## Influence of Entropy Changes on First Passage Time in the Thermodynamics of trajectories

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For thermodynamics of trajectories, an ensemble containing dynamical activity and first-passage time (*FPT*) random variables is considered. The dependence of the average *FPT* on the total non-negative change in entropy is obtained. The same dependencies obtained for dynamic activity, dispersion of dynamic activity and *FPT*, as well as for the correlation of dynamic activity and *FPT*. Application of the obtained results to model systems makes it possible to obtain dependences of entropy changes containing a stationary nonequilibrium state and equilibrium states. To relate changes in entropy to the conjugate parameter of the *FPT*, three models of distribution functions are used, which are applied to classical two-level and three-level systems, as well as to a quantum two-level system.

Key-words: first-passage time; thermodynamics of trajectories; entropy changes

## 1. Introduction

In the description of nonequilibrium phenomena, the so-called approach of "thermodynamics of trajectories" is used [1-28]. In this approach, the behavior of time-ordered dynamic events is characterized similarly to the thermodynamic description of configurations in space. In a non-equilibrium situation, an analog of equilibrium thermodynamic quantities and relations is used, but for the dynamic case, trajectories, rather than states or configurations, become the object of consideration. The role of volume in this case is played by time.

Using the methods of large deviations (*LD*) [28], ensembles of trajectories can be classified according to dynamic order parameters and their conjugate fields. This is Ruelle's thermodynamic formalism [27], applied to the space of trajectories, not configurations. Quantities similar to the free energy density and entropy density have been identified and used to understand the rare dynamical behavior of systems, both classical [7–21] and quantum [22–26]. This approach has been effectively used in describing the dynamics of glassy systems [14, 29–31]. Statistical ensembles with fluctuating times of the deployment of trajectories were considered in [32]. *FPT* for dynamic ensembles of trajectories is considered in [33].

The paper [2] single out two types of variables - A and B, trajectory observables. Observables of types A and B can be negative or positive in general. An observable of type A jumps by discrete amounts at every configuration change; an example is the total current (which increases or decreases by 1 at every configuration change) in lattice gas models. Similarly, an observable of type B can be the time integral of a positive or negative function or a function that changes time. In [33], focus on trajectory observables defined in terms of the jumps in a trajectory, this is called counting observables. A more general definition of fluctuations of observables of the trajectory Xis given in [34]. An example is the total number of changes in the trajectory configuration or dynamic activity [8, 2, 12], sometimes also called "traffic" or "frenesy" [42-44]. Dissipation bounds and current fluctuations are considered in [35-41]. The behavior of the dynamic activity Kis investigated in the article. For variables of this kind and for *FPT*, ensembles of trajectories are obtained. The problem of the first passage occupies a prominent place in natural science since *FPT* is a key characteristic of the kinetics of any process [45–84]. *FPT* plays an important role in many areas of physics and applied mathematics, chemistry, protein folding, and even credit risk modeling.

In the thermodynamics of trajectories, an *s*-ensemble is singled out, in which the random variable is a time-additive value *A*, for example, dynamic activity *K*, and the time  $\tau$  of the deployment of trajectories is fixed, and an *x*-ensemble, in which the values *A* or *K* are fixed, and the random variable is time  $\tau$ . In [33], the time  $\tau$  is considered as *FPT*. In this article, this approach is used. In *x*-ensemble the random time  $\tau$  is *FPT* when a fixed value of *K* is reached. In [32] a generalization of the *x*-ensemble was obtained for multiple observables. In the present article, one more generalization of such an ensemble is carried out.

In articles [83-84, 52-53], *FPT* is considered as a thermodynamic variable and included in the generalized Gibbs distribution. This approach is also applicable to ensembles of trajectories and variables of type A and B. Similar results were obtained in [33, 9] for the joint distribution of activity parameters and process time. The behavior of *FPT* has its characteristics associated with many factors. One of the main factors is the change in entropy, which consists of intrasystem changes in entropy  $\Delta s_{sys}$  and the exchange of entropy with the environment  $\Delta s_m$ . The effect of entropy change on the behavior of a non-equilibrium system is studied. The change in entropy during the *FPT* time is included in the consideration. Three models of the partition function are considered. Dependences on the total entropy change in the system of such quantities as mean *FPT*, *FPT* variance, correlation of *FPT* and dynamic activity are calculated. These dependencies essentially depend on the interaction with the environment and change when the sign of the entropy flows describing the exchange of the system with the environment changes.

Typically, average *FPT* values are calculated from the Laplace transform of the *FPT* probability density by differentiating the Laplace transform and then setting the Laplace transform parameter to zero. In [83-84], the Laplace transform of the probability density *FPT* acts as the nonequilibrium part of the partition function, and the Laplace transform parameter is not equal to zero. The main idea of this article is that the parameter *x* (in notation [2, 32]) or  $\gamma = x$  (in notation [83-84]) which conjugate to the random variable time  $\tau$  or *FPT* associated with changes in entropy and is equal to zero only in equilibrium, as is shown in [83-84]. The presence of a non-zero value of  $\gamma$  corresponds to taking into account the change in entropy during the *FPT*. The impact of this accounting can be significant [85-86]. Any nonequilibrium process, including the *FPT* process, occurs with a change in entropy, which is taken into account in this article. Just as the inverse temperature parameter  $\beta = 1/k_BT$  conjugate to the random energy is not equal to zero in the general case, so the parameter  $\gamma$  (or *x*) is equal to zero only in the equilibrium case. Therefore, in the dependences of the moments of random variables *FPT* (or  $\tau$ ), of the dynamic activity *K*, as well as the parameters *M* from (22)-(28) in the general case, non-zero values of  $\gamma = x$  be taken into account.

The article introduces a statistical ensemble with fluctuating values of *FPT* and dynamic activity *K* in the form (29) (or (39), (80)). With the help of this ensemble, for the first time, explicit dependences of the average values, variances, and correlations of random variables *FPT* and *K* on the total change in entropy  $\Delta s_{tot} = \Delta s_{sys} + \Delta s_m$  (38) during the *FPT* time (or  $\tau$ ) are determined. The total change in entropy is associated with the parameter  $\gamma$ , and the dependences of the value  $\gamma$  on  $\Delta s_{tot}$ . The dependences of the moments of random variables *FPT* and *K* on the parameter  $\gamma$  (or *x*) conjugate to *FPT* are expressed through the dependences of these moments on the total change in entropy during the time *FPT* (or  $\tau$ ). Expressions for the correlation between dynamic activity and

*FPT* are obtained. It is physically obvious that such a correlation is not zero. In [32], a similar dependence of the quantity  $\langle \tau \rangle / \langle K_1 \rangle$  on the parameter *x* was obtained in Fig. 3a) in a more complex way using Monte Carlo simulation. Such dependences of system parameters on the total change in entropy during *FPT* were previously unknown. The results obtained can be considered as an application of distributions from [83, 84] to the thermodynamics of trajectories. The application of this approach to specific physical problems was carried out, for example, in [85-86].

The article is organized as follows. Section 2 provides information on the thermodynamics of trajectories: *s*-ensembles and *x*-ensembles. In Section 3, a joint distribution of K and *FPT* activities was obtained, from which the average values of *FPT* and K, their second moments, variances, and correlations between them were recorded. In the fourth section, dependencies of the first and second moments of distributions on the change in entropy are obtained, and curves are calculated for given numerical values of parameters. The fifth section contains brief conclusions.

### 2. Thermodynamics of trajectories, s-ensembles and x-ensembles

The formalism of nonequilibrium thermodynamics along trajectories is similar to the equilibrium thermodynamic formalism [27]. This article considers fluctuations of such dynamic variables as dynamic activity in a glassy system, integrated over a long-time t and a large (but finite) system. In [2], the statistical properties of evolution and the dynamic history of the system are studied. Equilibrium thermodynamics considers the probability distribution over the configurations of a large system. In trajectory thermodynamics, the thermodynamic formalism is applied to probability distributions over trajectory motion histories.

In [2, 9, 32, 49, 50] the classical stochastic system is described by the Master Equation

$$\partial_t \left| P(t) \right\rangle = W \left| P(t) \right\rangle. \tag{1}$$

The vector  $|P(t)\rangle$  represents the probability distribution at time t,  $|P(t)\rangle = \sum_{C} P(C,t)|C\rangle$ , where

P(C,t) describes the probability that the system is in configuration *C* at time *t*, and  $\{|C\rangle\}$  is the orthonormal basis of the configuration,  $\langle C|C'\rangle = \delta_{CC'}$ . For concreteness, we will focus on continuous-time Markov chains, but generalizations of what we describe below are simple. The master operator *W* is the matrix

$$W = \sum_{C' \neq C} w(C \to C') |C'\rangle \langle C| - \sum_{C} R(C) |C\rangle \langle C|.$$
<sup>(2)</sup>

Here  $w(C \to C')$  is the rate of transition from *C* to *C'*, and  $R(C) = \sum_{C'} w(C \to C')$  is the rate of exit from *C*. In this description, the expectation of the operator *T* is defined as  $\langle T(t) \rangle = \langle -|T|P(t) \rangle$ , where  $\langle -| = \sum_{C} \langle C|$  (such that  $\langle -|P(t) \rangle = 1$  due to conservation of probability).

In the Boltzmann-Gibbs theory, the macroscopic features of large systems are characterized by defining the statistical properties (mean and fluctuations) of extensive observables, such as the energy or number of particles. The microcanonical approach considers the properties of a system with a fixed total energy *E*. Such properties are determined from the counting factor of the number of configurations with energy *E* and the number of particles *N*, representing the size (volume) of the system. In the limit of large sizes  $(N \rightarrow \infty)$ , the entropy density  $s(e)=lim_{N\rightarrow\infty}(1/N)ln\Omega(eN,N)$  is determined, which is the relative weight of configurations with energy *E*, where *N* represents the size (the volume) of the system. In a dynamic context, the history of the system is considered between

the initial time  $\tau=0$  and the end time  $\tau$ . Instead of considering the statistics of the energy *E*, we study the observed *A*, which is extensive over the observation time  $\tau$ . The dynamic analog of the quantity  $\Omega(E,N)$  is the probability distribution of this observable; the value  $\Omega_{dyn}(A, \tau)$  is equal to the fraction of histories with a given value of the time-extensive observable *A*.

At the mathematical level, the choice of the observable *A* is somewhat arbitrary, although the application of the thermodynamic formalism requires that the quantity  $\log \Omega_{dyn} (A = a\tau, \tau) / \tau$ have a finite limit for large times  $\tau$ . Given this limitation, the choice of the order parameter *A* is determined by physical representations: we must use an observable that reveals the main physical processes occurring in the system. For example, in non-equilibrium systems in contact with two reservoirs of particles, we can define *A* as the total particle flux: the number of particles transferred from one reservoir to the other between times 0 and  $\tau$ . In the context of glassy phenomena, we consider observables that measure the "activity" or "complexity" of history [7, 8, 12].

In the Boltzmann-Gibbs approach, the canonical ensemble is defined in terms of the partition function

$$Z(\beta, N) = \sum_{E} \Omega(E, N) e^{-\beta E} , \qquad (3)$$

which characterizes the system at a given temperature  $\beta^{-1}$ . Phase transitions depend on intensive free energy  $f(\beta) = -\lim_{N \to \infty} \ln Z(\beta, N) / \beta N$  singularities. The dynamical analog of this thermodynamic partition function (3) is

$$Z_A(s,\tau) = \sum_A \Omega_{dyn}(A,\tau) e^{-sA} , \qquad (4)$$

where we have introduced an intensive field *s* conjugate to *A*. This field will play a role analogous to the inverse temperature  $\beta$ . The dynamic partition function  $Z_A(s, \tau)$  is the central object of Ruelle's thermodynamic formalism [27]. A correspondence is established between the thermodynamic limit of a large system size  $(N \rightarrow \infty)$  and the limit of a long time  $(\tau \rightarrow \infty)$  in Ruelle's formalism. In [2], systems are considered for which a large time limit must be taken at a fixed system size: in some cases, a second limit of the large system size *N* is taken. If we consider systems without thermodynamic phase transitions, then no singular behavior arises when passing to the limit of large *N* at a fixed  $\tau$ . In this case, we expect the limits of large *N* and large  $\tau$  to commute, but in the general case, this is not the case. In this article, the limit of large  $\tau$  is taken after finding the average values.

The duration of the history of the system is characterized by its length  $\tau$ . The probability of measuring the value A for an observable A in a history of length  $\tau$  is

$$\Omega_{dyn}(A,\tau) = \sum_{C} P(C,A,\tau).$$
(5)

The value  $P(C, A, \tau)$  (generalize the probability  $P(C, \tau)$ ) is defined as the probability of being in configuration *C* at time  $\tau$ , having measured a value *A* of the time-extensive variable between 0 and  $\tau$ .

The sequence of configurations  $C_0 \rightarrow ... \rightarrow C_K$  and the sequence of jump times  $t_1, ..., t_K$  determine the history of the system with duration  $\tau$ . Time record of configurations and waiting times of jumps between them, observed up to the moment of time  $\tau$ , describe the trajectory of total time  $\tau$ . If such a trajectory is denoted by  $X_{\tau}$ , then  $X_{\tau} = (C_0 \rightarrow C_{t_1} \rightarrow ... C_{t_n})$ , where  $C_0$  is the initial configuration, and  $t_i$  is the time when the transition from  $C_{t_{i-1}}$  to  $C_{t_i}$  occurs (so that the waiting time of the *i*-th jump is  $t_i - t_{i-1}$ ). The trajectory  $X_{\tau}$  changes configurations only *n* times (and  $t_n \leq \tau$ , i.e., there was no jump between  $t_n$  and  $\tau$ ). Between the moments  $t_k$  and  $t_{k+1}$  the system remains in configuration  $C_k$ .

