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SURVIVAL PROBABILITY APPROACH TO THE RELAXATION OF A MACROSCOPIC SYSTEM IN THE DEFECT-DIFFUSION FRAMEWORK

Abstract. The main objective of this paper is to present a new probabilistic model underlying the universal relaxation laws observed in many fields of science where we associate the survival probability of the system's state with the defect-diffusion framework. Our approach is based on the notion of the continuous-time random walk. To derive the properties of the survival probability of a system we explore the limit theorems concerning either the summation or the extremes: maxima and minima. The forms of the survival probability that result from the scheme under consideration are in agreement with the characteristics of empirical data. Moreover, the proposed approach allows us to indicate their origins.

1. Introduction. We present a new probabilistic approach to model the irreversible stochastic transition that a system undergoes as a whole due to the transitions of individuals (atoms, molecules, etc.) The idea is to incorporate the empirical knowledge on evolution in course of time of physical systems driven by external forces to a nonequilibrium excited state. Our considerations are based on the assumption that the transition of the system from its initial state occurs under the diffusion of defects (such as microscopic cavities or random orientations of crystallites) [11]. For other approaches see [9, 12, 15, 17].

We consider a macroscopic physical system consisting of a large number of objects individually taking part in the transition. The transition of the system from a nonequilibrium state A imposed at $t = 0$ to the relaxed state B at some $t > 0$ occurs as a consequence of the first transition of individuals.

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The nonincreasing empirical function $\Phi(t)$ ($\Phi(0) = 1$, $\Phi(\infty) = 0$) defined by the change of some physical parameter that discriminates between the states A and B is called the *relaxation function* and has the meaning of the survival probability of A. The experimental evidence [1, 4, 6] indicates that in the majority of cases the forms of the response functions $f(t) := -d\Phi(t)/dt$ that satisfactorily fit the data follow either the so-called short-time fractional power law, i.e.,

$$\lim_{t\to 0} f(t)/t^{-a} = \text{const} \quad \text{for some } 0 < a < 1, \tag{1}$$

or both short and long-time fractional power laws:

$$\lim_{t\to 0} f(t)/t^{-a_1} = \text{const} \quad \text{for some } 0 < a_1 < 1, \tag{2}$$

$$\lim_{t\to \infty} f(t)/t^{-a_2-1} = \text{const} \quad \text{for some } 0 < a_2 < 1. \tag{3}$$

The transition of an individual object from its excited state to the equilibrium occurs under the diffusion of defects. Each object (target) in the system is surrounded by an appropriately large number of defects. When the defects meet an excited state prepared at $t = 0$ (a dipole, stress, etc.) the latter is allowed to relax. We take into account all the nearest defects which at $t = 0$ are at the same distance from the target considered (all sited on a sphere of the random radius L (see Fig. 1)). We assume that they can reach the target diffusing in one direction along the line segment joining the defect and the target. We model this movement by means of a rescaled continuous-time random walk (CTRW) (see also [8, 11]).

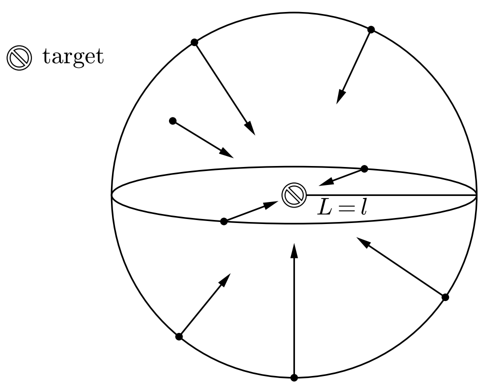

Fig. 1. The defect-diffusion model

The objective of this paper is to derive the form of the survival probability of the system's state A and to find its relationship with the parameters characterizing the movements of defects. In order to familiarize the reader with the notions used further and to justify the consecutive steps that we perform, we sketch briefly the stochastic scenario of our defect-diffusion model:

