Generalized relation between the relative entropy and dissipation for nonequilibrium systems

Pegah Zolfaghari, Somayeh Zare, and Behrouz Mirza[*]
Department of Physics, Isfahan University of Technology, Isfahan 84156-83111, Iran

Recently, Kawai, Parrondo, and Van den Broeck have related dissipation to time-reversal asymmetry. We generalized the result by considering a protocol where the physical system is driven away from an initial thermal equilibrium state with temperature β_0 to a final thermal equilibrium state at a different temperature. We illustrate the result using a model with an exact solution, i.e., a particle in a moving one-dimensional harmonic well.

I. INTRODUCTION

Irreversible thermodynamic processes are the ones that cannot be closed. In other words, the system and its surroundings never return to their original states. There are a number of features associated with such processes which include (i) dissipation; (ii) asymmetry in the arrow of time; and (iii) broken equilibrium. In recent years, some relations have been stated between dissipation and time-reversal asymmetry [1–10]. Here, we will focus on the relation obtained by Kawai, Parrondo, and Van den Broeck (KPV), which is expressed by the following [5],

$$\beta \langle W_{diss} \rangle \geq D[\rho_F(z,t) \parallel \rho_R(z^*, \tau - t)]. \tag{1}$$

In this relation, $\langle W_{diss} \rangle$ is the average work dissipated during the process in which the system evolved from one canonical equilibrium state at a temperature T into another at the same temperature. Based on the second law, the average work performed on the system must exceed the difference between the free energy in the initial equilibrium state and that in the final equilibrium one, i.e. $\langle W \rangle \geq \Delta F = F_B - F_A$ [11]. The dissipated work is defined as $\langle W_{diss} \rangle = \langle W \rangle - \Delta F$. $D(\rho_F(z,t) \parallel \rho_R(z^*, \tau - t))$ denotes the relative entropy [12], a measure of the distinction between ρ_F, i.e. the time-dependent phase-space density, during the forward process $(A \to B)$ and ρ_R, i.e. the time-dependent phase-space one, during the reverse process $(B \to A)$. $z = (\mathbf{x}, \mathbf{p})$ designates a point in the phase space, and the asterisk denotes the reversal of momenta, $\mathbf{p} \longrightarrow -\mathbf{p}$. For the case of the Hamiltonian dynamics, where the system evolves deterministically, Eq. (1) is an equality; i.e., the average dissipated work can be expressed by [7],

$$\begin{aligned} \beta \langle W_{diss} \rangle &= \int dz \rho_F(z,t) \ln[\frac{\rho_F(z,t)}{\rho_R(z^*, \tau - t)}] \\ &= D[\rho_F(z,t) \parallel \rho_R(z^*, \tau - t)]. \end{aligned} \tag{2}$$

Consider a system that is driven far from equilibrium by a protocol, where the inverse temperature of the initial and final equilibrium states are β_0 and β_τ, respectively. Our goal is to generalize Eq. (2) to this kind of process. A basic motivation to study this generalized relation is its possible application to the evolution of black holes that we will discuss elsewhere.

This will be attempted in Sec. 2. In Sec. 3, we will consider two solvable models for the generalized equation.

II. GENERALIZATION OF KPV EQUATION

We consider a system that is initially coupled with a reservoir in the reverse temperature β_0. The reservoir is then removed. Subsequently, from $t = 0$ to a later time $t = \tau$, the external forces are turned on according to some arbitrary but predetermined schedule, or protocol, λ_t. The microscopic evolution of the system during this time interval is described by the trajectory $z_t = (\mathbf{p}, \mathbf{q})$. The Hamiltonian of the system is denoted by $H(\lambda_t, z_t)$. At time $t = \tau$, the system is coupled with a reservoir in the reverse temperature β_τ, again. Similar to the derivation of the Crooks equality [7], we consider two processes which are labeled forward (F) and reverse (R). The initial phase-space densities for the forward and reverse processes are given by $(I \equiv F$ or $R)$

$$\rho_0^I(z_0, \lambda_0) = \frac{1}{Z_0} \exp[-\beta_0 H(z_0^I, \lambda_0)], \tag{3}$$

and $Z_t = \int dz_t \exp[-\beta_t H(z_t, \lambda_t)]$ is partition function at time $t = 0$ or $t = \tau$. It should be noted that temperature is only defined for the initial and final states and not for any state between the two. By combining Eq. (3) and definition of the partition function, we get

$$\frac{\rho_0^F}{\rho_0^R} = \frac{Z_\tau}{Z_0} \exp[\beta_\tau H(z_0^R; \lambda_\tau) - \beta_0 H(z_0^F; \lambda_0)]. \tag{4}$$