If we consider the statistics of time-extensive observables [7, 8], then we can study the properties of dynamics. "Dynamic activity" K, defined as the total number of configuration changes per trajectory [8, 2, 12], is one such observed trajectory. In [34] the fluctuations of observables of the trajectory X written in the form

$$A(t) = \sum_{x \neq y} a_{xy} N_{xy}(t),$$
 (6)

where  $a_{xy}$  are arbitrary real numbers with  $\sum |a_{xy}| > 0$ , and  $N_{xy}(t)$  are the elementary fluxes, that is, the number of jumps from x to y up to time t in  $X_{\tau}$ . For a time-integrated current the coefficients are antisymmetric, while for counting observables (such as the activity), they are symmetric. The value of K is (6) by  $a_{xy}=1$ . Below we will consider a special case of arbitrary values A, dynamic activity K. We can return to the general case. Its distribution over all trajectories  $X_{\tau}$  of total time  $\tau$  is

$$P_{\tau}(K) = \sum_{X_{\tau}} \delta(K - \hat{K}[X_{\tau}]) P(X_{\tau}), \qquad (7)$$

where the probability  $P(X_{\tau})$  is the probability to observe this trajectory out of all the possible ones of total time  $\tau$ .

The operator  $\hat{K}$  counts the number of jumps in a trajectory. The distribution  $P_{\tau}(K) = \Omega_{dyn}(K,\tau)$  (4)-(5). For large  $\tau$  this probability acquires a large deviations form [8, 21, 28],

$$P_{\tau}(K) \sim e^{-\tau \varphi(K/\tau)} \,. \tag{8}$$

Equivalent information is contained in the generating function (4),

$$Z_{\tau}(s) \equiv \sum_{K} e^{-sK} P_{\tau}(K) = \sum_{X_{\tau}} e^{-s\hat{K}[X_{\tau}]} P(X_{\tau}), \qquad (9)$$

whose derivatives give the moments of the activity,  $\langle K^n \rangle = (-1)^n \partial_s^n Z_t(s)_{|s=0}$ . For large  $\tau$  the generating function also acquires a *LD* form [28, 8],

$$Z_{\tau}(s) \sim e^{\tau \theta(s)} \,. \tag{10}$$

The following behavior  $\hat{P}_A(C,s,t) = \sum_A e^{-sA} P(C,A,t)$  is assumed in the large time limit as

 $\hat{P}_A(C,s,\tau) \sim R_0(C,s)e^{\tau\theta_A(s)}$  where  $\theta_A(s)$  is the largest eigenvalue of  $W_A$  [2] and  $R_0(C, s)$  is the associated right eigenvector. Thus, for large times,

$$Z_A(s,\tau) = \sum_C \hat{P}(C,A,\tau) \sim e^{\tau \theta_A(s)}, \qquad (11)$$

the function  $\theta_A(s)$  is considered as a (negative) dynamic free energy per unit time. Probability conservation implies  $Z_A(0,\tau)=1$ , so  $\theta(0)=0$  for all stochastic systems.

From (10), the scaled cumulant generation function for the activity is determined, i.e., the *n*-th activity cumulant (per unit time)

$$\frac{\left\langle \left\langle K^{n} \right\rangle \right\rangle}{\tau} = (-1)^{n} \frac{\partial^{n}}{\partial s^{n}} \theta(s)_{|s=0}, \qquad (12)$$

where  $\langle \langle . \rangle \rangle$  indicates cumulant (mean, variance, etc.). It thus contains the full statistical information about *K*.

Entropy and free energy in the Boltzmann-Gibbs theory are connected through the Legendre transformation (as can be seen from (3)). The function  $\theta(s)$  from (10) is a dynamical analog of the free energy density  $f(\beta)$ . Just like thermodynamic potentials, the *LD* functions  $\varphi(k)$  and  $\theta(s)$  are related by a Legendre-Fenchel transformation [8, 27]

$$\varphi(k) = -\min_{s} (\theta(s) + sk) \tag{13}$$

together with the inversion formula

$$\theta(s) = -\min_{k} (\varphi(k) + sk). \tag{14}$$

The above applies to the so-called *s*-ensembles, in which the time  $\tau$  of history of the system with duration  $\tau$  is fixed [2, 32]. In [32], *x*-ensembles are introduced in which *K* is fixed and the time fluctuates. If we denote by  $Y_K$  a trajectory  $Y_K = (C_0 \rightarrow C_{t_1} \rightarrow ... \rightarrow C_K)$ , where the number of configuration changes is fixed to be *K*, but the time  $\tau$  of the final *K*-th jump fluctuates from trajectory to trajectory. From (1)-(2) the probability of  $Y_K$  is

$$P(Y_{K}) = p_{0}(C_{0}) \prod_{i=1}^{K} e^{-(t_{i}-t_{i-1})R(C_{t_{i-1}})} W(C_{t_{i-1}} \to C_{t_{i}}),$$
(15)

where  $t_0=0$  and  $t_K=\tau$ . The distribution  $P_K(\tau)$  of total trajectory length  $\tau$  for fixed activity K is

$$P_{K}(\tau) = \sum_{Y_{\tau}} \delta(\tau - \hat{\tau}[Y_{K}]) P(Y_{K}) = \sum_{C_{0} \dots C_{K}} p_{0}(C_{0}) \prod_{i=1}^{K-1} \int_{0}^{t_{i+1}} e^{-(t_{i} - t_{i-1})R(C_{t_{i-1}})} W(C_{t_{i-1}} \to C_{t_{i}}).$$
(16)

For large *K* this probability has a *LD* form,

$$P_{K}(\tau) \sim e^{-K\Phi(\tau/K)}.$$
(17)

The corresponding moment generating function for  $\tau$  is

$$Z_{K}(x) = \int_{0}^{\infty} d\tau e^{-x\tau} P_{K}(\tau) = \sum_{Y_{K}} e^{-x\hat{\tau}[Y_{K}]} P(Y_{K}), \qquad (18)$$

 $\langle \tau^n \rangle = (-1)^n \partial_x^n Z_K(x)_{|x=0}$ . For large *K* the generating function also has a *LD* form,

$$Z_K(x) \sim e^{K_g(x)}.$$
 (19)

Equation (18) is the partition sum for the ensemble of trajectories with probabilities

$$P_{x}(Y_{K}) \equiv Z_{K}^{-1}(x)e^{-x\hat{\tau}[Y_{K}]}P(Y_{K}).$$
(20)

The function g is the functional inverse of  $\theta$  and vice versa [32]

$$\theta(s) = g^{-1}(s), \quad g(\gamma) = \theta^{-1}(\gamma), \qquad s = g(\gamma), \quad \gamma = \theta(s).$$
(21)

We replace g(x) with g(y) (to use the notation  $\gamma$  from [83-84] for the parameter conjugate to *FPT*).

## 3. Joint distribution for activity and FPT

Above we considered *s*-ensembles and *x*-ensembles. This section, following [32], examines the generalization of the *x*-ensemble to multiple observables. Next, a joint distribution was obtained for random variables of dynamic activity K and of fluctuating total time. This distribution is obtained using the conditional probability formula and the effective parameter  $s_{ef}$ .

Consider now the statistics of first-passage times (*FPT*) (also called stopping times) [45-84]. This is the time when a certain observed trajectory first reaches the threshold value. In the thermodynamics of trajectories, in this situation, ensembles of trajectories with total fixed time are replaced by ensembles of trajectories of fluctuating total time.

In [32], the case is considered of the statistics of several different time-extensive quantities [2, 12]. For example, one could think of counting, instead of the total activity, the total number of certain kind of transitions, or the time integral of a certain quantity such as the energy. Let's say that there are *N* different dynamical observables, which we denote collectively by the vector  $\vec{M} = (M_1, ..., M_N)$ . Under the dynamics Eqs. (1)-(2) there will be a joint probability for observing a combination of these  $\vec{M} = (M_1, ..., M_N)$  quantities,  $P_{\tau}(\vec{M})$ . For large  $\tau$  this joint probability will have a *LD* form, generalized (8),

$$P_{\tau}(\vec{M} / \tau) \sim e^{-\tau \tilde{\Phi}(\vec{M} / \tau)}, \qquad (22)$$

where the *LD* function now depends on the whole vector of intensive observables  $(M_1/\tau; ...; M_N/\tau)$ . The corresponding moment generating function for  $\vec{M}$  also has a *LD* form at large  $\tau$  [28],

$$Z_{\tau}(\vec{s}) \equiv \sum_{\vec{M}} e^{-\vec{s} \cdot \vec{M}} P_{\tau}(\vec{M}) \sim e^{\tau \Theta(\vec{s})}, \qquad (23)$$

where for each observable  $M_n$  there is a counting field  $s_n$ , collected in the vector  $\vec{s} \equiv (s_1, ..., s_N)$ , and where the *LD* function  $\Theta(\vec{s})$  is a now function of this whole vector. The *LD* function  $\Theta(\vec{s})$  is the largest eigenvalue of the deformed master operator (2) [32]. Eq. (23) and the equation for the deformed master operator define an  $(\tau; \vec{s})$ -ensemble for a general set of dynamical order parameters  $\vec{M}$  [32]. There is an equivalent construct for studying the statistics of  $\vec{M}$  in trajectories where the total activity K is fixed. The probability of observing  $\vec{M}$ , together with a total time  $\tau$ , for a fixed and large K has the form, generalized (17),

$$P_{K}(\tau / K, \vec{M} / K) \sim e^{-K\tilde{\Phi}(\tau / K, \vec{M} / K)}.$$
(24)

The corresponding moment generating function is

$$Z_{K}(x,\vec{s}) \equiv \sum_{\vec{M}} \int_{0} d\tau e^{-x\tau - \vec{s}\vec{M}} P_{K}(\tau,\vec{M}) \sim e^{KG(x,\vec{s})}.$$
(25)

Average values are determined in the same way as was done in expressions (12), (18),  $\frac{\langle \tau \rangle}{K} = -\frac{\partial}{\partial x} G(x, \vec{s})_{|\vec{s}, x=0}, \quad \frac{\langle M_i \rangle}{K} = -\frac{\partial}{\partial s_i} G(x, \vec{s})_{|x, \vec{s}=0}.$  Equations (24) and (25) define a generalized x-

ensemble [32]. In the case where  $\vec{M}$  corresponds only to the activity *K* the function G(x, s) = g(x) - s, and Eqs.  $\theta(\vec{s}) = x_*(\vec{s})$ ,  $G(x_*(\vec{s}), \vec{s}) = 0$  reduce to (21).

As in [9], suppose that the system starts in an initial state  $\psi$ . For a random waiting time  $t_w$  the system evolves continuously, so that its unnormalised state at time  $t < t_w$  is  $exp(-iH_{eff}t)\psi$ , where  $H_{eff}$  is a non-selfadjoint effective Hamiltonian. At the time of detection, a click with label  $i=1,...,N_L$  is recorded, and the system's conditional state is updated by applying a jump operator  $L_i$ . A full detection process is given by a finite measurement trajectory  $X = ((t_1, i_1),...,(t_n, i_n))$ , where  $0 \le t_1 \le \le t_n$ . Each such trajectory has the final time  $T[X]=t_n$ , and a total number of jumps K[X]=n. There are some natural ways of obtaining finite trajectories. The first one repeats the single detection process K times. This corresponds to the x-ensemble. This scheme has an associated state transformation given by,  $J[X]=J(t_{w,n},i_n) \cdot J(t_{w,2},i_2)J(t_{w,1},i_1)$ , where  $t_{w,n}=t_n-t_{n-1}$ ,  $t_{w,1}=t_1$  are the waiting times between the detection events, or quantum jumps. In words, given a trajectory X resulting from this process, the system is at the end in state  $J[X]\psi$ ;  $J[t_w,i]=L_ie^{-t_wH_{eff}}$  is the jump operator effecting the total change  $\psi \rightarrow J[t_w,i]\psi$ .

