \tag{2}$$

where

$$\begin{aligned}B_0(p) &= \left(p\tilde{I}_{n_0} + r\tilde{I}_{n_r}\right)\left\{1 - \frac{1}{2}\left[(1-\lambda_N)\,\tilde{I}_0 - \tilde{I}_1\right]\right\} + \\ &+ \frac{1}{2}\left(p\tilde{I}_{N-n_0} + r\tilde{I}_{N-n_r}\right)\left[(1-\lambda_N)\,\tilde{I}_N - \tilde{I}_{N+1}\right] + \\ &+ \frac{1}{2}r\lambda_N\left(\tilde{I}_{n_0}\tilde{I}_{N-n_r} - \tilde{I}_{n_r}\tilde{I}_{N-n_0}\right),\end{aligned} \tag{3a}$$

$$\begin{aligned}B_N(p) &= \left(p\tilde{I}_{N-n_0} + r\tilde{I}_{N-n_r}\right) \times \\ &\times \left\{1 - \frac{1}{2}\left[(1-\lambda_0)\,\tilde{I}_0 - \tilde{I}_1\right]\right\} + \\ &+ \frac{1}{2}\left(p\tilde{I}_{n_0} + r\tilde{I}_{n_r}\right)\left[(1-\lambda_0)\,\tilde{I}_N - \tilde{I}_{N+1}\right] + \\ &+ \frac{1}{2}r\lambda_0\left(\tilde{I}_{N-n_0}\tilde{I}_{n_r} - \tilde{I}_{n_0}\tilde{I}_{N-n_r}\right).\end{aligned} \tag{3b}$$

Here $\lambda_{0,N} = q_{0,N}/k$ and

$$\begin{aligned}\Delta(p) &= \left\{1 - \frac{1}{2}\left[(1-\lambda_0)\,\tilde{I}_0 - \tilde{I}_1 - \frac{r\lambda_0}{p}\tilde{I}_{n_r}\right]\right\} \times \\ &\times \left\{1 - \frac{1}{2}\left[(1-\lambda_N)\,\tilde{I}_0 - \tilde{I}_1 - \frac{r\lambda_N}{p}\tilde{I}_{N-n_r}\right]\right\} - \\ &- \frac{1}{4}\left[(1-\lambda_0)\,\tilde{I}_N - \tilde{I}_{N+1} - \frac{r\lambda_0}{p}\tilde{I}_{N-n_r}\right] \times \\ &\times \left[(1-\lambda_N)\,\tilde{I}_N - \tilde{I}_{N+1} - \frac{r\lambda_N}{p}\tilde{I}_{n_r}\right].\end{aligned} \tag{4}$$

In Eqs. (3)–(4), the Laplace transforms of modified Bessel functions $\tilde{I}_m(s) = \tilde{I}_{-m}(s) = \left(s - \sqrt{s^2-1}\right)^{|m|}/\sqrt{s^2-1}$ are taken with $s = 1 + (p+r)/2k$. Solution (2) corresponds to the most general problem formulation and becomes visibly simpler in the "symmetrical" cases ($q_0 = q_N = k$), or for semi-infinite or infinite chains, and also in the popular case of resets to the initial node ($n_0 = n_r$) [7–9]. Laplace transforms (2) can hardly be inverted; nevertheless, they are sufficient for calculating practically all relevant process observables. Before proceeding to the latter, we note that these calculations can be significantly simplified by using the so-called renewal equations [2, 4].

2.2. Renewal equations

These equations relate the solutions of resetting problems with the solutions of those without resetting (the corresponding processes without resetting are often termed "underlying"). For example, when the probability of the walker's presence in the chain is conserved, $\sum_n \rho_n(t) = 1$ (in particular, in an infinite chain without sinks), the solution can be written at once,

$$\rho_n\left(t|n_0,n_r,r\right) = e^{-rt}\rho_{u,n}\left(t|n_0\right) + r\int_0^t e^{-r\tau}\rho_{u,n}\left(\tau|n_r\right)\mathrm{d}\tau, \tag{5}$$

from simple considerations. Namely, the first term in the r.h.s. of Eq. (5) is the probability e^{-rt} of no resets till time t, multiplied by the propagator of underlying process $\rho_{u,n}\left(t|n_0\right)$ started at node n_0. The second term is the probability $re^{-r\tau}$ of the last reset at time τ multiplied by the propagator of underlying process $\rho_{u,n}\left(\tau|n_r\right)$ started at node n_r in the time interval $(t-\tau,\ t)$. Equation (5) shows, in particular, that the resetting causes a non-zero stationary distribution (so-called non-equilibrium steady state, NESS)

$$\rho_n^{\mathrm{st}}\left(n_r,r\right) = r\int_0^\infty e^{-rt}\rho_{u,n}\left(t|n_r\right)\mathrm{d}\,t, \tag{6}$$

which does not depend on the initial conditions. For an infinite chain, the underlying process propagator is well known, $\rho_{u,n}\left(t|n_m\right) = e^{-2kt}I_{|n-m|}\left(2kt\right)$, so that $\rho_n^{\mathrm{st}}\left(n_r,r\right) = (r/2k)\,\tilde{I}_{|n-n_r|}\left(1+r/2k\right)$ [7, 8], what is a discrete analog of its continuous counterpart $\rho_r^{\mathrm{st}}\left(x|x_r\right) = \sqrt{r/4D}\exp\left(-|x-x_r|\sqrt{r/D}\right)$ with a cusp at $x = x_r$ [1]. However, the asymptotic $r \to \infty$ is now power-like, $\rho_n^{\mathrm{st}}(n_r, r\to\infty) \simeq (r/k)^{-|n-n_r|}$.