- Let θ denote the survival time of an individual target in its imposed state. We will say that the target has not relaxed until time $t > 0$ if none of the N defects that surround it has covered the distance L. This way we associate the survival probability of an individual with the probability of $\{\max\{\overline{R}_1(t), \dots, \overline{R}_N(t)\} < L\}$, where $\overline{R}_j(t)$ is the distance covered by the jth defect until time t.
- The system consists of a large number M (we also allow this number to be random Z_M) of targets with i.i.d. survival times $\theta_1, \dots, \theta_M$. We identify the survival probability of the entire system with the probability of its first passage [7–10, 15–17], i.e.,

  $$\mathrm{P}(\widetilde{\theta} \geq t) = \mathrm{P}(\min\{\theta_1, \dots, \theta_M\} \geq t),$$

  where $\widetilde{\theta}$ denotes the effective survival time of the imposed state A (the effective waiting time for the entire system).

The article is structured as follows: In Section 2 we introduce the notion of the rescaled continuous-time random walk and study its asymptotic properties. In Section 3 we express the survival probability of an individual and of the entire system in terms of the rescaled CTRW, and basing on extreme-value theory together with the results obtained in Section 2 we derive formulas for the survival probabilities. Finally, in Section 4 we discuss the results obtained in the context of the physical phenomenon of relaxation.

2. Rescaled continuous-time random walk as a model of movement of defects. The notion of the continuous-time random walk (CTRW) was introduced by Montroll and Weiss [14] as a walk with random time intervals between subsequent jumps (see Fig. 2). Since then it has been applied

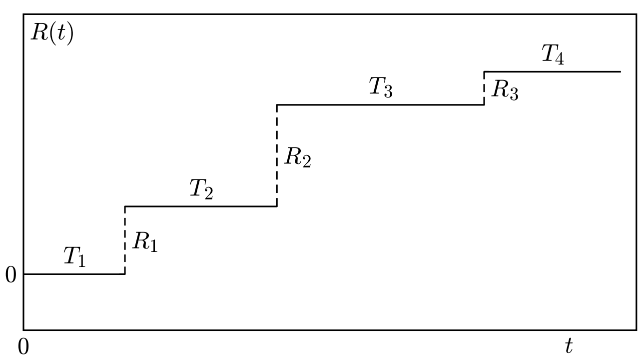

Fig. 2. An exemplary trajectory of the CTRW with the jumps performed in one direction

to model a wide variety of phenomena connected with anomalous diffusion. The definition of this stochastic process can be formulated as follows:

Definition 2.1 (see [8]). Let $(T,R)=\{(T_i,R_i), i=1,2,\ldots\}$ be a sequence of i.i.d. random vectors such that $T_i>0$ with probability 1. The random variable T_i is usually interpreted as a waiting time of a moving particle for the ith jump, and R_i indicates both the length and direction of the ith jump. The *continuous-time random walk* $\{\widetilde{R}(t), t\geq 0\}$ generated by (T,R) is defined to be the random sum

$$\widetilde{R}(t)=\sum_{i=1}^{N_T(t)} R_i, \tag{4}$$

where $\{N_T(t), t\geq 0\}$ is the counting renewal process corresponding to T. More precisely, $\widetilde{R}(t)=S_R(N_T(t))$, where $S_R(n)$ and $S_T(n)$ denote the partial sums of the sequences $R=\{R_i, i=1,2,\ldots\}$ and $T=\{T_i, i=1,2,\ldots\}$, respectively (defined as $S_R(0)=S_T(0)=0$, and $S_R(n)=\sum_{i=1}^n R_i$ and $S_T(n)=\sum_{i=1}^n T_i$ for $n=1,2,\ldots$), and

$$N_T(t)=\max\{k : S_T(k)\leq t\}. \tag{5}$$

Further considerations are restricted to the jump parameters with the following properties:

Assumption 1. $(T,R)=\{(T_i,R_i), i=1,2,\ldots\}$ is a sequence of i.i.d. random vectors such that R_i and T_i are independent positive random variables for which

$$\mathrm{P}(R_i\geq r)\overset{r\to\infty}{\sim}(r/b_R)^{-\alpha} \quad \text{for some } 0<\alpha<1,\ b_R>0, \tag{6}$$

$$\mathrm{P}(T_i\geq t)\overset{t\to\infty}{\sim}(t/b_T)^{-\lambda} \quad \text{for some } 0<\lambda<1,\ b_T>0. \tag{7}$$