We are interested in quantities obtained by incrementing with some amount at the addition of each particle. Such a quantity is of the form  $F[X] = \sum_{n=1}^{K[X]} F(t_{w,n}, i_n)$ , where  $F(t_w, i)$  is a (possibly vector-valued) quantity depending only on a single waiting time  $t_w$ , and some property of the system we are monitoring, say "spin" *i*. The most important ways of truncating an infinite trajectory, leading to statistical ensembles of field particles are with either fixed dynamic activity *K* and fluctuating  $\tau$ , or fixed the time  $\tau$  and fluctuating *K*, obtained by taking  $F(t_w,i)=t_w$  and  $F(t_w,i)=1$ , respectively. We can also measure a "spin" operator  $\hat{M}$  corresponding to  $F(t_w,i)=M(i)$ , where *M* is some (in general vector-valued) quantity depending on *i*. The associated probability distributions are given by  $P_K(T, M):=tr[\rho^{FC}_K \delta((T,M)-(\hat{T},\hat{M}))]$ , where  $\rho^{FC}_K$  is reduced density matrix on the output alone of the output space  $F^{out}$  [9]. The associated generating functions are given by  $Z_K(x, c) := tr[\rho^{FC}_{\ K} e^{-x\hat{T}-c\hat{M}}] = tr[\rho^{T^K}_{\ x,c}(I)]$ , written in terms of the deformed generators  $T_{x,c}$ and  $W_{s,c}$  [9] obtained from T and W (2) by replacing J[X] and  $V_{\tau}[X]$  with  $J_{x,c}[X]$  and  $V_{\tau s,c}[X]$  [9], where [32]  $T_x = \sum_{C' \neq C} \frac{w(C \to C^{*})}{x + R(C)} |C^{*}\rangle \langle C|$ ,

$$T_{x,c} = (xId + R)^{-1} \left( \sum_{i=1}^{N_L} e^{-cM(i)} L_i^{\dagger}(\cdot) L_i \right),$$
(26)

the inverse  $(xId + R)^{-1} = \int_0^\infty dt (e^{-it(H_{eff} - ix/2)^{t}}) (\cdot) e^{-it(H_{eff} - ix/2)}$  exists whenever  $\left\| e^{-it(H_{eff} - ix/2)} \right\| \le 1$ , which holds for all  $x > x_{min}$ , where  $x_{\min} = 2Im\lambda_0 \le 0$  and  $\lambda_0$  is the eigenvalue of  $H_{eff}$  with maximum imaginary part.

The elements of  $T_x$  represent the Laplace transforms of the factors in the integrand of (16), since in (18) and (25)  $Z_K(x)$  is the Laplace transform of  $P_K(\tau)$ . Then the LD function g(x) corresponds to the logarithm of the largest eigenvalue  $T_x$ . We restrict to  $x > x_{\min}$  subsequently;  $H_{\text{eff}}$  is a nonselfadjoint *effective Hamiltonian* (for open quantum systems),  $H_{eff} = H - (i/2) \sum_i L_i^* L_i$ , where H is a selfadjoint operator interpreted as the system's Hamiltonian when isolated from the environment. At the time of detection, a click with label  $i=1, ..., N_L$  is recorded, and the system's conditional state

is updated by applying a jump operator  $L_i$ .

Similar expressions are written in [9] for  $W_{s,c}$ ,  $P_{\tau}(K, M)$ ,  $Z_{\tau}(s, c)$  for fixed volume *T* and fluctuating *K*. We now suppose that  $T_{x,c}$  has a unique eigenvalue  $e^{g(x,c)}$  equal to its spectral radius.

We assume, that  $\vec{M} = K$ ,  $M_1$ , where  $M_1$  is some quantity depending on "spin" operator *i* [9]. We write the distribution of the values  $\tau$ , K,  $M_1$  in the form

$$P_{s,x,c}(\tau, K, M_1) = e^{-sK} e^{-x\tau - cM_1} P(\tau, K, M_1) / Z(s, x, c),$$
(27)

where

$$Z(s, x, c) = \sum_{M_1} \sum_{K} \int_0^\infty d\tau e^{-sK} e^{-x\tau - cM_1} P(\tau, K, M_1) \,.$$
(28)

Distributions of the form (27)-(28) were obtained, for example, in [87]. In [52, 53, 83-84] the joint distribution of *FPT* and system energy was obtained. Similar operations were carried out in [88], where distributions were obtained whose form is closer to the results of [52, 83-84] than to (29).

The value of  $M_I$  depends on the "spin" operator [9]  $i_n$  in  $(t_{w,n}, i_n)$ . Let us assume that the value of  $M_I$  is fixed at the value  $i_n$ . In this case, the value of K is also fixed. We assume that the values of  $i_n$ ,  $M_I$ , and K are sufficiently large for the relation  $Z_K(x,c) \sim e^{g(x,c)}$  to hold. At fixed values of  $M_I$ , the factor  $e^{-cM_1}$  in the denominator and numerator (27) is reduced, the relation is fulfilled  $\sum_M P(\tau, M_1, K) = P(\tau, K) = P(\tau | K) P(K) = P_K(\tau) P(K),$ 

where the conditional probability formula equal  $P(\tau, K) = P(\tau|K)P(K)$ ,  $P(\tau|K) = P_K(\tau)$  to is used. We equate the conditional probability  $P(\tau|K)$  and the probability  $P_K(\tau)$  from (16)-(18). Thus, the value of *K* is fixed in the conditional probability, but then these fixed values of *K* are averaged. It is assumed that there is an ensemble of systems with fixed values of *K*. Integration over  $\tau$  in (28) leads at large *K* to the expression (18), (19),  $\int_0^{\infty} d\tau e^{-x\tau} P_K(\tau) = e^{Kg(x)}$ , deformed generators [9]  $T_{x,c}$  (26) act, and partition function (27) takes the form (7)-(9)

$$Z = Z_{\tau}(s_{ef}) = \sum_{K} e^{-K(s-g(x))} P(K), \quad s_{ef} = s - g(x).$$
<sup>(29)</sup>

From equality (29) we obtain that  $s_{ef} = s - g(x) = 0$ , by (21). But for  $s_{ef} = 0$ , the values of *s*, g(x), and  $\gamma$  are not equal to zero. We consider expression (29) as a formal relation; for small values

of  $\tau$  (values of *K* are large, the *LD* function g(x) is already used), when the equations for the eigenvalues of a transfer matrix operator  $W_{s,c}$  [9, 32] should take into account other eigenvalues, except for the largest ones, and  $s_{ef} = s - g(x) \neq 0$ . From expression (29) we find the average values and second moments, and then, after differentiation, we set  $s_{ef} = s - g(x) = 0$ .

This corresponds to the fact that we pass to the limit of large values of the time  $\tau$  after taking derivatives and determining the moments, as in the nonequilibrium statistical operator (*NSO*) method [89–91]. In the *NSO* method, calculations are also made for large volumes, and then the passage to the limit  $\varepsilon \rightarrow 0$  is carried out. In [92], it was shown that  $\varepsilon = 1/\overline{T}$ , where  $\overline{T}$  is the average lifetime of the system, analogue of quantity  $\tau$ . Also, in expressions (30)-(34), at first large, but finite values of *K*, corresponding to a large volume, are chosen, and at the end - large values of  $\tau$ , corresponding to large *FPT*  $\overline{T}$ . Hence, using relation (29), we obtain expressions for the average values and second moments:

$$\left\langle K \right\rangle = -\frac{\partial \ln Z_{s_{ef}}}{\partial s_{ef}} \frac{\partial s_{ef}}{\partial s} \Big|_{s_{ef}=0} = \left\langle K_0 \right\rangle.$$
(30)

From (18)-(19) we have  $\ln Z_{K}(\gamma) = Kg(\gamma)$ ,

$$\langle \tau_{\gamma} \rangle = -K \frac{\partial g(\gamma)}{\partial \gamma}, \quad K = \langle K_0 \rangle,$$
(31)

$$D_{K} = \left\langle K^{2} \right\rangle - \left\langle K \right\rangle^{2} = \frac{\partial^{2} \ln Z_{s_{ef}}}{\partial s^{2}} = D_{K_{0}} = \left\langle K_{0}^{2} \right\rangle - \left\langle K_{0} \right\rangle^{2}, \qquad (32)$$

$$D_{\tau} = \left\langle \tau^2 \right\rangle - \left\langle \tau \right\rangle^2 = \frac{\partial^2 \ln Z_{\gamma}}{\partial \gamma^2} = K \frac{\partial^2 g(\gamma)}{\partial \gamma^2}.$$
(33)

The derivative of  $lnZ(s_{ef})$  (29) with respect to  $\gamma$  leads to the identity

$$\langle \tau \rangle = -\frac{\partial \ln Z(s_{ef})}{\partial \gamma} = -\frac{\partial \ln Z(s_{ef})}{\partial s_{ef}} \frac{\partial s_{ef}}{\partial \gamma} = \langle K_0 \rangle \frac{\langle \tau \rangle}{K}, \quad \frac{\partial s_{ef}}{\partial \gamma} = -\frac{\partial g(\gamma)}{\partial \gamma}, \quad \langle K_0 \rangle = K.$$

Mixed derivatives of  $lnZ(s_{ef})$  (29) allows one to obtain a correlation between the parameters *K* and  $\tau$ 

$$D_{K\tau} = \langle K\tau \rangle - \langle K \rangle \langle \tau \rangle = \frac{\partial^2 \ln Z_{s_{ef}}}{\partial s \partial \gamma} = \frac{\partial}{\gamma}_{|s} \left( \frac{\partial \ln Z_{s_{ef}}}{\partial s}_{|\gamma} \right) = \frac{\partial^2 \ln Z_{s_{ef}}}{\partial s^2} \frac{\partial s_{ef}}{\partial \gamma} = D_{K_0} \frac{\langle \tau_{\gamma} \rangle}{K}.$$
 (34)

This approach, together with relations (21), makes it possible to find the parameters  $\tau$  and K that are undefined in expressions (10) and (19):  $\tau = \tau_0 = \langle \tau_{\gamma=0} \rangle$ ,  $K = K_0 = \langle K_{\gamma=0} \rangle$ . As shown in [93], from the theory of random processes it follows that the value  $K = K_0$  is equal to the value of the boundary that the *FPT* of a random process with a fixed value of K reaches. You can write expressions for higher order correlators.

Let us check the fulfillment of the inequality  $\langle \tau \rangle_A / \sqrt{\operatorname{var}(\tau)} \leq \sqrt{K_A}$  obtained in [7] for expressions (30)-(34). In the notation of this article  $\langle \tau \rangle_A = \tau_0$ ,  $\operatorname{var}(\tau) = D_\tau |_{\gamma=0}$ ,  $K_A = K_0$ . For the two-level models discussed below and for the three-level model, strict inequality is satisfied.

# **4.** Dependences of the first and second moments of random variables of activity and FTP on changes in entropy

All real physical processes, which are modeled by stochastic processes, occur with a change in entropy. The changes in entropy plays an important role in calculating the average of the first-passage time [83-86]. The average *FTP* at zero value of the Laplace transforms argument of the density distribution of the *FTP*, which is usually used to determine the average value of the *FTP*, does not reflect the influence of real processes on the average *FTP*.

Expressions (30)-(34) include the parameter  $\gamma$ , which equal x in [2, 32], of Laplace transform argument in (18), (25), (28), (39). In this section, the parameter  $\gamma$  is associated with the total entropy change in the system during the *FPT*. Then the moments of random variables *FPT* and K (mean values, variances, correlations) are expressed through the parameter  $\gamma$  and the total change in entropy in the system during the *FPT* time. Let us describe the algorithm for expressing moments (30)-(34) through the total change in entropy. The total change in entropy  $\Delta s_{tot}$  consists of the change in the entropy of the system  $\Delta s_{sys}$  and the exchange of entropy with the environment  $\Delta s_m$ ,  $\Delta s_{tot} = \Delta s_{sys} + \Delta s_m$ . Expressions (30)-(34) depend on the parameter  $\gamma$ . The values of  $\Delta s_{sys}$  and  $\Delta s_m$  also depend on the parameter  $\gamma$ . Let us write down the relation  $\Delta s_{tot} = \Delta s_{sys}(\gamma) + \Delta s_m(\gamma)$  and consider it as an equation for the parameter  $\gamma$ , depending on  $\Delta s_{tot}$ ,  $\gamma(\Delta s_{tot})$ . Solving this equation, we obtain  $\gamma(\Delta s_{tot})$  and substitute it into expressions (30)-(34).

In this article, for the same thermodynamic quantity, which is conjugate to a random *FPT*, different notations are used, namely the notation  $\gamma$  in expressions (21), (31)-(34), and the notation x in expressions (18)-(20), (27)-(29). This is because an attempt is made to connect the results obtained for x-ensembles in [2, 32], where the notation x is used, with the results of articles [52-53], [83-84], where the notation  $\gamma$  is used. In both cases, in the statistical system, the *FPT* is considered as a random thermodynamic parameter, and the parameter  $\gamma$  (or x) is conjugate to the random thermodynamic variable *FPT*, as in distributions (20), (27), (39).