In the presence of absorption/decay processes the last renewal equation is formulated for the survival probability $Q(t) = \sum_n \rho_n(t)$. From considerations similar to those used for deriving Eq. (5), one can deduce that

$$Q_r\left(t|n_0,n_r\right) = e^{-rt}Q_u\left(t|n_0\right) + r\int_0^t e^{-r\tau}Q_r\left(t-\tau|n_0,n_r\right)Q_u\left(\tau|n_r\right)\mathrm{d}\,\tau, \tag{7}$$

where Q_u (Q_r) corresponds to the underlying (resetting) process, respectively.

2.3. Expressions for observables

The Laplace transformation of Eq. (7) gives:

$$\tilde{Q}_r(p|n_0,n_r) = \frac{\tilde{Q}_u(p+r|n_0)}{1 - r\tilde{Q}_u(p+r|n_r)}. \quad (8)$$

Eq. (8) greatly simplifies calculations of the main observables (MFPTs and CVs). The survival probability $Q(t)$ is directly related to the distribution $f(t)$ of first passage times: $Q(t) = 1 - \int_0^t f(t')\,\mathrm{d}t'$, or, in Laplace transforms, $\tilde{Q}(p) = \left[1 - \tilde{f}(p)\right]/p$. The corresponding MFPT, in its turn, is simply $\int_0^\infty t f(t)\mathrm{d}t = \tilde{Q}(p=0)$. Then from Eq. (8), it follows that the MFPT $\langle T_r\rangle$ in the presence of resetting reads:

$$\langle T_r(n_0,n_r)\rangle = \frac{\tilde{Q}_u(r|n_0)}{1 - r\tilde{Q}_u(r|n_r)} = \frac{1-\tilde{f}_u(r|n_0)}{r\tilde{f}_u(r|n_r)}. \quad (9)$$

This way of calculating MFPT is much easier than finding the derivative of $\tilde{f}_r(p)$ in the limit $p \to \to 0$ according to the standard definition $\langle T^k\rangle = = (-1)^k \left[\mathrm{d}^k \tilde{f}(p)/\mathrm{d}p^k\right]_{p=0}$. Calculating CV becomes visibly simpler, as well. In terms of $\tilde{f}_u$ and $\tilde{f}_r$, Eq. (8) can be re-written as

$$\tilde{f}_r(p|n_0,n_r) = \frac{p\tilde{f}_u(p+r|n_0) + r\tilde{f}_u(p+r|n_r)}{p + r\tilde{f}_u(p+r|n_r)}. \quad (10)$$

Derivation of (10) with respect to p leads to Eq. (9), while the second derivative taken at $p=0$ is the mean square of the first passage time and reads:

$$\left.\frac{\mathrm{d}^2\tilde{f}_r(p|n_0,n_r)}{\mathrm{d}p^2}\right|_{p=0} = \left\langle T_r^2(n_0,n_r)\right\rangle = = 2\frac{\left(1-\tilde{f}_u(r|n_0)\right)\left(1+r\frac{\mathrm{d}\tilde{f}_u(r|n_r)}{\mathrm{d}r}\right)+r\tilde{f}_u(r|n_r)\frac{\mathrm{d}\tilde{f}_u(r|n_0)}{\mathrm{d}r}}{r^2\left(\tilde{f}_u(r|n_r)\right)^2}, \quad (11)$$

so that the standard deviation is

$$\sigma_r(n_0,n_r) = \left[\left\langle T_r^2(n_0,n_r)\right\rangle - \langle T_r(n_0,n_r)\rangle^2\right]^{1/2} = = \left[1 + 2r\left(\frac{\mathrm{d}\tilde{f}_u(r|n_r)}{\mathrm{d}r} + \tilde{f}_u(r|n_r)\frac{\mathrm{d}\tilde{f}_u(r|n_0)}{\mathrm{d}r} - \tilde{f}_u(r|n_0)\frac{\mathrm{d}\tilde{f}_u(r|n_r)}{\mathrm{d}r}\right) - \tilde{f}_u^2(r|n_0)\right]^{1/2} \Big/ \left(r\tilde{f}_u(r|n_r)\right)$$

and the coefficient of variation –

$$\mathrm{CV}_r(n_0,n_r) = \frac{\sigma_r(n_0,n_r)}{\langle T_r(n_0,n_r)\rangle} = = \left[1 + 2r\left(\frac{\mathrm{d}\tilde{f}_u(r|n_r)}{\mathrm{d}r} + \tilde{f}_u(r|n_r)\frac{\mathrm{d}\tilde{f}_u(r|n_0)}{\mathrm{d}r} - \tilde{f}_u(r|n_0)\frac{\mathrm{d}\tilde{f}_u(r|n_r)}{\mathrm{d}r}\right) - \tilde{f}_u^2(r|n_0)\right]^{1/2} \Big/ \left(1 - \tilde{f}_u(r|n_r)\right). \quad (12)$$