According to the definition of free energy given by $F(\lambda_t) = -\beta_t^{-1} \ln Z(\lambda_t)$, Eq. (4) can be rewritten as follows:

$$\frac{\rho_0^F}{\rho_0^R} = \exp[-\Delta(\beta F)] \exp[\beta_\tau H(z_0^R; \lambda_\tau) - \beta_0 H(z_0^F; \lambda_0)]. \tag{5}$$

Note that $\Delta(\beta F) = \beta_\tau F_\tau - \beta_0 F_0$. Assume that the work performed on the system is defined by [7, 13–15]

$$W[z_t] = \int_0^\tau dt \dot{\lambda} \frac{\partial H}{\partial \lambda}(z_t, \lambda_t). \tag{6}$$

Then, based on this definition, we have [7]

$$W[z_t] = H(z_\tau^F; \lambda_\tau) - H(z_0^F; \lambda_0). \tag{7}$$

Using Eq. (7), Eq. (5) can be simplified as

$$\frac{\rho_0^F}{\rho_0^R} = \exp[-\Delta(\beta F) + \beta_\tau W + (\beta_\tau - \beta_0)H_0], \qquad (8)$$

where $H_0 \equiv H(z_0^F; \lambda_0)$. We can rewrite Eq. (8) as

$$\ln(\frac{\rho_0^F}{\rho_0^R}) = -\Delta(\beta F) + \beta_\tau W + (\beta_\tau - \beta_0)H_0. \qquad (9)$$

We can use the definition of average as, $\int dz_0 \rho_0(z_0) A = <A>_{\rho_0}$, where, A is an arbitrary normalized function $[\int dz_0 A(z_0, 0) = 1]$. Therefore, we can write equality (9) as

$$\int dz_0 \ln(\frac{\rho_0^F}{\rho_0^R})\rho_0^F = \langle\ln(\frac{\rho_0^F}{\rho_0^R})\rangle_{\rho_0^F} =$$
$$-\Delta(\beta F) + \beta_\tau \langle W \rangle_{\rho_0^F} + (\beta_\tau - \beta_0)\langle H_0 \rangle_{\rho_0^F}. \qquad (10)$$

Since the phase-space density is conserved along any Hamiltonian trajectory, i.e., $\rho_0^F = \rho^F$ and $\rho_0^R = \rho^R$ and based on the definition of the relative entropy

$$\int dz \rho_F(z,t) \ln[\frac{\rho_F(z,t)}{\rho_R(z^*, \tau-t)}] = D[\rho_F(z,t) \parallel \rho_R(z^*, \tau-t)], \qquad (11)$$

we obtain the following generalized form of Eq. (2):

$$D(\rho^F \parallel \rho^R) = -\Delta(\beta F) + \beta_\tau \langle W \rangle_{\rho_0^F} + (\beta_\tau - \beta_0)\langle H_0 \rangle_{\rho_0^F}. \qquad (12)$$

The above expression is valid for the deterministic trajectories of the system, including information about every degree of freedom. If only partial information about the system is available, the relative entropy is reduced and we will have an inequality.

Since $z = (q, p)$ in deterministic dynamics represents all position and momentum variables and, $\rho(q, p)$ surrounds the phase-space trajectory going through $z = (q, p)$, Therefore, we can consider a partition of the entire phase space [5].This partition is described by a sequence $z_0, z_1, ...z_n$. Corresponding phase space distributions for the forward and backward processes are given by

$$\rho_n^F = \int_{z_n} \rho_0^F(p,q)dqdp, \qquad \rho_n^R = \int_{z_n^*} \rho_0^R(p,q)dqdp. \qquad (13)$$

By integrating Eq. (9) over z_n we obtain

$$\langle\exp[-\beta_\tau W - (\beta_\tau - \beta_0)H_0]\rangle_n^F =$$
$$\frac{\int_{z_n} \rho_0^F(p,q)\exp(-\beta_\tau W - (\beta_\tau - \beta_0)H_0)dqdp}{\rho_n^F}$$
$$= \frac{\rho_n^R}{\rho_n^F} \exp[-\Delta(\beta F)]. \qquad (14)$$

Now, by using $\langle\exp(-x)\rangle \geq \exp\langle-x\rangle$, we can rewrite Eq. (14) as:

$$\langle\beta_\tau W + (\beta_\tau - \beta_0)H_0\rangle_n^F \geq \Delta(\beta F) + \ln\frac{\rho_n^F}{\rho_n^R}. \qquad (15)$$

By performing an average over the different subsets, we will have

$$\langle\beta_\tau W + (\beta_\tau - \beta_0)H_0\rangle^F = \Sigma_n \rho_n^F \langle\beta_\tau W + (\beta_\tau - \beta_0)H_0\rangle_n^F. \qquad (16)$$

