Entropy production rate of diffusivity fluctuations under diffusing diffusivity equation

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Abstract. Entropy production rate is discussed for diffusivity fluctuations of RNA-protein particles in cytoplasm of a living cell. The rate under the diffusing diffusivity equation is shown to become positive. The lower bound on the rate that suppresses the entropy production is also presented.

1. Introduction

In a recent experimental study in Ref. [1], RNA-protein particles, which are messenger RNA molecules fluorescently labeled with a protein, have been found to exhibit an exotic diffusion phenomenon in living cells. The cells studied there are of two different types: one is Escherichia coli cell (i.e., a bacterium), and the other is Saccharomyces cerevisiae cell (i.e., a yeast). The experimental observations have shown, in cytoplasm of each cell, that the mean square displacement of the RNA-protein particle, which is denoted here by $x^2$, takes

$$x^2 \sim Dt^\alpha$$

for elapsed time, $t$, at the level of individual trajectory of the particle. Here, $D$ stands for the diffusivity (i.e., the diffusion coefficient) and $\alpha$ is termed the diffusion exponent.

The values of $\alpha$ seem to be approximately equal to a certain constant, which has a positive value less than unity for each cell type. Such a phenomenon is called anomalous diffusion [2], which is receiving much attention in the literature [3,4].

The diffusivity, however, fluctuates in a wide range. $D$ obeys the following exponential law:

$$P(D) \sim \exp \left( -\frac{D}{D_0} \right)$$

with $D_0$ being a typical value of the diffusivity. This distribution is robust in the sense that it holds for the different cell types mentioned above. Thus, this implies the existence of a universal feature of diffusivity fluctuations.

The exponential distribution in equation (2) has played a crucial role for describing non-Gaussian distribution of the displacements of the RNA-protein particles [1] (see also, for example, Refs. [5,6] for similar discussions). Such a distribution has been obtained by the superposition of the Gaussian distribution of the displacements with respect to the distribution in equation (2). It may be worthwhile to mention that this procedure has been discussed based on the concept
2. Entropy associated with diffusivity fluctuations

In Ref. [10], the entropy associated with diffusivity fluctuations is given by the following Shannon entropy:

\[ S[P] = - \int dD P(D) \ln P(D). \] (3)

Here, \( P(D) dD \) is the probability of finding the diffusivity in the interval \([D, D + dD]\). (It is noticed that \( S \) is determined up to an additive constant as known for an entropy of a continuous distribution.) The same symbol \( P \) as that in equation (2) is used for this probability density, but it will not cause confusion. As discussed in Ref. [10], \( S \) is obtained as follows (see Refs. [12, 13] for an original discussion and a recent relevant work in the context of the diffusion exponent, respectively). Suppose that a medium for diffusion of the RNA-protein particles, which is regarded as the cytoplasm, is virtually divided into many small local blocks, in which the particles exhibit anomalous diffusion. The diffusivity fluctuates depending on these local blocks. Such a fluctuation varies slowly but is assumed to be approximately constant. Then, consider a number of replicas of the medium, each of which is discriminated from each other in terms of the local property of diffusivity fluctuations. As a measure of uncertainty about how the diffusivity locally fluctuates over the cytoplasm, the entropy is introduced as the logarithm of the number of replicas, which is divided by the number of local blocks in the medium. A point in the discussion is that the local blocks are statistically independent from each other in terms of the diffusivity, since the diffusivity is obtained through equation (1) from independent trajectory. The entropy introduced in this way turns out to take the form of the Shannon entropy, which is discrete, and accordingly its continuum limit is written by equation (3).

As shown in Ref. [10], the exponential distribution can be derived by the maximum entropy principle [14] with \( S \) in equation (3): together with the normalization constraint, \( \int dD P(D) = 1 \), the maximum entropy distribution is found to be given by \( \hat{P}(D) \propto e^{-\lambda D} \), where \( \lambda \) is a positive Lagrange multiplier associated with the constraint on the average of the diffusivity, \( \int dD P(D) D = \bar{D} \). Thus, it is obvious that this fluctuation distribution with \( \lambda = 1/D_0 \) is identical to the distribution in equation (2).

3. Entropy production rate

Let us relax the assumption mentioned above, and accordingly diffusivity fluctuations vary slowly. Therefore, the fluctuation distribution that deviates slightly from the exponential distribution seems to tend to approach the exponential distribution.

To discuss dynamical evolution of the fluctuation distribution, we employ the diffusing diffusivity equation proposed in Ref. [11] (see also, for example, Refs. [15,16] for recent developments). This equation, which is of the advection-diffusion type with respect to the diffusivity, offers a description of time evolution of the fluctuation distribution.