Thus, Eqs. (11), (12) contain only the first derivatives of distribution $\tilde{f}_u$ for the underlying process, taken at $p = r$. Note that, in the obtained expressions (9), (12) for observables, the possibility of different initial and resetting nodes ($n_0 \neq n_r$) is preserved, while they often ignore it, assuming $n_0 = n_r$ 'by default'. However, this distinction does matter except the stationary distributions like (6). For example (see also below), suppose that the optimal value r^*, which minimizes MFPT $\langle T_r\rangle$, exists. This means that $(\mathrm{d}/\mathrm{d}r)\langle T_r(n_0,n_r)\rangle|_{r^*} = 0$. Differentiating Eq. (9), one has:

$$r^*\left[\frac{\mathrm{d}\tilde{f}_u(r|n_r)}{\mathrm{d}r} + \tilde{f}_u(r|n_r)\frac{\mathrm{d}\tilde{f}_u(r|n_0)}{\mathrm{d}r} - \tilde{f}_u(r|n_0)\frac{\mathrm{d}\tilde{f}_u(r|n_r)}{\mathrm{d}r}\right]_{r^*} = = \tilde{f}_u(r^*|n_r)\left[\tilde{f}_u(r^*|n_0) - 1\right].$$

Using this condition in (12) leads to the following variation coefficient under optimal resetting:

$$\mathrm{CV}_{r^*}(n_0,n_r) = = \frac{\left[1+2\tilde{f}_u(r^*|n_r)\left(\tilde{f}_u(r^*|n_0) - 1\right) - \tilde{f}_u^2(r^*|n_0)\right]^{1/2}}{1-\tilde{f}_u(r^*|n_0)},$$

which turns into the 'universal' property $\mathrm{CV}_{r^*} = 1$ [10] in the case $n_0 = n_r$ only.

2.4. When is the resetting advisable?

The coefficient of variation is often associated with the condition of the expediency of the resetting, i.e., with the ability of the latter to improve the search by diminishing the MFPT. Usually, this condition is derived by expanding the MFPT in a series near $r = 0$ [4, 11]:

$$\langle T_r(n_0, n_r)\rangle = a_0 + a_1 r + a_2 r^2 + \dots . \tag{13}$$

Obviously, a_0 is the MFPT in the absence of a resetting, $\langle T(n_0)\rangle$. It is also clear that the resetting is beneficial, if $\langle T_r(n_0, n_r)\rangle_{r\to 0}$ is less than $\langle T(n_0)\rangle$, that is, if $a_1 < 0$. Expand the r.h.s. of Eq. (9) near $r = 0$, bearing in mind that $\tilde{f}_u(0|n) = 1$ and $\left(\mathrm{d}^k/\mathrm{d}r^k\right)\tilde{f}_u(r|n)\,|_{r=0} = (-1)^k \left\langle T^k(n)\right\rangle$:

$$\langle T_{r\to 0}(n_0, n_r)\rangle = \langle T(n_0)\rangle + [\langle T(n_r)\rangle \langle T(n_0)\rangle - \\ - \frac{1}{2}\left\langle T^2(n_0)\right\rangle]r + O\left(r^2\right). \tag{14}$$

Comparing (13) and (14) gives the sought beneficial condition:

$$\langle T(n_r)\rangle \langle T(n_0)\rangle < \frac{1}{2}\left\langle T^2(n_0)\right\rangle . \tag{15}$$

If nodes n_0 and n_r coincide, then condition (15) turns into $\langle T(n_0)\rangle^2 < (1/2)\left\langle T^2(n_0)\right\rangle$, or

$$\mathrm{CV}_u^2(n_0) > 1. \tag{16}$$

Condition (16) that implies a sufficiently wide (fat-tailed) distribution $f_u(t)$ of first passage times in the underlying process is often proposed as 'universal' (or at least sufficient, see, e.g., [4, 11]). In fact, it (as well as aforementioned condition $\mathrm{CV}_{r^*} = 1$) is such only in the case of the resetting to the initial node (what is practically never noted). The general "benefit criterion", as it follows from (15), reads:

$$\mathrm{CV}_u^2(n_0) > 2\frac{\langle T(n_r)\rangle}{\langle T(n_0)\rangle} - 1. \tag{17}$$

In other words, the cases are possible when $\mathrm{CV}_u^2 > 1$, but the resetting is not beneficial, and vice versa, it is advisable, while $\mathrm{CV}_u^2 < 1$ (see Section 3 for an example). In both cases, nevertheless, criterion (17) remains valid.