Here and further on, we use the symbol "$\sim$" to specify the asymptotic behavior, i.e. $f(x)\overset{x\to a}{\sim} bx^c$ means $\lim_{x\to a} f(x)/bx^c=1$. Conditions (6) and (7) signify that the random variables R_i and T_i, respectively, have heavy tails and are sufficient for the respective random variables to belong to the domain of attraction of the one-sided Lévy-stable law with the index of stability equal to the heavy-tail exponent. Therefore, R_i and T_i satisfying Assumption 1 belong to the domains of attraction of the random variables $\mathcal{S}_\alpha$ and $\mathcal{S}_\lambda$, respectively, where $\mathcal{S}_a$ with $0<a<1$ denotes the completely asymmetric Lévy-stable random variable with Laplace transform $\psi_a(s)=\mathrm{E}(\exp(-s\mathcal{S}_a))=\exp(-s^a)$ [18]. (We will denote by $\mathcal{S}_a(x)$ the corresponding distribution function.)

In the following definition we introduce the notion of the rescaled CTRW constructed from the CTRW generated by independent and heavy-tailed jump parameters (T,R). We use this transformation of CTRW to model the migration of defect in the defect-diffusion approach to explain the relaxation mechanism. The procedure of rescaling allows us to derive the distribution of the defect position at any fixed $t > 0$.

DEFINITION 2.2. For any fixed $t > 0$ we define

$$\overline{R}(t) := \lim_{c\to\infty} \frac{\widetilde{R}(ct)}{c^{\lambda/\alpha}} \tag{8}$$

as a weak limit, if it exists. The resulting stochastic process $\{\overline{R}(t), t \geq 0\}$ will be called the *rescaled CTRW generated by* (T, R).

PROPOSITION 2.1. *If* (T, R) *satisfies Assumption* 1, *then* $\overline{R}(t)$ *is well defined and*

$$\overline{R}(t) \stackrel{d}{=} t^{\lambda/\alpha} A \frac{\mathcal{S}_\alpha}{\mathcal{S}_\lambda^{\lambda/\alpha}}, \tag{9}$$

where A *is the constant*

$$\left(\frac{b_R^\alpha \Gamma(1-\alpha)}{b_T^\lambda \Gamma(1-\lambda)}\right)^{1/\alpha},$$

and the Lévy-stable random variables $\mathcal{S}_\alpha$, $\mathcal{S}_\lambda$ *are independent.*

Proof. Condition (9) is in fact a limit theorem for the CTRW $\widetilde{R}(ct)$ and is analogous to the result obtained for the CTRW in [7, 12]. ■

Below we derive the asymptotic properties of the rescaled CTRW at any fixed time $t > 0$. This result will be used in the following section, since it permits obtaining the distribution of the maximum of an appropriately constructed sequence of i.i.d. random variables which are independent rescaled CTRW's at fixed time $t > 0$.

THEOREM 2.1. *Fix* $t > 0$. *Under Assumption* 1 *the tail of the distribution of* $\overline{R}(t)$ *has the following asymptotic property*:

$$\mathrm{P}(\overline{R}(t) \geq x) \stackrel{x\to\infty}{\sim} B(t) x^{-\alpha}, \tag{10}$$

where

$$B(t) = t^\lambda \frac{\sin \pi\lambda}{\pi\lambda} \frac{b_R^\alpha}{b_T^\lambda}.$$