Therefore, in expression (19), where the function g(x) appears - an *LD* function depending on the argument x from [2, 32], it is possible to replace  $x=\gamma$  using the notation from [83-84]. By relation (21) the argument  $\gamma$  is related to the cumulant  $\theta(s)$ . We express this argument  $\gamma$  in terms of the change in entropy over the *FPT* time. The value of K from (19) is assumed to be proportional to the average value of K from expression (12). By setting s=0 here, we assume that the random process  $\tau$  changes accordingly. Let us denote it by  $\tau_0$  at s=0. When  $s \neq 0$ , the dependence of the parameter K on the argument  $\gamma$  has the form

$$\langle K \rangle = \langle K_s \rangle = \langle K_\gamma \rangle = -\frac{\partial \theta(s)}{\partial s} \tau.$$
 (35)

Subsequent calculations will be carried out for a two-level model. In [32-33] classical twolevel system is described as follows. The operator  $W_s$  is  $W_s = \begin{pmatrix} -\eta & e^{-s}\kappa \\ e^{-s}\eta & \kappa \end{pmatrix}$ , where  $W_s = \sum_{C' \neq C} e^{-s} w(C \to C') |C'\rangle \langle C| - \sum_{C} R(C) |C\rangle \langle C|$ ,  $W_s$  [2, 8] is deformed operator W (2) and  $\theta(s)$  (36) is its largest eigenvalue;  $\eta \neq \kappa$  are transition rates. In two-level system where there are only two configurations,  $C \in \{0,1\}$ , and the transition rates are,  $W(0 \to 1) = \kappa$  and  $W(1 \to 0) = \eta$ . From  $\theta(s)$ 

configurations,  $C \in \{0,1\}$ , and the transition rates are,  $W(0 \to 1) = \kappa$  and  $W(1 \to 0) = \eta$ . From  $\theta(s)$ we can obtain the activity value. For the average activity per unit time, we obtain expressions (35)-(37) as expected. For the case  $\kappa = \eta$  the *LD* function reduces to  $\theta(s) = \eta(e^{-s/2} - 1)$ , which is the cumulant generating function for a Poisson process with rate  $\eta$ . Similarly, the operator  $T_x$  (26) for this problem reads,  $T_x = \begin{pmatrix} 0 & \kappa / (x + \kappa) \\ \eta / (x + \eta) & 0 \end{pmatrix}$ , and from its largest eigenvalue, we obtain the *LD* 

function  $g(\gamma)$  (36). This function g is indeed the inverse of the function  $\theta(s)$  (36). The moments of the total time  $\langle \tau \rangle$  are obtained from  $g(\gamma)$ . In particular, the average total time, scaled by the number of jumps, is  $\langle \tau \rangle_{K} / K = -g(0) = (\kappa + \eta) / \kappa \eta$ , which is the inverse of (37). Analogous relations between the moments of K in the fixed  $\tau$  ensemble and those of  $\tau$  in the fixed K ensemble can be obtained by Eq. (21).

For a two-level classical system [32, 33] in [33] expressions obtained

$$g(\gamma) = -\ln(1 + \gamma a_1 + \gamma^2 a_2), \quad a_1 = \frac{\eta + \kappa}{\eta \kappa}, \quad a_2 = \frac{1}{\eta \kappa};$$
  

$$\theta(s) = \frac{1}{2} \left[ \sqrt{(\eta - \kappa)^2 + 4\eta \kappa e^{-s}} - (\eta + \kappa) \right].$$
(36)

From (10), (12) we obtain

$$\frac{\langle K_0 \rangle}{\tau} = \frac{1}{a_1} = \frac{\eta \kappa}{\eta + \kappa} = -\frac{\partial \theta(s)}{\partial s}\Big|_{\gamma = 0, s = 0}.$$
(37)

Below we will in the calculations limit ourselves to the value  $K = K_0 = \langle K_{\gamma=0} \rangle$ , although there are also possibilities for the value of *K* to depend on  $\gamma$  (Appendix A).

#### 4A. Example: classical two-level system, partition function (39)

Let's consider changes in entropy. The total change in entropy  $\Delta s_{tot}$  consists of the change in the entropy of the system  $\Delta s_{sys}$  and the exchange of entropy with the environment  $\Delta s_m$ ,

$$\Delta s_{tot} = \Delta s_{sys} + \Delta s_m \,. \tag{38}$$

The Gibbs/Shannon entropy of distribution of the form (27)-(28) [52-53], [83-84], [94], [88]

$$p_{s\gamma} = e^{-sK - \gamma \tau_{\gamma}} / Z_{s\gamma}, \quad Z_{s\gamma} = Z(s,\gamma) = Z_s Z_{\gamma}, \tag{39}$$

$$Z_s = Z_\tau(s) = \sum_K e^{-sK} P_\tau(K) \sim e^{\tau\theta(s)}, \quad Z_\gamma = Z_K(\gamma) = \int_0^\infty d\tau e^{-\gamma\tau} P_K(\tau) \sim e^{K_S(x)}$$

is equal to

$$= s_{sys} = -\left\langle \ln p_{s\gamma} \right\rangle = s \left\langle K_{\gamma} \right\rangle + \gamma \left\langle \tau_{\gamma} \right\rangle + \ln Z_{s\gamma}, \tag{40}$$

where the average values are

 $S_{\gamma}$ 

$$\langle K_{\gamma} \rangle = -\partial \ln Z_s / \partial s = \langle K_{s=g(\gamma)} \rangle.$$
 (41)

Entropy (40) includes the total average values  $\langle K_{\gamma} \rangle$  and  $\langle \tau_{\gamma} \rangle$ , and not the ratios  $\langle K_{\gamma} \rangle / \tau$  and  $\langle \tau_{\gamma} \rangle / K$ . The quantities  $lnZ_s$  and  $lnZ_{\gamma}$  also contain the parameters  $\tau$  and K. This complicates the problem due to the uncertainty of the expressions for K and  $\tau$  (paragraph after (34)).

The Gibbs/Shannon entropy (40) is naturally generalizable to nonequilibrium states, since it remains well-defined even when p(x) is not the Boltzmann distribution [94], [95]. The Clausius relation  $\Delta S \ge -Q/T$  (where Q is heat) which relates the change  $\Delta S$  in the entropy of a system to the heat Q exhausted into an ideal thermal reservoir at temperature T should hold for this choice of the entropy in a broad class of Markovian stochastic processes on a finite set of states [96]. Expressions (42)-(45) were obtained in [10] from Gibbs entropy (Shannon entropy). There are different types of entropy. For example, thermodynamic entropy and information entropy. They are not identical to each other. However, many works, for example, [89-91], [94-96], [101-103], show analogies between these quantities and effectively use their proximity. In general, the formulation of the entropy production problem is not universal. This depends on the dynamic laws governing the system, as well as on the underlying physical system itself. We will assume that for the entropy inside the system expression (40), (A3) is valid, and for the exchange of entropy with the environment expressions (42)-(45) are satisfied.

The partition function (39) differs from expression (29) and is written from expression (28) if the value of *K* is from the conditional probability  $P(\tau|K)$  and  $e^{Kg(x)}$  is not averaged over *K* (assuming, for example, this value *K* is equal to the mean value), as was done in [32], although the approach leading to the expression (29) is more consistent. Quantity (40) is equal to the entropy of the system  $s_{sys}$ , the value  $\langle \tau_{\gamma} \rangle$  from (31), (A2). A distribution of the form (39) was obtained in [88], as *sx*-ensemble. This distribution differs from the distribution obtained in [52, 83-84] by replacing the pair of conjugate quantities  $\beta u$  (the product of the inverse temperature  $\beta$  and energy *u*) by *sK* (activity *K* and the conjugate field *s*).

In [97], the change in K activity is associated with the production of entropy in the system and with the exchange of entropy between the system and the environment. With a single transition  $C \rightarrow C'$ , the change in entropy is

$$\Delta s_1(C,C') = \ln[w(C \to C') / w(C' \to C)].$$

$$\tag{42}$$

where  $w(C \rightarrow C')$  is the rate of the jump process. The change in entropy during the exchange with the medium while moving along the trajectory  $Y_K(C_0 \rightarrow C_1 \rightarrow ... \rightarrow C_K)$  is

$$\Delta s_m[C(t)] = \sum_{\alpha=1}^{K} \Delta s_1(C_{\alpha-1}, C_{\alpha}), \qquad (43)$$

as *K* changes from  $K_0$  to  $K_{\gamma}$ ,

$$\Delta s_{m(K_0K_{\gamma})}[C(t)] = \sum_{\alpha=K_0}^{K_{\gamma}} \Delta s_1(C_{\alpha-1}, C_{\alpha}), \qquad (44)$$

where we sum over all configuration changes. The corresponding dynamical partition function is [10, 97]

$$Z(\lambda,\tau) = \left\langle e^{-\lambda s_m} \right\rangle \sim e^{\tau \theta(\lambda)}, \qquad (45)$$

where  $\lambda$  is the parameter conjugate to  $s_m$ . In analogy with the activity, the mean entropy production rate in the  $\lambda$ -ensemble is given  $\langle s_m \rangle / \tau = -\partial \theta(\lambda) / \partial \lambda$ . Assuming that the quantity  $\Delta s_1 = \Delta s_1(C_{\alpha-1}, C_{\alpha})$  is constant, expression (45) takes the form

$$\Delta s_{m(K_0K_{\gamma})}[C(t)] = \Delta s_1(\langle K_{\gamma} \rangle - \langle K_{\gamma=0} \rangle).$$
(46)

Using expression (39) and the results of [98] (43), we obtain for the term from (38), when  $\langle s_m \rangle = -\tau \partial \theta(\lambda) / \partial \lambda$ ,  $\tau = \tau_0$ ,  $\Delta \langle s_m \rangle = \langle s_{m|K_{\gamma}} \rangle - \langle s_{m|K_0} \rangle = -\tau [\partial \theta(\lambda) / \partial \lambda |_{\lambda=\gamma} - \partial \theta(\lambda) / \partial \lambda |_{\lambda=0}]$ , (47)

Expression (47) coincides with (46) at  $\Delta s_1 = (+/-)1$  [60].

Expressions (42)-(45) were obtained in [97] for the thermodynamics of trajectories, expanding the *s*-ensemble approach to driven systems based on the results obtained in [10]. In [98] noted the difficulties of physical interpretation of general definitions entropy production for specific physical systems. In [98] as well as in [99] entropy production obtained for the Markov jump process. Expressions (42)-(45) for Egs. dynamics (1)-(2) were used in [100] for the connection between gauge invariance in stochastic dynamics and fluctuation theorems. These

issues are also discussed in [101-103], and in other works. In [94], notes the important role of the "microscopic reversibility relation" in terms of the thermodynamic entropy of the environment since it encodes the time-reversibility of the full microscopic dynamics in a coarse-grained stochastic dynamic. In general, the formulation of the entropy production problem is not universal. This depends on the dynamic laws governing the system, as well as on the underlying physical system itself.

Let us express the parameter  $\gamma$  in terms of the change in entropy. Let us expand the expressions from relation (36) into a series in  $\gamma$  up to the power  $\gamma^2$ :

$$\ln(1 + \gamma a_1 + \gamma^2 a_2) = \gamma a_1 - \gamma^2 c_3 + \dots, \ c_3 = a_1^2 / 2 - a_2,$$

$$\frac{a_1 + 2\gamma a_2}{1 + \gamma a_1 + \gamma^2 a_2} = a_1 - \gamma 2c_3 + \gamma^2 a_1(2c_3 - a_2) + \dots.$$
(48)

If in (40) we used expansions (48), then

$$\Delta \langle s_{sys} \rangle / \langle K_0 \rangle = (\langle s_0 \rangle - \langle s_\gamma \rangle) / \langle K_0 \rangle = \gamma^2 [2a_2 - a_1^2] = \gamma^2 a_s,$$
(49)

where  $a_s = [2a_2 - a_1^2]$ 

For further estimates, we need to know the explicit form of the function  $g(\gamma)$ . Let us consider an example of a classical two-level system [32, 33] (a quantum system can also be considered) with a function  $g(\gamma)$  of the form (36). Up to  $\gamma^2$ , from (47), (48), we obtain

$$\left\langle \Delta s_m \right\rangle = \gamma^2 (\pm a_m) + \gamma (\pm b_m), \tag{50}$$

where  $a_m = 4a_2^2 / a_1^2 - a_2$ ,  $b_m = a_1 - 2a_2 / a_1$ . The sign in (50) depends on whether flows enter the environment (+ sign) or exit the system into the environment (- sign). The plus or minus sign is determined by the flow sign: into the system from the environment or vice versa - from the system to the environment.

Using expression (36) leads to a transcendental equation for the parameter  $\gamma$ . If we expand into a series and restrict ourselves to quadratic terms in  $\gamma$ , then from (38), (49), (50) we obtain an equation for  $\gamma$  of the form

$$a\gamma^{2} + b\gamma + d = 0, \ a = -(a_{s} \pm a_{m}), \ b = -(\pm)b_{m}, \ d = \Delta \langle s_{tot} \rangle / \langle K_{0} \rangle.$$
(51)

The coefficients of this equation depend on the sign of expressions (50), (51).

The solution of equation (51) has the form

$$\gamma = [\pm \sqrt{b^2 - 4da} - b] / 2a,$$
 (52)

where the parameters *a* and *b* from expressions (50), (51), depending on the sign, take the values
$$a_{+} = -a_{s} - a_{m}, \quad a_{-} = -a_{s} + a_{m}, \quad (53)$$

where 
$$a_{+} = -(a_{s} + a_{m}) = a_{1}^{2} - a_{2} - 4a_{2}^{2} / a_{1}^{2}, a_{-} = -(a_{s} - a_{m}) = a_{1}^{2} - 3a_{2} + 4a_{2}^{2} / a_{1}^{2}$$
,  
 $b_{+} = -b_{m}, b_{-} = b_{m}, b_{+} < 0, b_{-} > 0$ , as for model (36)  $2a_{1}^{2} - 5a_{2} > 0, 7a_{1} / 2 + 3a_{2} / a_{1} > 0$ .