2.5. Splitting probabilities

Now, we turn to calculating the observables on the base of solutions (2), bearing in mind that $f(t)$ is nothing but $q_0\rho_0(t)$ or $q_N\rho_N(t)$ in the cases of a single sink at node 0 or N, respectively. If there are two sinks at both edges (reaching any of the two targets), then $f(t)$ is simply $q_0\rho_0(t) + q_N\rho_N(t)$. We are interested in MFPT (9) and CV (12) for which we can use $\tilde{f}_u(p)$, that is, solutions (2)–(4) with $r = 0$. In the case of a finite chain with two sinks at its edges, there exist additional important observables, such as the splitting probabilities W_0 and W_N (cf. [12, 13]) of the exit through the corresponding terminal node; obviously, $W_0 + W_N = 1$. They are simply

$$W_0 = q_0\int_0^\infty \rho_0(t)\mathrm{d}t = q_0\tilde{\rho}_0(p\to 0), \\ W_N = q_N\int_0^\infty \rho_N(t)\mathrm{d}t = q_N\tilde{\rho}_N(p\to 0). \tag{18}$$

In addition, apart from the unconditional MFPT, there exist its conditional analogs $\langle t_0\rangle$ and $\langle t_N\rangle$ related to the times of reaching the corresponding target (cf. [14]). Their distribution functions are the corresponding normalized flows:

$$f_0(t) = \frac{q_0\rho_0(t)}{\int_0^\infty q_0\rho_0(t)\mathrm{d}t} = \frac{\rho_0(t)}{\tilde{\rho}_0(0)}, \\ f_N(t) = \frac{q_N\rho_N(t)}{\int_0^\infty q_N\rho_N\mathrm{d}t} = \frac{\rho_N(t)}{\tilde{\rho}_N(0)},$$

so that [9]

$$\langle t_0\rangle = -\left.\frac{\mathrm{d}\ln\tilde{\rho}_0(p)}{\mathrm{d}p}\right|_{p=0}, \quad \langle t_N\rangle = -\left.\frac{\mathrm{d}\ln\tilde{\rho}_N(p)}{\mathrm{d}p}\right|_{p=0}. \tag{19}$$

3. Calculation of Observables in Particular Cases

In this section, we list the results for several important illustrative versions of our rather multi-parametric system defined by Eq. (1) [1]. A special emphasis is made on the new features of observables due to the possible distinctions between n_0 and n_r (and also between q_0 and q_N). It is useful to begin with the case of an infinite chain. This is practically the only case for which one can obtain the explicit time evolution (5). In spite of the absence of terminal targets, one can pose a question about MFPT, implying the first reaching of a certain (say, zeroth) node after starting at node n_0. However, finding the corresponding $f_r(t)$ implies the solution of an auxiliary problem

[1] Partially, they were presented in works [7–9].

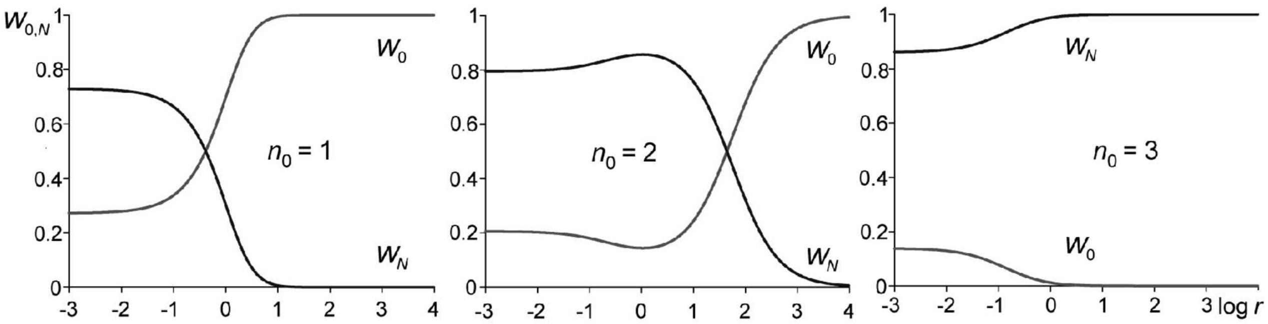


Fig. 1. Splitting probabilities for $N = 5$, $k = 0.5$, $q_0 = 0.05$, $q_N = 5$; $n_0 = n_r$ [9]

for a *semi-infinite* chain ($n = 0, 1, 2, ...$) with a sink $q_0 = k$ at the zeroth node and an implied target at node $n = -1$, so that $f_r(t|n_0, n_r) = k\rho_0(t|n_0, n_r, r)$. In this case, following the receipt of Section 2, we can obtain [9]:

$$\langle T_r(n_0, n_r)\rangle = \frac{1}{r}\left(\phi^{n_0+1} - 1\right)\phi^{n_r-n_0}, \tag{20}$$

where $\phi = 1 + (r/2k) + \sqrt{(r/k) + (r/2k)^2}$. It is easy to check that this MFPT is infinite both for $r = 0$ (what is well known for diffusion along an infinite line and remains valid for an infinite chain) and for $r \to \infty$[2]. Consequently, it has a minimum at some finite optimal r^*. This is a second (after the emergence of the non-equilibrium steady state) main resetting effect. In comparison with the case $n_0 = n_r$, MFPT (20) contains a factor $\phi^{n_r-n_0}$, and, since $\phi > 1$, it increases (if $n_r > n_0$) or decreases (if $n_r < n_0$) the MFPT for identical n_r, n_0. But even in the case where n_0 is close (or even equal!) to zero and $n_r \gg n_0$, there exists the optimal resetting rate r^* minimizing the MFPT – so important is the elimination of detrimental trajectories to the infinite side of the chain. In passing, we note that our consideration is applicable in the case of an initial node adjacent to the target, whereas such a case is impossible in the continuous model (there is no analog of an adjacent point).

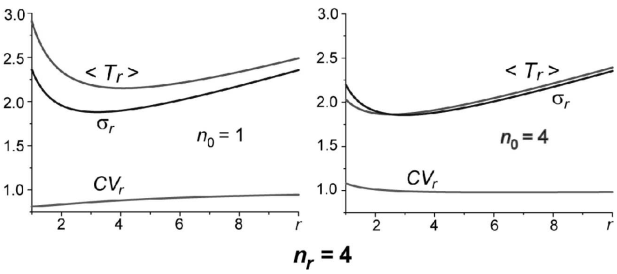
Proceed to finite chains. First, consider symmetrical boundary conditions, i.e., $q_0 = q_N$. Here, calculations of the splitting probabilities (18) are straightforward since we simply take solutions (2) in the limit $p \to 0$. If, in addition, $n_0 = n_r$, then, with r growing, domination of one (whose edge is closer to n_r) of W_0, W_N becomes only stronger, so that, for $r \to \infty$, the corresponding splitting probability reaches 1, while the other – 0. As for the MFPT, its behavior is more complex. In short chains and for not so intense sinks, the optimal resetting rate r^* could be absent (for $N = 2$, r^* does not exist for any q_0 [7, 8]). This essentially differs from the results in the corresponding continuous model in which r^* always exists for n_0 close to any of the interval ends [14].

The difference of the resetting and initial nodes, $n_0 \neq n_r$, causes an interesting effect of inversions of the splitting probabilities. For instance, in a chain with seven nodes ($N = 6$), $W_0(r \to \infty|n_0, n_r = 2) \to 1$ for any n_0 (because n_r is closer to node 0). However, for $n_0 \geqslant 4$, when $W_0(r = 0|n_0, n_r = 2) < W_N(r = 0|n_0, n_r = 2)$, increasing r eventually leads to inverting this inequality. The MFPT behavior is also changed. While, with identical $n_0 = n_r$, the optimal rate r^* exists for $n_0 = 1, 5$ (those close to the edges) only, here, for example, for $n_r = 1$, it exists for any n_0 (except, of course, terminal nodes), see [9] for corresponding graphics.

Now, consider the asymmetrical boundary conditions, $q_0 \neq q_N$. Here, interesting effects emerge even in short chains with identical initial and resetting nodes (see the example for $N = 2$ in [7, 8]). Take, for instance, the case $N = 5$ with q_0 and q_N differing by two orders. Placing n_0 closer to the left end ($n_0 = 0, 1, 2$), one has a pronounced inversion of W_0 and W_N with r growing; however, for $n_0 \geqslant 3$, it disappears (see Fig. 1). The possibility of such inversion as a resetting control ability can be important in various applications.

The MFPT in such a chain with six nodes exhibits four qualitatively different behaviors with r growing, depending on n_0 (see Fig. 8 in [9]).

[2] Except the case $n_r = 0$ when, obviously, $\langle T_{r\to\infty}(n_0, n_r = 0)\rangle = 1/k$.



a *b*

Fig. 2. MFPT, standard deviation and coefficient of variation as functions of r for a finite chain with $N = 5$, $k = 1$, $q_0 = 0.1$, $q_N = 10$ and $n_r = 4$. $n_0 = 1$ (*a*); $n_0 = n_r = 4$ (*b*)

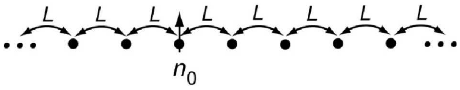


Fig. 3. Tight binding model. Initial condition: the walker is on node n_0

The difference of n_0 and n_r does not add new shapes of $W_{0,N}(r)$ except some details. For instance, for $N = 5$, the placement $n_r = 2$ permits inversion for any n_0 from 0 to 5, but $n_r = 3$ eliminates it for all n_0. The unconditional MFPT exhibits a more various behavior: with $n_r = 2$, r^* is absent for all n_0, while, with $n_r = 4$, it appears for any n_0. For different conditional MFPT behaviors, see the examples in [9].