Finally, considering Eqs. (15) and (16) yields the following generalized relations:

$$\langle\beta_\tau W + (\beta_\tau - \beta_0)H_0\rangle^F - \Delta(\beta F) \geq \int \ln(\frac{\rho_n^F}{\rho_n^R})d\rho_n^F, \qquad (17)$$
$$\langle\beta_\tau W + (\beta_\tau - \beta_0)H_0\rangle^F - \Delta(\beta F) \geq D(\rho_n^F \parallel \rho_n^R). \qquad (18)$$

Equation (18) is the basic result of this Brief Report. In Sec. 3, we will consider an example that corresponds to an exact equality as in Eq. (12).

III. PARTICLE IN A MOVING HARMONIC WELL

In this section, we analyze Eq. (12) for a particle with mass m which is trapped in a harmonic well with a spring constant k. The Hamiltonian of the particle is given by

$$H(x, p, \lambda) = \frac{p^2}{2m} + \frac{k}{2}(x - \lambda)^2. \qquad (19)$$

We will consider processes during which the center of the well is moved either rightward or leftward at a constant speed, u. These correspond to the forward and reverse protocols, $\lambda_F(t) = ut$ and $\lambda_R(t) = u(\tau - t)$, where τ is the total time interval. Along this time interval, the initial and final reverse temperatures are β_0 and β_τ, respectively, during the forward process, and vice versa during the reverse process. We consider two dynamics for this example: Hamiltonian dynamics and Langevin dynamics.

A. Hamiltonian dynamics

In this section we assume that the system is thermally isolated from environment after the initial equilibration stage. Explicit expressions for the initial equilibrium densities are given by the following Gaussian distributions:

$$\rho_F(z, 0) = \frac{\beta_0}{2\pi}\sqrt{\frac{k}{m}}\exp[-\beta_0(\frac{p^2}{2m} + \frac{kx^2}{2})], \qquad (20)$$
$$\rho_R(z, 0) = \frac{\beta_\tau}{2\pi}\sqrt{\frac{k}{m}}\exp[-\beta_\tau(\frac{p^2}{2m} + \frac{k}{2}(x - u\tau)^2)]. \qquad (21)$$

By considering that in this situation the system evolves under the Hamiltonian dynamics, the equations of motions are given by

$$\dot{x}_F = \frac{p_F}{m}, \qquad \dot{p}_F = -k(x_F - ut), \qquad (22)$$
$$\dot{x}_R = \frac{p_R}{m}, \qquad \dot{p}_R = -k(x_R - u\tau + ut). \qquad (23)$$

Due to the Gaussian nature of the initial densities [Eqs. (20) and (21)] and the linearity of the equations of motion, the distribution remains Gaussian for all times. Therefore, according to the relations of means and covariances for two-dimensional Gaussian distributions, $(f_G(z) = \frac{1}{2\pi\sqrt{det\sigma}}\exp[\frac{1}{2}(z-\bar{z})^T.\sigma^{-1}.(z-\bar{z})])$, [7] and consider that the relative entropy between two Gaussian distributions, $f_G(z)$ and $g_G(z^*)$, is

$$D[f_G(z) \parallel g_G(z^*)] = -1 + \frac{1}{2}[\ln(\frac{\det\sigma_g}{\det\sigma_f}) + Tr(\sigma_g^{-1}.\sigma_f^*)]$$
$$+ \frac{1}{2}(\bar{z}_f^* - \bar{z}_g)^T.\sigma_g^{-1}.(\bar{z}_f^* - \bar{z}_g), \quad (24)$$

where $\sigma_{xp}^* = -\sigma_{xp}$ and all other elements of σ^* are unaltered [16]. We have

$$D[\rho_F(z,t) \parallel \rho_R(z^*, \tau - t)] = -1 + \ln(\frac{\beta_0}{\beta_\tau}) + (\frac{\beta_\tau}{\beta_0})$$
$$+ \beta_\tau m u^2[1 - \cos(w\tau)]. \quad (25)$$

By considering the relations for means and variances that we obtain here, we can say that the means and variances are the same with the results in Ref. [7]; the only difference is that here we have β_0 in $t = 0$ and β_τ in $t = \tau$. Also, according to the following relations

$$\langle W \rangle_{\rho_0^F} = -uk \int_0^\tau [\bar{x}_F(t) - ut]$$
$$= uk \int_0^\tau [\frac{\sin(wt)}{w}]$$
$$= mu^2[1 - \cos(w\tau)], \quad (26)$$

$$\langle H_0 \rangle_{\rho_0^F} = \frac{1}{\beta_0}, \qquad -[\Delta(\beta F)] = \ln(\frac{\beta_0}{\beta_\tau}). \quad (27)$$