Proof. For the function

$$H(t) := \mathrm{E}\left(\exp\left(-t^{\alpha/\lambda}\left(\frac{\mathcal{S}_\alpha}{\mathcal{S}_\lambda^{\lambda/\alpha}}\right)^{-\alpha/\lambda}\right)\right),$$

we have

$$\begin{aligned} H(t) &= \mathrm{E}\left(\exp\left(-t^{\alpha/\lambda} \frac{\mathcal{S}_\lambda}{\mathcal{S}_\alpha^{\alpha/\lambda}}\right)\right) = \mathrm{E}\left(\exp\left(-t^\alpha \frac{1}{\mathcal{S}_\alpha^\alpha}\right)\right) \\ &= \mathrm{P}\left(\Gamma_1 \geq t^\alpha \frac{1}{\mathcal{S}_\alpha^\alpha}\right) = \mathrm{P}(\Gamma_1^{1/\alpha} \mathcal{S}_\alpha \geq t), \end{aligned}$$

where Γ_1 is a random variable distributed according to the standard exponential law, independent of S_α. Therefore by [3, Chapter XIII]

$$\text{(11)}\quad \int_0^\infty e^{-st}H(t)\,dt = \frac{1-\mathrm{E}(\exp(-s\Gamma_1^{1/\alpha}\mathcal{S}_\alpha))}{s} = \frac{1-\mathrm{E}(\exp(-s^\alpha\Gamma_1))}{s}$$
$$= \frac{1-(1+s^\alpha)^{-1}}{s} \overset{s\to 0}{\sim} s^{\alpha-1}.$$

By the Tauberian theorems condition (11) implies

$$H(t) \overset{t\to\infty}{\sim} \frac{1}{\Gamma(1-\alpha)}\,t^{-\alpha}.$$

As a consequence, the Laplace transform of the random variable $\mathcal{S}_\lambda/\mathcal{S}_\alpha^{\alpha/\lambda}$ satisfies

$$\text{(12)}\qquad \mathrm{E}\Big(\exp\Big(-t\,\frac{\mathcal{S}_\lambda}{\mathcal{S}_\alpha^{\alpha/\lambda}}\Big)\Big) \overset{t\to\infty}{\sim} \frac{1}{\Gamma(1-\alpha)}\,t^{-\lambda}$$

since $\mathrm{E}(\exp(-t\mathcal{S}_\lambda/\mathcal{S}_\alpha^{\alpha/\lambda})) = H(t^{\lambda/\alpha})$. Again by the Tauberian theorems, condition (12) implies

$$\text{(13)}\qquad \mathrm{P}\Big(\frac{\mathcal{S}_\lambda}{\mathcal{S}_\alpha^{\alpha/\lambda}} \le z\Big) \overset{z\to 0}{\sim} \frac{z^\lambda}{\Gamma(1-\alpha)\Gamma(\lambda+1)}.$$

Property (13) together with Proposition 2.1 leads to

$$\mathrm{P}(\overline{R}(t)\ge x) = \mathrm{P}\Big(\frac{\mathcal{S}_\lambda}{\mathcal{S}_\alpha^{\alpha/\lambda}} \le \Big(\frac{x}{t^{\lambda/\alpha}A}\Big)^{-\alpha/\lambda}\Big) \overset{x\to\infty}{\sim} t^\lambda\,\frac{\sin\pi\lambda}{\pi\lambda}\,\frac{b_R^\alpha}{b_T^\lambda}\,x^{-\alpha},$$

which is equivalent to (10). ∎

In the following section we focus on the survival probability of the system's imposed state in the defect-diffusion framework. We will attribute the rescaled CTRW properties to the behavior of all defects in the system. We will propose a suitable definition of the survival probability, and derive its forms.

3. The rescaled CTRW approach to the survival probability. Consider a family $\{(T^{(jk)}, R^{(jk)}),\ j,k = 1,2,\ldots\}$ of independent random sequences

$$(T^{(jk)}, R^{(jk)}) = \{(T_i^{(jk)}, R_i^{(jk)}), i = 1,2,\ldots\},$$

such that for any fixed pair $j,k = 1,2,\ldots$ the sequence $(T^{(jk)}, R^{(jk)})$ satisfies Assumption 1 with the same parameters α, λ, b_R and b_T. For a fixed $t>0$ and $j,k = 1,2,\ldots,$ let $\overline{R}_{jk}(t)$ be defined as in Definition 2.2 by means of $(T^{(jk)}, R^{(jk)})$.