Now, turn to the coefficient of variation and "benefit criterion" (17). The plots of calculated CV_r together with that of σ_r and $\langle T_r\rangle$ are presented in Fig. 2 for a chain with $N = 5$, $k = 1$, $q_0 = 0.1$, $q_N = 10$ and $n_r = 4$ in the two illustrative cases: for non-coincident $n_0 = 1$ and coincident $n_0 = 4$.

One can see that, in both cases, r^* exists, and the resetting is beneficial. However, it follows from the left plot that $\langle T_r(1,4)\rangle$ is always larger than $\sigma_r(1,4)$, including the case $r = 0$. Calculations give $\langle T(1)\rangle = \langle T_{r=0}(1,4)\rangle = 10.364$ whereas $\sigma_u(1) = \sigma_{r=0}(1,4) = 9.110$, so that $\mathrm{CV}_u(1) = \mathrm{CV}_{r=0}(1,4) = 0.879 < 1$. According to the "universal" criterion $\mathrm{CV}_u^2 < 1$, the resetting should not be beneficial; nevertheless, in this case of $n_0 \neq n_r$, it is, and criterion (16) loses its universality,, as well as the relationship $\mathrm{CV}_{r^*} = 1$. However, the obtained above improved criterion (17) remains valid. Indeed, $\langle T(4)\rangle = \langle T_{r=0}(4,4)\rangle = 4.464$, and it is easy to check that inequality (17) holds. At the same time, for coincident $n_0 = n_r = 4$, as can be seen from the right plot in Fig. 2, $\mathrm{CV}_u^2 > 1$, and criterion (16), as well as the "universal" relationship $\mathrm{CV}_{r^*} = 1$, works, since, for the optimal value $r^* = 2.53$ the values of the MFPT and standard deviation coincide, $\sigma_{r^*=2.53}(4,4) = \langle T_{r^*=2.53}(4,4)\rangle = 1.862$.

With this, we finish a short list of the peculiarities of classical random walks in a regular chain, which appear due to the Poissonian resetting, and attempt to consider quantum walks in the same structure.

4. Quantum Walks

One can try to consider the resetting influence on quantum migration along a 1D lattice. For this, the tight binding model with the Hamiltonian

$$H = L\sum\nolimits_n \left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right) \tag{21}$$

looks as a proper starting point. Here, $|n\rangle$ represents a particle-walker state localized on the node n, and L is the integral of jumps between the nearest neighbours, see Fig. 3. It is supposed that $\langle m|n\rangle = \delta_{mn}$.

Although it might seem that we can proceed along the lines similar to those in the previous Sections, it will be clear soon that this way brings some initial results only. The quantum character of walks poses not so simple and still highly debated questions.

To illustrate this, let us begin with an infinite chain, when n's in Eq. (21) are integers from $-\infty$ to $+\infty$. In this case, the Schrödinger equation $\mathrm{d}\,|\Psi(t)\rangle/\mathrm{d}t = -iH\,|\Psi(t)\rangle$ ($\hbar = 1$) for the wave function $|\Psi(t)\rangle = \sum_n c_n(t)\,|n\rangle$ immediately reduces to the canonical relationship for Bessel functions, so that, under initial condition $|\Psi(0)\rangle = |n_0\rangle$, the solution is

$$c_n(t|n_0) = (-1)^{n-n_0} J_{n-n_0}(2Lt). \tag{22}$$

Underlying propagator (22) is the base for solving numerous problems concerning the particle motion under various boundary conditions, in the presence of irregularities (sinks or traps), *etc.*, when the quantum nature of motion sometimes leads to counter-intuitive results (see, e.g., [12]). The evolution for the probability to find the particle on node n is given by the diagonal element of the density matrix $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$. According to Eq. (22), it reads:

$$\rho_{nn}(t|n_0) = |c_n(t|n_0)|^2 = J^2_{n-n_0}(2Lt), \tag{23}$$

and, as distinct from the classical case, its decay to 0 in the limit $t \to \infty$ is accompanied by oscillations. A more essential distinction can be seen after calculating the mean square displacement, MSD $= \sum_n (n - n_0)^2 \rho_{nn}(t|n_0)$. Using Eq. (23), one can obtain that

$$\text{MSD} = 2L^2t^2. \tag{24}$$

Eq. (24) points the ballistic character of quantum propagation with "velocity" $L\sqrt{2}$ while in the classical counterpart MSD $\sim t$. This feature looks promising for the supposed efficiency of quantum search algorithms, quantum computing, so on.