If in (52) we choose the + sign in front of the square root, then we get two solutions depending on the signs in (51). Let's denote them

$$\gamma_{1(+)(+)} = \left[\sqrt{b_{+}^{2} - 4da_{+}} - b_{+}\right] / 2a_{+} = \left[\sqrt{1 - 4da_{+}} / b_{m}^{2} + 1\right]b_{m} / 2a_{+} > 0.$$
(54)

The first subscript (+) in (54) denotes the sign before the square root in (52), and the second plus sign corresponds to the sign choice in (50)-(51). At  $\Delta \langle s_{tot} \rangle = 0$ , expression (54) is equal to  $b_m / a_+ \neq 0$ . Then expressions (49), (50) are not equal to zero, but  $\Delta \langle s_m \rangle = -\Delta \langle s_{sys} \rangle$ . This is a stationary nonequilibrium state (at  $\Delta \langle s_{tot} \rangle = 0$ ) as defined in [104]. In [105] it is shown that  $\gamma \sim \sigma_s$ , the production of entropy in the system;  $\sigma_s \sim \Delta \langle s_{sys} \rangle / \langle \tau_{\gamma} \rangle$ , and  $\gamma \sim q$ , flows in the system. This case describes nonequilibrium stationary states when  $\Delta \langle s_{tot} \rangle = 0$ , but  $\Delta \langle s_{sys} \rangle \neq 0$ ,  $\Delta \langle s_m \rangle \neq 0$ ,  $\Delta \langle s_m \rangle \neq 0$ ,  $\Delta \langle s_{sys} \rangle = -\Delta \langle s_m \rangle$ , [93]. For the "–" sign in (51), we obtain the solution

$$\gamma_{1(+)(-)} = \left[\sqrt{1 - 4da_{-}/b_{m}^{2}} - 1\right]b_{m}/2a_{-}, \qquad \Delta \langle s_{tot} \rangle \ge 0.$$
(55)

At  $\Delta \langle s_{tot} \rangle = 0$ , expression (55) vanishes. Then expressions (49), (50) also vanish. This is the equilibrium state (at  $\Delta \langle s_{tot} \rangle = 0$ ).

If in (52) we choose the sign "-" in front of the square root, then we also obtain two solutions depending on the signs in (51)-(52):

$$\gamma_{2(-)(+)} = \left[-\sqrt{1 - 4da_{+} / b_{m}^{2}} + 1\right]b_{m} / 2a_{+},$$
(56)

$$\gamma_{2(-)(-)} = -\left[\sqrt{1 - 4da_{-} / b_{m}^{2} + 1}\right]b_{m} / 2a_{-}, \qquad \Delta \langle s_{tot} \rangle \ge 0.$$
(57)

For negative values of  $\gamma$ , the convergence condition of the Laplace transforms of the *FPT* distribution, partition function  $Z_{\gamma}$  from (39), must be satisfied. At large times, the time distributions tend to an exponential distribution of the form  $\tau_0^{-1} \exp(-\tau/\tau_0)$ ,  $\tau_0 = \langle \tau_{\gamma=0} \rangle$ . For the Laplace transform by  $\gamma$  of an exponential distribution of the *FPT* with mean value  $\tau_0$ , at  $\gamma < 0$  the condition

$$\gamma + 1/\tau_0 > 0 \tag{58}$$

must be satisfied. In case (57), for the convergence of  $Z_{\gamma}$ , the condition  $\Delta \langle s_{tot} \rangle \ge 0$  must be satisfied. For the parameter values chosen below the values  $\gamma_{(-)(-)}$  (57) are not realized. For case  $\gamma_{(+)(+)}$  (56), condition (58) leads to a constraint of the form d < 0.00676 for values of the parameters  $\eta=5$ ,  $\kappa=1.25$  as in [33].

The condition of positivity of the radical expression must also be satisfied, which also imposes a boundedness condition on *d* of the form  $d < b^2 / 4a$ . For the case of a positive sign in (50) and for values of the parameters  $\eta=5$ ,  $\kappa=1.25$ , this condition gives the limitation d<0.1567. For the case of a negative sign in (50) d<0.1863.

If we substitute  $\Delta \langle s_{tot} \rangle = 0$  into equation (51), then we obtain the equation for  $\gamma$ ,

$$\gamma[\gamma(a_s \pm a_m) \pm b_m] = 0.$$
<sup>(59)</sup>

The first root of this equation is  $\gamma=0$ . Substituting this root into expressions (50), (49) gives that  $\Delta \langle s_{sys} \rangle = \Delta \langle s_m \rangle = 0$ . This situation describes an equilibrium state (55), (56). The second root of equation (59) is  $\gamma = \mp b_m / (\pm a_m + a_s)$ . In this case  $\Delta \langle s_{sys} \rangle \neq 0$ ,  $\Delta \langle s_m \rangle \neq 0$ , but  $\Delta \langle s_{tot} \rangle = 0$ . This is a stationary non-equilibrium state  $\gamma_{(+)(+)}$ . State (57) not realized. It can be seen from (36) that at  $\gamma = 0$ , s = 0. This case corresponds to a phase transition [2, 12]. When the dynamics have two phases, an active one for s<0 and an inactive one for s>0 [2, 12]. The used model (36) leads to the existence of two equilibrium states, one of which (55) is possible in range of entropy changes d<0.1567, and the second is possible only in a narrow range of entropy changes defined by expression (58). A stationary nonequilibrium state was also obtained, in which the values  $\gamma = 0$ , s = 0. are not reached, and no phase transition occurs. Thus, the system has an active phase (55) with  $\gamma > 0$ , s < 0 and an inactive phase (56) with  $\gamma < 0$ , s > 0 which is limited. The transition between them occurs with a change in the branch  $\gamma$  from (55) to (56) and back through

the equilibrium state, in which s = 0,  $\Delta \langle s_{tot} \rangle = \Delta \langle s_{sys} \rangle = \Delta \langle s_m \rangle = 0$ . In addition, there is an active phase (54)  $\gamma > 0$ , s < 0, a stationary nonequilibrium state without a phase transition.

If we consider not the average, but the random total change in entropy, then this value can be negative, not exceeding the Boltzmann constant. Then the exchange of entropy with the medium should be considered as a random variable.

Below, as in expressions (30)-(34), we consider the observables dynamic activity *K* and *FPT*, the first and second moments of these observables, and the correlation between them. The *s*-tilted probability density of *x* satisfies of relation  $f_s(x) \sim e^{sx} f(x)$ . The expressions obtained below for the moments depend on the parameter  $\gamma$  associated with the change in entropy. The equations of motion also are modified to create a tilted or twisted equation of motion. The function  $\theta(s)$  can be obtained by deforming the master operator W(2) and replacing it with  $W_s$  [10, 28]. In particular, for the case of activity, this deformed operator is considered in [2, 8, 12], for *FPT* the deformed generators are  $T_{x,c}$  (26) (by  $x=\gamma$ ). The scaled cumulant generating function  $\theta(s)$  and the rate function  $\varphi(a)$  (8) are related by a Legendre transform,  $\varphi(a)=-min_s[\theta(s)+sa]$  (13), that is,  $\varphi(a)=-\theta[s(a)]-s(a)a$ , with *s* and *a* related through  $a(s)=-\theta'(s)$ .

Let us illustrate the obtained results of dependences on entropy change. Let us write out the ratios according to which Figures 1-3 were built. A two-level model (36) is used with the values of the parameters  $\eta$ =5,  $\kappa$ =1.25, as in [33]. To avoid ambiguity in determining the values of *K* and  $\tau$  in (39)-(41), we take the values of *K* equal to  $K_0$ . Let value  $K_0$ =100. From (30)-(34) we have (at  $K = \langle K_{\tau} \rangle \approx \langle K_0 \rangle$ )

$$\langle T \rangle = \langle \tau_{\gamma} \rangle \simeq \langle K_{0} \rangle \frac{\partial g(\gamma)}{\partial \gamma} = \langle K_{0} \rangle \frac{a_{1} + 2\gamma a_{2}}{1 + \gamma a_{1} + \gamma^{2} a_{2}} = 10^{2} \frac{1 + 0.32\gamma}{1 + \gamma + 0.16\gamma^{2}}, \quad \langle K_{0} \rangle = 100,$$

$$D_{K_{0}} = \frac{\eta \kappa (\eta^{2} + \kappa^{2})}{(\eta + \kappa)^{3}} \langle T_{0} \rangle = 0.68 \langle T_{0} \rangle = 0.68 \langle K_{0} \rangle, \quad \langle T_{0} \rangle = \langle K_{0} \rangle a_{1},$$

$$D_{T} = \langle K_{0} \rangle \frac{2(-a_{2} + a_{1}^{2} / 2 + \gamma a_{1} a_{2} + \gamma^{2} a_{1} a_{2})}{(1 + \gamma a_{1} + \gamma^{2} a_{2})^{2}}, \quad a_{1} = 1,$$

$$(61)$$

$$CorrTK = \langle TK \rangle - \langle T \rangle \langle K \rangle = 0.68 \langle K_0 \rangle \frac{a_1 + 2\gamma a_2}{1 + \gamma a_1 + \gamma^2 a_2}, \qquad (62)$$

where  $\langle T \rangle = \langle \tau \rangle$  is the average *FPT*,  $D_{K_0} = \langle K_0^2 \rangle - \langle K_0 \rangle^2$  is the variance of  $K_0$ ,  $D_T = \langle T^2 \rangle - \langle T \rangle^2$  is the variance of *FPT*, and *CorrTK* is the correlation (34) between *T* and *K*. The value of  $\gamma$  in (60)-(62) can be of the form (54)-(56). For model (36) with parameter values  $\eta=5$ ,  $\kappa=1.25$ , the values (54)-(56) are:

 $\gamma_{1(+)(+)} = 0.461[\sqrt{1-6.381d} + 1], \quad \gamma_{2(-)(+)} = 0.546[\sqrt{1-5.384d} - 1], \quad \gamma_{1(+)(-)} = 0.461[1-\sqrt{1-6.381d}], \quad d = \Delta \langle s_{tot} \rangle / \bar{K}_0.$ (63) The condition for the radical expression to be positive limits the quantity *d*. So, *d*<1/6.381=0.1567. Figures 1-3 show the behavior of the average *FPT*  $\langle T \rangle$  (60), dispersions of *FPT* (61), and correlator (69) depending on  $\gamma_{1(+)(+)}, \gamma_{2(-)(+)}$  (63) and parameter  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$ .



Fig. 1. The behavior of  $\langle T(d) \rangle$  (60) [full (blue)],  $DT(d) = D_T(d)$  (61) [dashed (green)], CorrTK(d) = Co(d) (62) [dot-dash (red)] at  $\gamma = \gamma_{I(+)(+)}$  (54), (63) from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  in the range 0 < d < 0.156.



Fig. 2. The behavior of  $\langle Tm(d) \rangle = \langle T(d) \rangle$  (60) [full (blue)],  $DTm(d) = D_T(d)$  (61) [dashed (green)], CorrTK(d) = Co/m(d) (62) [dot-dash (red)] at  $\gamma = \gamma_{I(+)(-)}$  (55), (63) from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  in the range 0 < d < 0.156.



Fig. 3. The behavior of  $\langle T(d) \rangle = T2$  (60) [full (blue)],  $DT2(d) = D_T(d)$  (61) [dashed (green)], CorrTK(d) = Corr2(d) (62) [dot-dash (red)] at  $\gamma = \gamma_{2(-)(+)}$  (56), (63) from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  in the range 0<d<0.00676 corresponding to the convergence of the Laplace transform of the *FPT* distribution  $Z_\gamma$ , obtained from (58).

We write the dependence of the average activity  $\langle K_{\gamma} \rangle$  on the parameter  $\gamma$  in the form

$$\langle K_{\gamma} \rangle \approx - \langle \tau_{0} \rangle \frac{\partial \theta(s)}{\partial s} |_{s=g(\gamma)} .$$
 Then  
 
$$\langle K_{\gamma} \rangle = \langle \tau_{0} \rangle \frac{\eta \kappa (1 + a_{1}\gamma + a_{2}\gamma^{2})}{(\eta + \kappa)\sqrt{1 + 4\eta\kappa(a_{1}\gamma + a_{2}\gamma^{2})/(\eta + \kappa)^{2}}} = \langle K_{0} \rangle \frac{1 + a_{1}\gamma + a_{2}\gamma^{2}}{\sqrt{1 + 4(a_{1}\gamma + a_{2}\gamma^{2})/a_{1}(\eta + \kappa)}} .$$
 (64)

Figure 4 shows the behavior of  $\langle K_{\gamma} \rangle$  (64) depending on  $\gamma_{I(+)(+)}$ , (63)  $\langle K_{\gamma^{1+}} \rangle$ ,  $\gamma > 0$ , s < 0 (active phase),  $\gamma_{I(+)(-)}$ , (63),  $\langle K_{\gamma^{1-}} \rangle$ , at  $\gamma < 0$ , s > 0 (inactive phase), and on  $\gamma_{2(-)(+)}$ , (63)  $\langle K_{\gamma^{2+}} \rangle$ ,

at  $\gamma > 0$ , s < 0 (active phase) in scale 0 < d < 0.156. Similar dependencies (but from *s*, not from  $\gamma$ ) were obtained in [2, 12].



Fig. 4. The behavior of  $\langle K_{\gamma} \rangle$  (64) from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  depending on  $\gamma_{I(+)(+)}$  (63),  $\langle K_{\gamma^{1+}} \rangle = KI +$  [full (blue)], depending on  $\gamma_{I(+)(-)}$  (63),  $\gamma > 0$ , s < 0 (active phase),  $\langle K_{\gamma^{1-}} \rangle = KI -$  [dashed (green)], and on  $\gamma_{2(-)(+)}$  (63),  $\langle K_{\gamma^{2+}} \rangle = K2 +$  [dot-dash (red)],  $\gamma < 0$ , s > 0 (inactive phase). Panel shows  $\langle K_{\gamma^{1-}} \rangle$ ,  $\langle K_{\gamma^{2+}} \rangle$ ,  $\langle K_{\gamma^{1+}} \rangle$  from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  in the range 0<d<0.156.