The left-hand side of Eq. (12) is equal to

$$\beta_\tau m u^2[1 - \cos(w\tau)] + (\beta_\tau - \beta_0)\frac{1}{\beta_0} + \ln(\frac{\beta_0}{\beta_\tau}). \quad (28)$$

So, we have

$$\beta_\tau \langle W \rangle_{\rho_o^F} + (\beta_\tau - \beta_0)\langle H_0 \rangle_{\rho_0^F} - \Delta(\beta F) =$$
$$(\beta_\tau - \beta_0)\frac{1}{\beta_0} + \ln(\frac{\beta_0}{\beta_\tau}) + \beta_\tau m u^2[1 - \cos(w\tau)]. \quad (29)$$

Therefore, comparison of Eqs. (25) and (29) yields the following equation for a Hamiltonian dynamics:

$$\beta_\tau \langle W \rangle_{\rho_0^F} + (\beta_\tau - \beta_0)\langle H_0 \rangle_{\rho_0^F} - \Delta(\beta F) =$$
$$D[\rho_F(z,t) \parallel \rho_R(z^*, \tau - t)], \quad (30)$$

which is a special case of Eq. (12).

B. Overdamped Langevin dynamics

In this section we consider a system that interacts with its environment so that we may use overdamped Langevin dynamics[7]. For the forward process the Fokker-Planck equation for $\rho_F(x,t)$ is

$$\frac{\partial}{\partial t}\rho_F(x,t) = \frac{k}{\gamma}\frac{\partial}{\partial x}[(x - ut)\rho_F(x,t)] + \frac{1}{\gamma\beta}\frac{\partial^2}{\partial x^2}\rho_F(x,t). \quad (31)$$

where γ is the friction coefficient. By the use of the means and variances for forward and reverse processes,

$$\bar{x}_F(t) = ut - \frac{\gamma u}{k}(1 - e^{-kt/\gamma}), \quad \sigma_F^2 = \frac{1}{\beta_0 k}, \quad (32)$$

$$\bar{x}_R(t) = u(\tau - t) + \frac{\gamma u}{k}(1 - e^{-k(\tau - t)/\gamma}), \quad \sigma_R^2 = \frac{1}{\beta_\tau k}, \quad (33)$$

we have the following results for the relative entropy and average work:

$$D[\rho_F(x,t) \parallel \rho_R(x, \tau - t)] = -1 + \ln(\frac{\beta_0}{\beta_\tau}) + (\frac{\beta_\tau}{\beta_0})$$
$$+ \frac{2\beta_\tau \gamma^2 u^2}{k}\{1 - e^{-k\tau/2\gamma}\cosh[\frac{k}{\gamma}(\frac{\tau}{2} - t)]\}^2, \quad (34)$$

$$\langle W \rangle_{\rho_0^F} = -uk \int_0^\tau [\bar{x}_F(t) - ut]$$
$$= \gamma u^2[\tau - \frac{\gamma}{k}(1 - e^{-k\tau/\gamma})]. \quad (35)$$

In this situation, we have to demonstrate the validity of inequality (18). We note that the left-hand side of this inequality is

$$\langle \beta_\tau W + (\beta_\tau - \beta_0)H_0 \rangle^F - \Delta(\beta F) = \beta_\tau \gamma u^2[\tau - \frac{\gamma}{k}(1 - e^{-k\tau/\gamma})] + (\beta_\tau - \beta_0)\frac{1}{\beta_0} + \ln(\frac{\beta_0}{\beta_\tau}), \quad (36)$$

and $D(\rho_n^F \parallel \rho_n^R)$ has a maximum value at $t = \tau/2$. Combining Eqs. (34) and (36) we have

$$\langle \beta_\tau W + (\beta_\tau - \beta_0)H_0 \rangle^F - \Delta(\beta F) \geq D(\rho_n^F \parallel \rho_n^R),$$

where the inequality is valid for any $\zeta = \frac{k\tau}{\gamma} \geq 0$. Therefore the validity of inequality (18) for overdamped Langevin dynamics

is demonstrated.

IV. CONCLUSION

We extended a known relation between the dissipated work and time-reversal asymmetry to a more general case by assuming a protocol which starts from an equilibrium state and moves to another equilibrium where the initial and final temperatures are different (it should be noted that we do not need to define temperatures between the two equilibria). Time-reversal asymmetry is more clear in this kind of process; however, the definition of dissipated work is not completely understood in this situation. It will be interesting to consider more general cases, as they will provide a better understanding of the relationship between the time-reversal asymmetry and dissipation and other aspects of non-equilibrium statistical mechanics.

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