Let us now introduce the resetting, which, as earlier, is implied to be Poissonian. Suppose that the system with Hamiltonian (21) is prepared in state $|\Psi(0)\rangle$ at $t = 0$. In the interval $[t, t + \mathrm{d}t]$, the system may return to the determined resetting state $|n_r\rangle$with probability $r\,\mathrm{d}t$, or, with the probability $1 - r\,\mathrm{d}t$, continue to evolve unitarily, obeying the Schrödinger equation, as $|\Psi(t)\rangle = \exp(-iHt)\,|\Psi(0)\rangle$:

$$|\Psi(t+\mathrm{d}t)\rangle = \begin{cases} |n_r\rangle \quad \text{with the probability } r\mathrm{d}t, \\ (1 - iH\mathrm{d}t)\,|\Psi(t)\rangle, \\ \quad \text{with the probability}(1 - r\mathrm{d}t). \end{cases}$$

Due to the resetting, the density matrix does not correspond to a pure state any longer and should be averaged on all possible resets in the interval [0, t]. This, in principle, can be done by summarizing the corresponding infinite series [15]. It is much simpler, however, to apply the last renewal equation (5), which retains its validity in the quantum case also [2]:

$$\rho_r(t|n_0, n_r) = e^{-rt}\rho_u(t|n_0) + r\int_0^t e^{-r\tau}\rho_u(\tau|n_r)\mathrm{d}\tau, \tag{25}$$

where $\rho_u(t|m)$ is the density matrix of the system with no resetting, so that $\rho_u(t|n_0) = e^{-iHt}\rho_u(0|n_0)\,e^{iHt}$, and $\rho_u(0|n_0) = |n_0\rangle\langle n_0|$. Obviously, the stationary density matrix $\rho_r^{\text{st}}(n_r)$ is

$$\rho_r^{\text{st}}(n_r) = r\int_0^\infty e^{-rt}\rho_u(t|n_r)\mathrm{d}t \tag{26}$$

and represents a non-equilibrium steady state with detailed balance violation caused by internal flows generated by resets. In our case, the density matrix for the underlying process $\rho_u(t|l) = \sum_{nm} c_n^*(t|l)c_m(t|l)$ includes amplitudes (22),, and its diagonal elements are given by Eq. (23). Then the evolution and stationary values of the probability of the walker presence at node n read:

$$P_n(t) \equiv [\rho_r(t|n_0, n_r)]_{nn} =$$
$$e^{-rt}J^2_{n-n_0}(2Lt) + r\int_0^t e^{-r\tau}J^2_{n-n_r}(2L\tau)\mathrm{d}\tau, \tag{27}$$

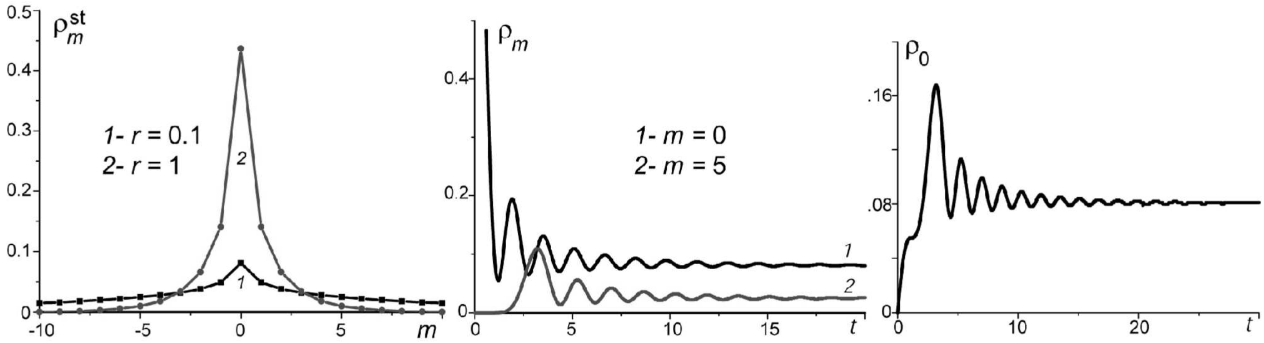
$$P_n^{\text{st}} = r\int_0^\infty e^{-rt}J^2_{n-n_r}(2Lt)\mathrm{d}t =$$
$$= \frac{r}{2\pi L}Q_{n-n_r-1/2}\left(\frac{r^2}{L^2} + 1\right), \tag{28}$$

where $Q_\nu(x)$ is the Legendre function of the second kind [16]. The same results derived in a more complex way were recently obtained in work [15].

Fig. 4 exemplifies the stationary distribution and evolution of some node occupation probabilities. The shape of the plot in Fig. 4, *a* is similar to that of the stationary distribution (6) for classical walks in an infinite chain with the resetting. With r growing, it becomes narrower around n_r, what is natural. However, its asymptotic for $r \to \infty$, as follows from (28), is somewhat different and proportional to r^{-2n} instead of r^{-n} mentioned above.