#### 4B. Example: classical two-level system, partition function (29)

Calculations Figs. 1-4 was carried out using expression (39), with a statistical sum of the form  $Z_{s\gamma} = Z(s,\gamma) = Z_s Z_{\gamma}$ ,  $Z_s = Z_r(s) = \sum_{\kappa} e^{-s\kappa} P_r(K) \sim e^{r\theta(s)}$ , (9), (10),  $Z_{\gamma} = Z_K(\gamma) \equiv \int_0^{\infty} d\tau e^{-\gamma\tau} P_K(\tau)_{|_{s=\gamma}} = e^{K_g(\gamma)}$ , (18), (19). If we calculate using expression (29), in which the partition function is equal to  $Z = Z_r(s_{ef}) = \sum_{\kappa} e^{-K(s-g(\gamma))} P(K)$ ,  $s_{ef} = s - g(\gamma)$ , and at large times  $Z_r(s_{ef})_{r\to\infty} \to 1$ ,  $\langle \tau \rangle_{\gamma} = -\langle K_0 \rangle \partial g(\gamma) / \partial \gamma$ ,  $\langle K \rangle_{\gamma} = \langle K \rangle_0$ , (30), (31) then  $\ln Z_r(s_{ef})_{s_{es}=0} = 0$ . Using expression (47) to determine  $\Delta s_m$ , (38), we obtain, using expressions (21), (36), an equation for determining the parameter  $\gamma$  through  $\Delta s_{tot}$  the signs "+" and "-" in  $\Delta s_m$ . This equation also has four solutions. These are functions  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  of the form

$$\begin{split} \gamma_{01(+)(+)} &= 4.38[\sqrt{1 - 0.67d} + 1], \quad \gamma_{01(+)(-)} = 4.38[-\sqrt{1 - 0.67d} + 1], \\ \gamma_{02(-)(+)} &= 9.05[1 + \sqrt{1 + 0.325d}], \quad \gamma_{02(-)(-)} = 9.05[1 - \sqrt{1 + 0.325d}], \quad d = \Delta \langle s_{tot} \rangle / \bar{K}_0. \end{split}$$
(65)

The designation 0 indicates that  $\ln Z_r(s_{ef})_{r\to\infty} \to 0$ . On Figs. 5-8 show the results of calculations with expressions (29), (65) corresponding to Figs. 1-4 obtained using expressions (39), (63). The behavior of the parameters  $\gamma$  does not change qualitatively. As in case (63), for case 1a) the quantities  $\gamma_{01(+)(+)}$  and  $\gamma_{02(-)(+)}$  describe the system in a stationary nonequilibrium state, for quantities 1b), 2a) equilibrium states  $\gamma_{01(+)(-)}$  and  $\gamma_{02(-)(-)}$  are possible, and the value  $\gamma_{02(-)(-)}$  (63) is realized only at small values of d < 0.0067. But for the partition function (29), the convergence condition differs from (58). Therefore, the question of the existence of the values  $\gamma_{02(-)(-)}$  and the boundaries of the value  $\gamma_{02(-)(+)}$  requires a separate study. Considering the closeness of the results obtained when using partition functions (39) and (29), we can assume that expression (65) can also be used to estimate the convergence of relation (29). The requirement that the radical expression in  $\gamma_{01(+)(+)}$  and  $\gamma_{02(+)(-)}$  be positive gives the condition d < 1.49.



Fig.5. The behavior of  $\langle T(d) \rangle$  (60) [full (blue)],  $DT(d) = D_T(d)$  (71) [dashed (green)], CorrTK(d) = CoO(d) (62) [dot-dash (red)] at  $\gamma = \gamma_{OI(+)(+)}$  (65) from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  in the range 0 < d < 1.4.

It can be seen that the first and second moments of *FPT*, the correlation of *FPT* and activity *K* behave in the same way as in Fig. 1, shifting in height.



Fig.6. The behavior of  $\langle TOm(d) \rangle = \langle T(d) \rangle$  (60) [full (blue)],  $DOTm(d) = D_T(d)$  (61) [dashed (green)], CorrTK(d) = Co/Om(d) (62) [dot-dash (red)] at  $\gamma = \gamma_{0I(+)(-)}$  (65) from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  in the range 0 < d < 1.4.

Fig. 6 for partition function (28)-(29) repeats the behavior of Fig. 2 for partition function (39). The general nature of the dependence remains.



Fig.7. The behavior of  $\langle T(d) \rangle = T02$  (60) [full (blue)],  $DT02(d) = D_T(d)$  (61) [dashed (green)], CorrTK(d) = Corr02(d) (62) [dot-dash (red)] at  $\gamma = \gamma_{02(-)(+)}$  (65) from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  in the range 0 < d < 15 (Fig 7a)) and at  $\gamma = \gamma_{02(-)(-)}$  (65) in the range 0 < d < 0.007 (Fig. 7b)). Fig. 7b) corresponded to the convergence of the Laplace transform of the *FPT* distribution  $Z_{\gamma}$ , obtained from (58).

In this case, there is agreement with Fig. 3. Curves in Fig. 7b) grow faster than in Fig. 3b).



Fig. 8. The behavior of  $\langle K_{\gamma} \rangle$  (64) from  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  depending on  $\gamma_{I(+)(+)}$  (65),  $\langle K_{\gamma^{1+}} \rangle = KI +$  [full (blue)], depending on  $\gamma_{I(-)(+)}$  (65),  $\gamma > 0$ , s < 0 (active phase),  $\langle K_{\gamma^{1-}} \rangle = K2 +$  [dot-dash (red)], and on  $\gamma_{2(+)(-)}$  (65),  $\langle K_{\gamma^{2-}} \rangle = KI -$  [dashed (green)],  $\gamma < 0$ , s > 0 (inactive phase). Panel (a) shows  $\langle K_{\gamma^{1+}} \rangle$ ,  $\langle K_{\gamma^{1-}} \rangle$ ,  $\langle K_{\gamma^{2-}} \rangle$  in the range 0<d<1.4. Panel (b) shows  $\langle K_{\gamma^{2--}} \rangle = K2 -$  on from  $\gamma_{2(-)(-)}$  (65) in the range 0<d<0.007 (Fig. 8b) corresponding to the convergence of the Laplace transform of the *FPT* distribution  $Z_{\gamma}$ , obtained from (58).

Thus, the results obtained using the calculations using expressions (29) and (39) are close, although the partition functions differ from each other. When deriving expression (29), fewer assumptions were made. Therefore, this expression may be preferable.

#### 4C. Example: classical three-level system

Three-level systems are present in many physical contexts. A spin-1 particle in an external magnetic field, three states of atoms or molecules bound by lasers or other interactions, three-level atom interacting with two classical monochromatic fields and oscillations between three neutrino flavors these are just a few different examples. We focused for simplicity on stochastic Markovian classical systems. Classical systems are only an approximation of the behavior of quantum systems in certain limits (e.g. large mass/energy, high temperature, long timescales). In [23] in three-level system the statistics of the number *K* of photons emitted from Level  $|1\rangle$  decays to  $|0\rangle$  with rate  $\kappa_1$  is obtained. Let us limit ourselves to a simple model, a special case of a three-level system, considered in [32]. As a simple example consider the classical three-level system with configurations  $|0\rangle$ ,  $|1\rangle$ ,  $|2\rangle$ . Suppose we only observe the jumps between configurations  $|2\rangle$  and  $|0\rangle$ . In the notation above (from (22)-(25)) we have N = 1, and  $\vec{M}$  is just  $K_{20}$ , the total number of

transitions between top and bottom levels. In the *s*-ensemble, the largest eigenvalue of the operator

$$W_{s_{20}} = \kappa \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ e^{-s_{20}} & 0 & -1 \end{pmatrix}$$
(66)

(where  $s_{20}$  is the field conjugate to  $K_{20}$ ,  $\kappa$  is the rate of jumps between configurations 2 and 0 associated to emission into the bath) gives the *LD* function,

$$\Theta(s_{s_{20}}) = \kappa(e^{-s_{20}/3} - 1), \qquad (67)$$

which is the cumulant generating function for the number of jumps  $K_{20}$  per unit time. In the *x*-ensemble context, the relevant operator is

$$T_{x,s_{20}} = \frac{\kappa}{x+\kappa} \begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 1\\ e^{-s_{20}} & 0 & 0 \end{pmatrix}.$$
 (68)

From its largest eigenvalue we obtain the *LD* function from (25)

$$G(\gamma, s_{20}) = -s_{20} + 3[\log \kappa - \log(\gamma + \kappa)].$$
(69)

This is the generating function for cumulants of both  $\tau/K$  and  $K_{20}/K$ ;

$$g(\gamma) = G(\gamma, s_{20} = 0) = 3[\log \kappa - \log(\gamma + \kappa)].$$
(70)

If we solve  $G(x_*, s_{20})=0$  for  $x_*$  we get,  $x_*(s_{20})=\gamma_*(s_{20})=\Theta(s_{20})$  above, in accordance with (21).

Let us consider the case corresponding to expression (29), when at large times the partition function is equal to unity. For the average value of K from (10), (12), (41), (67), (21) we obtain

$$\left\langle K_{\gamma} \right\rangle = -\tau \frac{\partial \Theta(s)}{\partial s}\Big|_{s=g(\gamma)} = \tau \frac{\kappa}{3} e^{-s_{20}/3}\Big|_{s_{20}=g(\gamma)} = \tau \frac{\kappa}{3} (1 + \frac{\gamma}{\kappa}).$$
(71)

This expression depends on the value of  $\tau$ , which is not specified in relation (10); it is only required to be large enough to satisfy the *LD* relations. Therefore, there is a certain arbitrariness in the choice of parameter  $\tau$ , the average value of which from (70) is equal to

$$\left\langle \tau_{\gamma} \right\rangle = -K \frac{\partial g(\gamma)}{\partial \gamma} = \frac{3K}{\kappa} \frac{1}{1 + \gamma/\kappa} = \tau_0 \frac{1}{1 + \gamma/\kappa}.$$
 (72)

If in expression (72) we choose  $K = \langle K_{\gamma=0} \rangle = K_0$ , then substituting this value of K into (72), followed by substituting (72) into (71), taking into account the relation  $\gamma = x = x_*$ ,  $e^{-s_{20}/3} = 1 + \gamma / \kappa$  leads to the expression  $\langle \tau_{\gamma=0} \rangle = 3K_0 / \kappa$ . If we substitute expression (72) into expression (71) with  $\tau = \langle \tau_{\gamma=0} \rangle = 3K_0 / \kappa$ , we obtain

$$\langle K_{\gamma} \rangle = K_0 (1 + \gamma / \kappa) .$$
 (73)

Differentiating expressions (72) by  $\gamma$  and (71) by *s*, we obtain relations for the dispersion  $D_{\tau}$  of the time  $\tau$  and for the dispersion  $D_K$  of dynamic activity *K*:

$$D_{\tau} = \frac{3K_0}{\kappa^2} \frac{1}{(1 + \gamma / \kappa)^2},$$
(74)

$$D_{\kappa} = \frac{K_0}{3} (1 + \gamma / \kappa) = \frac{\langle K \rangle}{3}.$$
(75)

Using expressions (34), (72), (75) we obtain

$$D_{\tau \kappa} = \frac{K_0}{\kappa} \frac{1}{(1 + \gamma / \kappa)} \,. \tag{76}$$

As above, in sections 4A), 4B), it is possible to find changes in entropy in the system  $\Delta s_{sys}$  using expressions (39) or (29). We use expression (29) as in Section 4B). We consider a simplified model at  $\kappa = 0.5$ ,  $K_0 = 100$ . For  $\Delta \langle s_{sys} \rangle$ , taking into account that at large times  $Z_\tau(s_{ef}) = 0$ , we obtain after expansion in a series in  $\gamma$  and restriction to quadratic terms:  $\Delta \langle s_{sys} \rangle = 9K_0(\gamma/\kappa)^2/2$ . Using expression (47), after expansion into a series we find:  $\Delta s_m = \pm K_0 \gamma/\kappa$ . Depending on the sign in front  $\Delta s_m$ , we obtain two quadratic equations with solutions: with the "+" sign in  $\Delta s_m$ :

$$\gamma / \kappa = [\pm \sqrt{1 + 18d} - 1] / 9, \quad d = \Delta s_{tot} / K_0,$$
(77)

and with the sign "-" in  $\Delta s_m$ :

$$\gamma / \kappa = [\pm \sqrt{1 + 18d} + 1] / 9.$$
 (78)

Condition (58) is not satisfied for solution (77)  $(\gamma_{(+)} / \kappa)(d)$  with a minus sign. For solutions  $(\gamma_{(+)} / \kappa)(d) = [\sqrt{1+18d} - 1]$ ,  $(\gamma_{(-)} / \kappa)(d) = [\sqrt{1+18d} + 1]$ , condition (58) is satisfied for all *d*. For  $(\gamma_{(-)} / \kappa)(d) = [-\sqrt{1+18d} + 1]$  condition (58) is satisfied for  $d < 1/\tau_0 + 9/2\tau_0^2$ . In [23] it is shown that for *s*>0 (which corresponds to values of  $\gamma < 0$ ) the cumulant  $\theta(s)$  takes constant value. But we are considering a very small segment for  $\gamma < 0$ , when this circumstance can be ignored. We rewrite the realized parameters in (77)-(78) in the form

 $(\gamma_{(++)} / \kappa)(d) = [\sqrt{1+18d} - 1]/9, (\gamma_{(++)} / \kappa)(d) = [\sqrt{1+18d} + 1]/9, (\gamma_{(--)} / \kappa)(d) = [-\sqrt{1+18d} + 1]/9.$  (79) The solution  $(\gamma_{(-+)} / \kappa)(d)$  describes stationary nonequilibrium states in which there is no equilibrium. For solutions  $(\gamma_{(++)} / \kappa)(d)$  and  $(\gamma_{(--)} / \kappa)(d)$ , equilibrium and phase transitions are possible.