We let $\{\theta_k,\ k = 1,2,\ldots\}$ be a sequence of i.i.d. positive random variables such that for any k the conditional probability of θ_k given a positive random variable L is

$$\text{(14)} \quad \mathrm{P}(\theta_k \geq t \mid L = l) = \lim_{N\to\infty} \mathrm{P}(A_N \max\{\overline{R}_{1k}(t), \ldots, \overline{R}_{Nk}(t)\} < l),$$

where

$$A_N = N^{-1/\alpha}\left(\frac{\sin \pi\lambda}{\pi\lambda}\,\frac{b_R^\alpha}{b_T^\lambda}\right)^{-1/\alpha},$$

while L is independent of $(T^{(jk)}, R^{(jk)})$ for any j,k and satisfies the condition

$$\text{(15)} \qquad \mathrm{P}(L < l) \overset{l\to 0}{\sim} (l/c_0)^\kappa, \qquad 0 < \kappa, c_0 = \text{const.}$$

THEOREM 3.1. *Let $\kappa \neq \alpha$. The survival probability of the imposed state of an individual kth target has the form*

$$\text{(16)} \qquad \mathrm{P}(\theta_k \geq t) = \mathrm{E}(\exp(-t^\lambda L^{-\alpha}))$$

and the survival probability of the system in state A is

$$\text{(17)} \quad \mathrm{P}(\widetilde{\theta} \geq t) = \lim_{M\to\infty} \mathrm{P}(B_M \min\{\theta_1, \ldots, \theta_M\} \geq t) = \exp(-t^{\eta\lambda}),$$

where $\eta = \min\{\kappa/\alpha, 1\}$, $B_M = bM^{1/\eta\lambda}$ and

$$b = \begin{cases} c_0^{-\kappa/\eta\lambda}(\Gamma(1-\eta))^{1/\eta\lambda}, & \eta < 1, \\ \mu^{1/\lambda}, & \eta = 1,\ \mu = \mathrm{E}(L^{-\alpha}). \end{cases}$$

Proof. By extreme-value theory [13, Chapter 1], the asymptotic property given in Theorem 2.1 implies that for any $k = 1, 2, \ldots,$

$$\begin{aligned} \lim_{N\to\infty} \mathrm{P}(A_N \max(\overline{R}_{1k}(t), \ldots, \overline{R}_{Nk}(t)) \leq l) &= \exp(-(l/t^{\lambda/\alpha})^{-\alpha}) \\ &= \exp(-t^\lambda l^{-\alpha}) \end{aligned}$$

and therefore $\mathrm{P}(\theta_k \geq t) = \mathrm{E}(\exp(-t^\lambda L^{-\alpha}))$, which proves (16).

Observe that condition (15) is equivalent to $\mathrm{P}(L^{-\alpha} > z) \overset{z\to\infty}{\sim} (zc_0^\alpha)^{-\kappa/\alpha}$. Hence, for $\kappa/\alpha > 1$ the expected value $\mu = \mathrm{E}(L^{-\alpha})$ is finite, and it follows from the Tauberian theorems that

$$\text{(18)} \qquad \mathrm{P}(\theta_k \leq t) = 1 - \mathrm{E}(\exp(-t^\lambda L^{-\alpha})) \overset{t\to 0}{\sim} \mu t^\lambda,$$

whereas for $\eta = \kappa/\alpha < 1$, the Tauberian theorems lead to

$$\text{(19)} \qquad \mathrm{P}(\theta_k \leq t) \overset{t\to 0}{\sim} c_0^{-\kappa}\Gamma(1-\eta)t^{\lambda\eta}.$$

Now (18) and (19) yield (17) by extreme-value theory. This technique does not apply to the case of $\kappa = \alpha$, which remains an open question. ∎

The following theorem corresponds to the case when we assume the number of targets that actively contribute to the relaxation process to be random, in particular to have negative binomial distribution. Some attempts to justify the ubiquity of this distribution in physics have been presented in [5]. By assuming the model in which Z_M follows the negative binomial law, we allow for the clustering in the number of targets in the system.