Quantitative characteristics of localization caused by introducing classical resetting stochasticity to a quantum system can be easily calculated with the use of Eqs (27), (28). In particular, the stationary mean displacement $\sum_n P_n^{\text{st}}(n - n_0) = n_r - n_0$, and the stationary mean square displacement $\text{MSD}^{\text{st}} = \sum_n P_n^{\text{st}}(n - n_0)^2$ is $4L^2/r^2$.

Regrettably,, the further advance in studying the classical resetting effects in quantum walks along a one-dimensional lattice seems hardly possible. First, there is a serious technical obstacle for finding the occupation probabilities even in chains with a single irregularity (e.g., an edge, a sink, *etc.*). There is no special problem to find the Laplace transforms of corresponding amplitudes $\tilde{c}_n(p)$ [12]. However, to invert them or to find with their help at least the Laplace transforms of the square of their moduli, i.e., $\tilde{\rho}_n(p)$, is a daunting task. Even a bigger obstacle, a fundamental one, roots in the impossibility to correctly define the MFPT. For example, in the just considered case of an infinite chain, it is impossible to formulate the auxiliary problem for a semi-infinite



a *b* *c*

Fig. 4. Stationary distribution of node occupation for different rates of resetting to node $n_r = 0$. $L = 1$. $r = 0.1$ (curve *1*); $r = 1$ (curve *2*) (*a*). Evolution of some occupation probabilities ($n_r = 0$, $r = 0.1$) (*b, c*). $n_0 = 0$ (*b*): ρ_0 (curve *1*), ρ_5 (curve *2*); $n_0 = 5$ (*c*)

chain with an *irreversible* transition from the terminal node to the target, since the corresponding transition rate cannot be built with the only parameter L of the quantum-mechanical resonance exchange. Consequently, one cannot correctly introduce the distribution function $f(t) = \kappa\rho_0(t)$, as it is completely unclear what is κ.

These reasons, as well as additional considerations concerning the peculiarities of quantum measurements, have led to the re-defining both the notion of the MFPT (replacing it for the mean time of the first *detection*) and the resetting itself (replacing it for *projective measurements* on a certain node). Currently, various approaches in this direction are intensively debated. This goes beyond the content of the present paper; for the corresponding latest works, see e.g., [3, 17, 18] and references therein.

5. Concluding Remarks

Random walks in a one-dimensional lattice belong to the basic models of the theory of stochastic processes, widely used for numerous applications in very diverse branches of science. The present work represents the most complete (up to date) analysis of the influence of the Poissonian resetting upon such random walks in chains of arbitrary length under arbitrary initial and boundary conditions. The exact analytic expressions for the dependence of the main observables (unconditional and conditional MFPTs, splitting probabilities, coefficients of variation) on the resetting rate allow one to reveal a variety of new resetting effects caused by different locations of the initial n_0 and resetting n_r nodes, or by different boundary conditions at the chain edges. In particular, the possibility of inverting the ratio W_0/W_N of the splitting probabilities by varying the resetting rate (that is, of converting an 'undesired' outcome into a 'desired' one) illustrates the resetting control abilities. The derived condition of the resetting expediency (generalization of the 'universal' criterion $\mathrm{CV}_u > 1$ for the case $n_0 \neq n_r$) shows that the resetting can improve the search even under a narrow distribution $f_u(t)$ of times of the first passage in the underlying process, when $\mathrm{CV}_u < 1$.

As for quantum walks, one can trace the influence of the classical resetting upon the course of nonequilibrium steady state formation in an infinite chain without sinks. However, attempts to introduce the observables similar to those in classical random walks demand re-defining the notions of both the MFPT and the resetting itself.

The present work, as well as practically all works in this field so far, is of mostly academic character [3]. Some aspects related to enzymatic catalysis and conformationally branched Michaelis–Menten schemes are discussed in [8, 9, 21]. A review of potential applications of the models with the stochastic resetting in a wide circle of multidisciplinary problems can be found in [4]. Although there is a lack of direct experiments on, for instance, (bio)molecular reactions or transport systems of molecular electronics, the first observations of diffusion with the reset-

[3] With the use of expressions presented, more specific statistical characteristics of random walks, like investigated in [19, 20], can be immediately calculated.

ting [22, 23], together with already developed technique of extracting statistical characteristics of single-molecular reactions, leave no doubt of using the cumulative theoretical results for various real systems with the resetting.

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Л.М. Христофоров

НЕПЕРЕРВНІ В ЧАСІ ВИПАДКОВІ БЛУКАННЯ З РЕСЕТИНГОМ В ОБМЕЖЕНОМУ ЛАНЦЮЖКУ

Детально проаналізовано модель класичних випадкових блукань з пуассонівським ресетингом в одновимірній ґратці в її загальному варіанті. Акцент зроблено на ефектах ресетингу, які виникають внаслідок різноманітності довільних початкових і граничних умов. Також обговорюється квантовий аналог моделі.

Ключові слова: випадкове блукання, низьковимірні ґратки, стохастичний ресетинг, доцільність ресетингу, квантові блукання.