Fig. 9. Behavior of functions (72)-(76)  $\langle \tau(d) \rangle$  (full, red),  $\langle K(d) \rangle$  (dashed, green),  $D_{\tau}(d)$  (dash-dotted, blue),  $D_{K}(d)$  (short dash, pink),  $D_{\tau K}(d)$  (dot, purple) depending on  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  when substituting parameter  $\gamma(d)/\kappa$  (79) into expressions (72)-(76). Range d=(0,...,10),  $(\gamma_{(++)}(d)/\kappa)$  on Fig. 9a),  $(\gamma_{(++)}(d)/\kappa)$  on Fig. 9b).

Figure 10 shows the dependence of average values and variances on  $(\gamma_{(+)}(d)/\kappa)$  (79) in the interval *d* values (0,...,0.0016). It can be seen that these values are constant over this interval. The calculation confirms the conclusions [23]. The same situation with Fig. 7b).



Fig. 10. Behavior of functions (72)-(76)  $\langle \tau(d) \rangle$  (full, red),  $\langle K(d) \rangle$  (dashed, green),  $D_{\tau}(d)$  (dash-dotted, blue),  $D_{K}(d)$  (short dash, pink),  $D_{\tau K}(d)$  (dot, purple) depending on  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  when substituting parameter ( $\gamma(-)(d)/\kappa$ ) (79) into expressions (72)-(76). Range d=(0,...,0.0016).

#### 4D). Example: the quantum two-level system, partition function (80)

In subsections 4A)-4C) distributions (29) and (39) were used. In this subsection we will use a distribution of the form

$$P_{M}^{sx}(K,\tau) = Z_{M}^{-1}(K,\tau)e^{-sK-x\tau}P_{M}(K,\tau),$$
(80)

where *M* is some fixed value, as in (27), the parameters *K* and  $\tau$  fluctuate;  $P_M(K, \tau)$  is the probability that an unbiased trajectory has a given duration  $\tau$  and the fluctuating observable reaches a certain value *K* by the time the other observable reaches its fixed value *M*. This distribution was obtained in [88], [52-53], [83-84], [32]. It is written from (27) after summation over  $M_I$ . The corresponding grand-partition function is (81) where the right-hand side takes the expected large deviation form with scaled-cumulant generating function (*SCGF*) G(s, x)

$$Z_{M}(K,\tau) = \sum_{K} \sum_{\tau} e^{-sK - x\tau} P_{M}(K,\tau) \sim e^{MG(s,x)},$$
(81)

we use the notation G, as in (25) [32}, in [88] the notation  $\varphi$  is used. SCGF from (19) is  $g(x)=G(s,x)_{x=0}$ . The average values are

$$\langle K \rangle = -\tau_0 \partial g(\gamma) / \partial \gamma, \quad \langle \tau \rangle = -K_0 \partial \theta(s) / \partial s.$$
 (82)

Let's apply these expressions to the quantum two-level system. The quantum two-level system corresponds to a system of two quantum levels  $|0\rangle$ ,  $|1\rangle$ , coherently driven on resonance at Rabi frequency  $\Omega$  and coupled to a zero-temperature bath [49]. The Hamiltonian, the single-jump operator, the super-operator  $W_s$ , the operator  $T_{x,s}$  (26), its largest eigenvalues are given, for example, in [32]. The largest eigenvalues  $G(s, \gamma)$ ,  $g(\gamma)$  coincide with expressions (67), (69), (70) of Section 4C), differing only in the parameter value. Accordingly, expressions (72)-(76), (77)-(79) also coincide. The parameter  $\kappa$  in 4C) is replaced by  $2\Omega$ . Let's put  $\Omega=1$  MHz. Then

$$\langle \tau_{\gamma_1} \rangle = 150 / (1 + \gamma_1), \quad \langle K_{\gamma_1} \rangle = 100(1 + \gamma_1), \quad \langle D_\tau \rangle = 75 / (1 + \gamma_1)^2,$$

$$\langle D_K \rangle = \langle K_{\gamma_1} \rangle / 3, \quad \langle D_{\tau K} \rangle = \langle \tau_{\gamma_1} \rangle / 3, \quad \gamma_1 = \gamma / 2\Omega = \gamma / 2.$$

$$(83)$$

For the largest eigenvalues we obtain the LD function from (10), (19), (25)

$$G(s, x) = -s - 3\ln(1 + \gamma / 2\Omega), \ \theta(s) = 2\Omega(e^{-s/3} - 1), \ g(\gamma) = -3\ln(1 + \gamma / 2\Omega).$$

We assume  $K_0 = M = 100$ . Entropy of the system  $\langle s_{sys} \rangle$  and  $\Delta \langle s_m \rangle$  are equal

$$\left\langle s_{sys} \right\rangle / M = s \left\langle K \right\rangle + \gamma \left\langle \tau \right\rangle + G(s,\gamma), \ \Delta \left\langle s_{sys} \right\rangle = -\left\langle s_{sys} \right\rangle, \ \Delta \left\langle s_m \right\rangle = -\tau_0 [\partial \theta(s) / \partial s - \partial \theta(s) / \partial s \Big|_{s=0}].$$

Since when using relation  $s = g(\gamma)$  (21), G(s,x)=0, then and  $\ln Z_M(K,\tau)=0$  as in (29). The behavior of the average and second moments (83) of the random variables  $\tau$  and K are shown in Fig. 11.



Fig. 11. Behavior of functions (83)  $\langle \tau(d) \rangle$  (full, red),  $\langle K(d) \rangle$  (dashed, green),  $D_{\tau}(d)$  (dash-dotted, blue),  $D_{K}(d)$  (short dash, pink),  $D_{\tau K}(d)$  (dot, purple) depending on  $d = \Delta \langle s_{tot} \rangle / \langle K_0 \rangle$  when substituting parameter  $\gamma(d)/2\Omega$  (79) into expressions (83). Range d=(0,...,10),  $(\gamma_{(++)}(d)/2\Omega)$  on Fig. 11a),  $(\gamma_{(-+)}(d)/2\Omega)$  on Fig. 11b).

The solution  $(\gamma_{(+)} / \kappa)(d)$  is not implemented, as in 4C). The negative branch of the solution at  $(\gamma_{(-)} / \kappa)(d)$  is constant, as in Fig. 10, but in the interval d=(0,...,0.0067).

In Appendix B, the parameter  $\gamma$  is associated with other parameters of the system, and the physical meaning of the parameter *s* and the associated parameter  $\gamma$  is also discussed.

## 6. Conclusion

In [83-84] *FPT* is considered as an independent thermodynamic variable present in the statistical ensemble. A similar situation arises in the thermodynamics of trajectories, when trajectories with random time (*FPT*) are studied [33], and the explicit form of the partition function is determined using the theory of large deviations with *LD* functions. The dependences of the average value of *FPT*, dispersions of *FPT* and dynamic activity, and correlation between *FPT* and dynamic activity on the total entropy change, consisting of intrasystem entropy production and entropy exchange with the environment, are found.

In [84], the Gibbs canonical ensemble was generalized to a nonequilibrium situation by introducing an additional thermodynamic parameter *FPT*. In the thermodynamics of trajectories, a similar procedure is carried out for *x*-ensembles (see, for example, [32, 33]). In this paper, the approach of paper [84] for determining the dependence of the mean *FPT* on the change in entropy is applied to the formalism of thermodynamics of trajectories. The joint distribution for the dynamic activity *K* (in this case generalizations to other counting observables are also possible) and *FPT* are considered. If in [84] the random variables energy and *FPT* are assumed to be independent, the partition function is divided into two factors, and the correlation between energy and *FPT* is equal to zero, then in this article, the dependence between random distribution parameters is determined. When using the theory of large deviations for large values of dynamic activity *K*, when the distribution for *FPT* is written in the form of an *LD* function, the case of relatively small values of *FPT* is considered, an expression for the partition function of the form (29) depending on  $s_{ef}$  (29) is obtained. The first and second moments of random variables are determined, including the correlation between the dynamic activity of *K* and *FPT*. After that, larger *FPT* values are assumed when  $s_{ef}=0$ .

The introduction noted the importance of *FPT*. In this case, it is important to know the patterns of *FPT* behavior, in particular, the dependence on entropy changes. The proposed approach will allow us to consider in detail various physical effects associated with changes in entropy in the system. Three model systems are calculated using three different distributions.

In all the examples considered in the article, the behavior of the moments differs. But everywhere (except 4B)) three branches of the dependences of the moments on the change in entropy are realized. Two branches belong to active states in which the parameter  $\gamma >0$  (s<0). In one of these branches, equilibrium states and a phase transition are possible; the second branch describes stationary nonequilibrium states, where there is no equilibrium and no phase transition. The solution with  $\gamma<0$  is close to equilibrium and exists only for very small changes in entropy. The calculation results in Section 4 confirm the conclusions of the theory [23].

The difference between this article and article [32] is that averaging is carried out over fixed values of K. The existence of an ensemble of systems with fixed values of K is assumed. One

of the results of this approach is the emergence of the possibility to find an expression for the correlation between the values of K and  $\tau$ . It is intuitively clear that such a correlation exists: the larger the *FPT*, the more events occur during this time.

In this article, the dependences of such quantities as the average values of dynamic activity and *FPT*, their variances and the correlation between them on the parameter conjugate with *FPT* are obtained in analytical form for three models of the partition function. The next important step is now taken. The parameter conjugate with *FPT* is associated with the overall change in entropy in the system, and the average values of dynamic activity and *FPT*, their variances and the correlation between them are expressed through the overall change in entropy in the system. This will allow you to evaluate the possibilities of influencing the system parameters. Suppose the dependencies, for example, of the average value of *FPT* on the total change in entropy, which may include control actions, are known. In that case, we can consider the possibilities of optimal control. In this article, some general regularities of such a process are obtained.

The dependences of the *FPT* moments on the change in entropy are calculated for three models of the partition function calculated using expressions (29), (39) and (80). A close behavior of the dependences of the *FPT* moments for partition functions is obtained. For partition function (29), one should use not condition (58), but the condition of convergence of expression (29). Condition (58) can be considered as an approximation for estimates (29), if we assume that the results obtained from expressions (39) and (29) are close.

The case of solutions of equations for the dependence of the parameter  $\gamma$  on the change in entropy, which corresponds to stationary nonequilibrium states, is also considered. In this case, zero and negative values of  $\gamma$  are not realized, there are only positive values of  $\gamma$  and the first and second moments of the distributions of activity and *FPT* corresponding to them. There is no phase transition, which occurs during the transition through the equilibrium state.

Above, we noted the analogy between the thermodynamics of trajectories and the method of nonequilibrium statistical operator. Both theories take into account the history of the system. At the same time, there are differences. Thus, time averaging is carried out in various ways. In the thermodynamics of trajectories, the theory of large deviations is used, and in the *NSO* method, only the principle of maximum entropy is used.

The results obtained are valid for simple classical two-level, three-level systems and quantum two-level system. For other systems, with other functions  $g(\gamma)$ , the results may differ. However, such general results as, for example, the limitation of the negative parameter  $\gamma$  by the convergence of the Laplace transform of the distribution *FPT*, remain valid.

There are also open questions. Thus, when considering model systems, various approximations of the form (29), (39), (80) were used. The question remains unclear: which approximation best describes the physical situation? What physical results correspond to distribution (29), as well as distribution (39)?

What is done in the article:

1). Using examples of classical two-level, three-level systems and quantum two-level system, it is shown how the states of these systems can be obtained by considering the behavior of the parameter  $\gamma$  (or *x*) conjugate to random time  $\tau$ . In this case, stationary nonequilibrium states and states in which equilibrium is achieved are distinguished.

2). The dependences of the moments (average values, variances, correlations) of the considered random variables (dynamic activity and observation time of the system) on the total change in the entropy of the system  $\Delta s_{tot}$  are obtained. Using the results obtained, one can consider the possibilities of increasing or decreasing moments as  $\Delta s_{tot}$  increases. The value  $\Delta s_{tot}$  includes

the change in entropy through exchange with the environment  $\Delta s_m$ . This quantity for the thermodynamics of trajectories is given in the form (42)-(45).

3). This approach allows us to more closely connect the results of thermodynamics of trajectories with nonequilibrium thermodynamics, in particular with stochastic thermodynamics. The connection between representation (42)-(45) with thermodynamic forces and flows is given, for example, in [101-102], [112]. Similar problems, for example, connections with heat and work, are considered in [111]. Knowing the influence of  $\Delta s_m$  on the behavior of the system, we can consider the impact of thermodynamic forces and flows on this behavior.