THEOREM 3.2. *Let a random sequence* $\{Z_M, M = 1, 2, \ldots\}$ *be independent of* $(T^{(jk)}, R^{(jk)})$ *and for any fixed* M *let* Z_M *be distributed according to the negative-binomial law with parameters* $c > 0$ *and* $p_M \in (0,1)$, *that is*,

$$\mathrm{P}(Z_M = m) = \frac{\Gamma(m+c)}{m!\Gamma(c)}(p_M)^c(1-p_M)^m, \qquad m = 0, 1, 2, \ldots \tag{20}$$

Assume additionally that $p_M \overset{M\to\infty}{\sim} D/M^d$ *for some positive constants* d *and* D. *Then the survival probability of the system in state* A *is*

$$\mathrm{P}(\widetilde{\theta} \geq t) = \lim_{M\to\infty} \mathrm{P}(B'_M \min\{\theta_1, \ldots, \theta_{Z_M}\} \geq t) = (1 + t^{\eta\lambda})^{-c}, \tag{21}$$

where $B'_M = (b/D^{1/\eta\lambda})M^{d/\eta\lambda}$.

Proof. We observe that for the sequence θ of positive random variables we may define $V(M) := (\min\{\theta_1, \ldots, \theta_M\})^{-1}$ and rewrite (21) as

$$\lim_{M\to\infty} \mathrm{P}\left(\frac{V(M)}{bM^{1/\eta\lambda}} \leq t\right) = \mathrm{P}(W_{\eta\lambda}^{-1} \leq t), \tag{22}$$

where $W_{\eta\lambda}$ is a random variable distributed according to the standard Weibull law. Moreover, we observe by [5] that

$$\lim_{M\to\infty} \mathrm{P}\left(Z_M \frac{D}{M^d} \leq z\right) = \Gamma_c(z), \tag{23}$$

where Γ_c is the standard gamma distribution function with the shape parameter c. Therefore, by [2], we deduce from (22) and (23) that

$$\lim_{M\to\infty} \mathrm{P}\left(\frac{V(Z_M)}{bD^{-1/\eta\lambda}M^{d/\eta\lambda}} \leq t\right) = \mathrm{P}(\Gamma_c^{1/\eta\lambda}W_{\eta\lambda}^{-1} \leq t), \tag{24}$$

where the random variables Γ_c and $W_{\eta\lambda}$ are taken to be independent. As a consequence of (24), we obtain

$$\begin{aligned}\lim_{M\to\infty} \mathrm{P}\left(\frac{b}{D^{1/\eta\lambda}} M^{d/\eta\lambda} \min\{\theta_1, \ldots, \theta_{Z_M}\} \geq t\right) &= \mathrm{P}\left(\frac{W_{\eta\lambda}}{\Gamma_c^{1/\eta\lambda}} \geq t\right)\\ &= \frac{1}{(1+t^{\eta\lambda})^c},\end{aligned} \tag{25}$$

which proves (21). ∎

4. Physical interpretation of the results. We have obtained the survival probability of the nonequilibrium state of the system, which is equivalent to the empirical relaxation function $\Phi(t) = \mathrm{P}(\widetilde{\theta} \geq t)$. We have, therefore, found the probabilistic scheme yielding two forms of relaxation functions, i.e.,

$$\Phi_1(t) = \exp(-(Ct)^{\eta\lambda}), \tag{26}$$

$$\Phi_2(t) = (1 + Dt^{\eta\lambda})^{-c}, \tag{27}$$

where C and D are positive constants. This result is of a significant importance as the functions (26) and (27) indeed exhibit the universal behavior. More precisely, formula (26) yields the short-time fractional power law (1) with $a = 1 - \eta\lambda$, whereas the relaxation function of the form (27) yields for $0 < c < (\eta\lambda)^{-1}$ both the short and long-time fractional power laws (2) and (3) with $a_1 = 1 - \eta\lambda$ and $a_2 = c\eta\lambda$. Moreover, the proposed approach allowed us to indicate the origins of the power-law characteristics. In the case of $\kappa < \alpha$ the parameters a, a_1 and a_2 depend on both spatial (by means of α and κ) and temporal (λ) characteristics of the system, whereas for $\kappa \geq \alpha$ they contain only the information on the temporal characteristics of the system. We notice that the randomness (via c) in the number of active participants does not influence the short-time system evolution. On the contrary, it causes the slowing down in the long-time behavior.

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