The diffusing diffusivity equation we consider here is given by

\[ \frac{\partial P(D, t)}{\partial t} = - \frac{\partial J(D, t)}{\partial D}, \] (4)
where \( P(D, t)dD \) is the probability of finding the diffusivity in the interval \([D, D + dD]\) at time \(t\) (the conventional time) and \( J(D, t) \) is the probability current given by

\[
J(D, t) = -\frac{\partial}{\partial D} \left[ k(D)P(D, t) \right] - s(D)P(D, t)
\]

(5)
satisfying the following reflecting boundary conditions

\[
J(0, t) = 0, \quad \lim_{D \to \infty} J(D, t) = 0.
\]

(6)

Here, \( k(D) (> 0) \) is the diffusivity of the diffusivity, whereas \(-s(D) (\leq 0)\) is the bias of the diffusion of the diffusivity. In the case [11] when \( k(D) \) and \( s(D) \) are respectively positive constants, \( k \) and \( s \), which satisfy \( D_0 = k/s \), equation (4) admits as its stationary solution the exponential distribution identical to equation (2).

Now, our interest is how the entropy

\[
S(t) = -\int dD P(D, t) \ln P(D, t)
\]

(7)
evolves in time. The entropy production rate is calculated as follows:

\[
\frac{dS}{dt} = \int dD \frac{[J(D, t)]^2}{k(D)P(D, t)} + \frac{d}{dt} \left\langle \frac{s(D)}{k(D)} D \right\rangle + \int dD \frac{J(D, t)}{k(D)} \left\{ \frac{s(D)}{k(D)} D + 1 \right\} \frac{dk(D)}{dD} - D \frac{ds(D)}{dD}
\]

(8)

where equations (4), (5), and the conditions in equation (6) have been used, and the rate is purposely expressed by the probability current and the average, \( \left\langle Q \right\rangle \equiv \int dDP(D, t)Q \).

In the case mentioned above, equation (8) is simplified to be

\[
\frac{dS}{dt} = \frac{1}{k} \int dD \frac{[J(D, t)]^2}{P(D, t)} + \frac{s d\langle D \rangle}{k dt}.
\]

(9)

The main result given in Ref. [10] is that this entropy production rate becomes manifestly positive: \( dS/dt > 0 \).

To see this, we employ the solution of equation (4) given as follows [17]:

\[
P(D, t) = \frac{1}{\sqrt{\pi kt}} \exp\left[ -\frac{(D + st)^2}{4kt} \right] + \frac{s}{k \sqrt{\pi}} e^{-\frac{s^2}{4kt}} \int_{s^2 - \frac{1}{4kt}}^{\infty} dy \exp(-y^2)
\]

(10)
satisfying the initial condition, \( P(D, 0) = \delta(D) \), which means that no trajectories of the RNA-protein particles exist over the cytoplasm at the initial time. From equations (4), (5), and the conditions in equation (6), the time derivative of \( \langle D \rangle \) is found to be given by

\[
\frac{d\langle D \rangle}{dt} = kP(0, t) - s,
\]

(11)

and accordingly equation (10) gives rise to

\[
\frac{d\langle D \rangle}{dt} = \frac{s}{2 \sqrt{\pi}} \int_{\frac{1}{2} \sqrt{\pi}}^{\infty} dy y^2 \exp(-y^2),
\]

(12)

showing that \( d\langle D \rangle/dt > 0 \). Thus, equations (9) and (12) lead to the main result about the positive entropy production rate.
4. Lower bound on the rate suppressing entropy production

Now, in terms of the fluctuation distribution, the entropy production rate in equation (9) can be rewritten by

$$\frac{dS}{dt} = k \int dD \frac{1}{P(D, t)} \left( \frac{\partial P(D, t)}{\partial D} \right)^2 - sP(0, t).$$  \hspace{1cm} (13)

The second term on the right-hand side offers the rate that tells us how the entropy production is suppressed. Using the solution in equation (10), we have the lower bound on this rate:

$$sP(0, t) > \frac{s^2}{2k}.$$  \hspace{1cm} (14)

Taking into account the tendency that $\langle D \rangle$ increases in time, it seems that the lower bound determines how such a tendency is suppressed, independently of time. It may be of interest to see the existence of the time-independent lower bound.

5. Conclusion

We have discussed the entropy production rate of diffusivity fluctuations of RNA-protein particles in cytoplasm of Escherichia coli cell as well as Saccharomyces cerevisiae cell and have shown the positivity of the rate under the diffusing diffusivity equation. Thus, the present approach offers a dynamical foundation for diffusivity fluctuations as the maximum entropy distribution. We have also presented the lower bound on the rate that suppresses the entropy production, which turns out to be time independent.

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