4). The analogy drawn in the article between distributions of thermodynamics of trajectories containing parameters  $sK+\gamma\tau$  with distributions of the form  $\beta u+\gamma\tau$  (where  $\beta$  is the inverse temperature, *u* is the internal energy density) [52, 83-84] makes it possible to transfer the methods used in thermodynamics of trajectories - obtaining stationary thermodynamic characteristics of the system from its dynamics using *LD* approaches, etc. - on distributions with  $\beta u+\gamma\tau$ .

## Appendix A. Non-zero values of the parameter $\gamma$ for the values of K and $\tau$ .

Let us expand the value  $s \neq 0$ ,  $\langle K \rangle = \langle K_s \rangle = \langle K_\gamma \rangle = -\frac{\partial \theta(s)}{\partial s} \tau$  (35) into a series in

 $\gamma$ , limiting ourselves to the linear term. Below we will see that this is enough to determine the value of  $\gamma$  from subsequent expressions in the expansion taking into account the degree of  $\gamma^2$ . To do this, consider the partition function (10), which includes the probability (7)-(8), and expand this probability  $P_{\langle \tau_{\gamma} \rangle}$ ,  $\tau = \langle \tau_{\gamma} \rangle$  into a series in  $\gamma$  in the neighborhood of  $P_{\langle \tau_{\gamma} \rangle | \gamma=0} = P_{\langle \tau_{0} \rangle}$ , taking into account the expression obtained from (9)-(10). From expression (8), we obtain, restricting ourselves to the first term in  $\gamma$ ,  $P_{\tau}(K) = e^{-\tau\varphi(K/\tau)}$ ,  $P_{\langle \tau_{\gamma} \rangle} \cong P_{\langle \tau_{\gamma} \rangle} / \partial \langle \tau_{\gamma} \rangle | \partial \langle \tau_{\gamma} \rangle / \partial \gamma |_{\gamma=0}$ ,  $\partial P_{\langle \tau_{\gamma} \rangle} / \partial \langle \tau_{\gamma} \rangle = P_{\langle \tau_{\gamma} \rangle} [-\varphi(K/\tau) + (K/\tau)(\partial \varphi(K/\tau) / \partial(K/\tau))], \tau = \langle \tau_{\gamma} \rangle$ . We believe  $\tau \neq \tau_0, \tau = \langle \tau_{\gamma} \rangle$ .

We take the explicit form of the function  $\varphi$  for the two-level classical system from [5]:  $\varphi(\kappa) = 3[\kappa \ln(\kappa/b) - (\kappa-b)], \quad b = 2\Omega/3 = \langle K \rangle / \tau$ . The calculation carried out gives the result

$$\langle K_{\gamma} \rangle = \langle K_0 \rangle - \gamma B_k,$$
 (A1)

where  $B_k = 6c_3 D_{K_0} / a_1$ ,  $c_3 = a_1^2 / 2 - a_2 = \frac{\kappa^2 + \eta^2}{2(\kappa \eta)^2}$ . Taking into account that  $\langle K_{\gamma} \rangle$  depends

on  $\gamma$ , from expressions (19), (A1), we obtain by  $K = \langle K_{\gamma} \rangle$ ,  $\ln Z_{\kappa}(\gamma) = \langle K_{\gamma} \rangle g(\gamma)$ ,

$$\left\langle \tau_{\gamma} \right\rangle = -\frac{\partial \ln Z_{\kappa}(\gamma)}{\partial \gamma} = -\frac{\partial \left\langle K_{\gamma} \right\rangle}{\partial \gamma} g(\gamma) - \left\langle K_{\gamma} \right\rangle \frac{\partial g(\gamma)}{\partial \gamma}.$$
 (A2)

For  $\Delta < \mathbf{s}_{m} >$  and  $< \tau_{\gamma} >$  we get  $\Delta \langle s_{m} \rangle = [\langle K_{0} \rangle \partial g(\gamma) / \partial \gamma_{|\gamma=0} - (\langle K_{0} \rangle - \gamma B_{k}) \partial g(\gamma) / \partial \gamma + B_{k} g(\gamma)] \partial \theta(\lambda) / \partial \lambda_{|\lambda=0}$ , and  $\langle \tau_{\gamma} \rangle = -\langle K_{\gamma} \rangle \partial g(\gamma) / \partial \gamma = -[\Delta \langle s_{m} \rangle / \Delta s_{1} + K_{0}] \partial g(\gamma) / \partial \gamma$ .

We obtain from (21), (31), (39)-(41),

$$\langle s_{\gamma} \rangle = \langle s_{sys} \rangle = -\langle \ln p_{s\gamma} \rangle,$$
 (A3)

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where  $\ln Z_s = \langle \tau_{\gamma} \rangle \theta(s)$ ,  $\ln Z_{\gamma} = \langle K_{\gamma} \rangle g(\gamma)$ . We will evaluate for  $\tau_0 \to \langle \tau_{\gamma} \rangle$ ,  $K_0 \to \langle K_{\gamma} \rangle$ . Since at s = 0,  $\theta(s) = 0$ ,  $\gamma = 0$ ,  $g(\gamma) = 0$ , then

$$\left\langle s_{0}\right\rangle = \left\langle s_{sys|\gamma=0}\right\rangle = s\left\langle K_{0}\right\rangle + \ln Z_{s|\gamma=0} = 0, \qquad (A4)$$

$$\Delta \langle s_{sys} \rangle = \langle s_0 \rangle - \langle s_\gamma \rangle = -s \langle K_\gamma \rangle - \gamma \langle \tau_\gamma \rangle - \ln Z_\gamma - \ln Z_s = -2g(\gamma) \langle K_\gamma \rangle - 2\gamma \langle \tau_\gamma \rangle.$$
(A5)

Using the relation obtained in [96] from the general expression (45) of the theory of large deviations,  $\langle s_m \rangle = -\langle \tau \rangle \partial \theta(\lambda) / \partial \lambda$ , assuming  $\lambda = 0$  (although arbitrary  $\lambda$  and the biased ensembles of trajectories are possible in [96]), from (47) (A1) we obtain

$$\Delta \langle s_m \rangle = \left[ -\langle K_0 \rangle a_1 + \left( \langle K_0 \rangle - \gamma B_k \right) \frac{a_1 + 2\gamma a_2}{1 + \gamma a_1 + \gamma^2 a_2} - B_k \ln(1 + \gamma a_1 + \gamma^2 a_2) \right] \frac{\partial \theta(\lambda)}{\partial \lambda}_{|\lambda=0}.$$
 (A6)

## Appendix B. Connection of parameter $\gamma$ with other system parameters

Above, the parameter  $\gamma$  was associated with a change in the entropy of the system. In the general case, changes in entropy caused by the exchange of entropy with the environment should be taken into account, as was done, for example, in Section 4. In addition to the above expression for the parameter  $\gamma$  through a change in entropy, there are other possibilities for determining the parameter  $\gamma$ .

In [52-53, 84] a distribution with random parameters of energy u and *FPT*  $T_{\gamma}$  is written. This distribution corresponds to expression (39) after replacing  $s \rightarrow \beta$ ,  $K \rightarrow u$ ,  $\tau \rightarrow T_{\gamma}$  (where  $\beta$  is the inverse temperature, u is the internal energy density) [52, 83-84]. It is important to note that these are different distributions. Although the parameter  $\gamma$  is conjugate to the random variable  $T_{\gamma}$  in both distributions, the second pair of variables  $\beta u$  differs from the pair sK in distribution (39). Equating these distributions corresponds to  $s=\beta$ , although this is just an analogy. For the distribution with  $\beta u$ , expressions (21), which are valid for distribution (39) and connecting the parameters  $\gamma$  and s, are not satisfied (apparently, it is possible to obtain analogues of these expressions). Therefore, below is given the physical meaning of the parameter  $\gamma$  for a distribution different from (39), not for the case of thermodynamics of trajectories, apparently, this is also only an analogy of the physical meaning of the parameter  $\gamma$  from distribution (39).

From distribution with  $\beta u$ , expressions for the internal entropy  $s_{\gamma}$  and the differential of this quantity are obtained:

$$s_{\gamma} = -\langle \ln \rho(z; u, T_{\gamma}) \rangle = \beta \langle u \rangle + \gamma \langle T_{\gamma} \rangle + \ln Z(\beta, \gamma); \ ds_{\gamma} = \beta d \langle u \rangle + \gamma d \langle T_{\gamma} \rangle. \tag{B1}$$

From (B1) we obtain (*T* is temperature,  $\beta \sim 1/T$ )

$$\gamma = \frac{\partial s_{\gamma}}{\partial \langle T_{\gamma} \rangle_{|\langle u \rangle}} = -\frac{\partial \langle u \rangle}{\partial \langle T_{\gamma} \rangle_{|s_{\gamma}}} (\frac{\partial \langle u \rangle}{\partial s_{\gamma}}_{|\langle \tau_{\gamma} \rangle})^{-1} = -\frac{1}{T} \frac{\partial \langle u \rangle}{\partial \langle T_{\gamma} \rangle_{|s_{\gamma}}}, \qquad \beta = \frac{\partial s_{\gamma}}{\partial \langle u \rangle_{|\langle \tau_{\gamma} \rangle}}, \tag{B2}$$

Since 
$$\partial \langle T_{\gamma} \rangle = -\chi_{t \in T_{\gamma}} \partial t$$
,  $\chi_{t \in T_{\gamma}} = \begin{cases} 1, t \in T_{\gamma} \\ 0, t \notin T_{\gamma} \end{cases}$ , then from (B2) we obtain that  
 $\gamma = \frac{1}{T} \frac{\partial \langle u \rangle}{\partial t} |_{s_{\gamma}} \chi_{t \in T_{\gamma}}.$ 

The expressions for  $\gamma$  and  $\beta$  are symmetrical. It is possible to further transform expression (B2).

Let us carry out the same operations for a distribution of the form (39), [90]

$$p_{s\gamma}(K,\tau) = e^{-sK-\gamma\tau} / Z_{s\gamma}, \quad Z_{s\gamma} = \sum_{K} \int d\tau e^{-sK-\gamma\tau} \omega(K,\tau), \quad (B3)$$

where, as in [85-86], the probability  $P(K, \tau)$  is denoted by  $\omega(K, \tau)$ . The Gibbs-Shannon entropy is written similarly to (B1) as

$$s_{\gamma} = -\left\langle \ln p_{s\gamma}(K,\tau) \right\rangle = s\left\langle K \right\rangle + \gamma\left\langle \tau \right\rangle + \ln Z_{s\gamma}, \quad ds_{\gamma} = sd\left\langle K \right\rangle + \gamma d\left\langle \tau \right\rangle. \tag{B4}$$

From (B4) we obtain

$$\gamma = \frac{\partial s_{\gamma}}{\partial \langle \tau \rangle_{|\langle K \rangle}} = -\frac{\partial \langle K \rangle}{\partial \langle \tau \rangle_{|s_{\gamma}}} \left( \frac{\partial \langle K \rangle}{\partial |s_{\gamma}|_{|\langle \tau \rangle}} \right)^{-1} = -s \frac{\partial \langle K \rangle}{\partial \langle \tau \rangle_{|s_{\gamma}}}.$$
(B5)

We write the quantity  $\frac{\partial \langle K \rangle}{\partial \langle \tau \rangle_{|_{S_{\gamma}}}}$  from (B5) in the form  $\frac{\partial \langle K \rangle}{\partial \langle \tau \rangle_{|_{S_{\gamma}}}} = -\frac{\partial s_{\gamma}}{\partial \langle \tau \rangle_{|_{\langle K \rangle}}} / \frac{\partial s_{\gamma}}{\partial \langle K \rangle_{|_{\langle \tau \rangle}}}$ .

Substituting these quantities into (B5), we obtain from (B4)

$$\gamma = -s \frac{\partial \langle K \rangle}{\partial \langle \tau \rangle_{|_{S_{\tau}}}} = s \frac{\gamma - \langle K \rangle / D_{K\tau}}{s - \langle K \rangle / D_{K}}.$$
(B6)

where  $D_K$  is dispersion of K (32),  $D_{K\tau}$  is a correlation between the parameters K and  $\tau$  (34).

Haven't used *LD* yet. If we use *LD*, then for a two-level system in (B6) it will be possible to substitute expressions (60)-(62) and obtain an equation for the parameter  $\gamma$ , expressed through the parameters  $\eta$  and  $\kappa$ , through the parameter *s*, which is also expressed through  $\gamma$  by expressions (21), and the value of *K*, which is assumed to be equal to the average value of  $K_0$  in accordance with (30).

There are other possibilities for determining the physical meaning of the parameter  $\gamma$ . Including for the situation when this parameter is related to the parameter *s* by relations (21). Although the *s*-field is not necessarily physically tunable, the singular features of the generating functions influence the shape of the overall distribution. The large deviation function behaves like a free energy function, where *s* plays the role of the inverse temperature. The time-extensive order parameter *K* is in the *count* of transitions between (coarse-grained) configurations, and *s* is a "counting" field. Activity *K* and counting field *s* are the extensive observable and its intensive conjugate field. Various aspects of the physical interpretation (critical values of the counting field *s*, the motion of the zeros of the moments generation function, etc.) of the parameter *s* are considered, for example in [106-114].

The topic of physical interpretation of the parameter *s* (and parameter  $\gamma$ ) is also touched upon in a number of other articles. This interpretation is ambiguous, depending on the physical system, the situation under consideration, the model used and other circumstances. Apparently, there is no universal physical meaning of the parameter *s* that is valid for all cases.

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