New Journal of Physics
The open access journal at the forefront of physics

PAPER • OPEN ACCESS

Thermodynamic uncertainty relation for underdamped dynamics driven by time-dependent protocols

To cite this article: Chulan Kwon and Hyun Keun Lee 2022 *New J. Phys.* **24** 013029

IOP Publishing New J. Phys. 24 (2022) 013029 https://doi.org/10.1088/1367-2630/ac2c8f

New Journal of Physics

The open access journal at the forefront of physics

Deutsche Physikalische Gesellschaft DPG
IOP Institute of Physics

Published in partnership with: Deutsche Physikalische Gesellschaft and the Institute of Physics

OPEN ACCESS

RECEIVED
9 June 2021

REVISED
24 September 2021

ACCEPTED FOR PUBLICATION
4 October 2021

PUBLISHED
18 January 2022

PAPER

Thermodynamic uncertainty relation for underdamped dynamics driven by time-dependent protocols

Chulan Kwon[1,*] and Hyun Keun Lee[2]

1 Department of Physics, Myongji University, Yongin, Gyeonggi-Do, 17058, Korea
2 Department of Physics, Sungkyunkwan University, Suwon, Gyeonggi-do 16419, Korea
* Author to whom any correspondence should be addressed.

E-mail: ckwon@mju.ac.kr

Keywords: thermodynamic uncertainty relation, underdamped dynamics, overdamped dynamics, Cramer–Rao inequality, non-equilibrium fluctuation, entropy production

Abstract

The thermodynamic uncertainty relation (TUR) for overdamped dynamics has recently been derived for general time-dependent protocols. However, its precedent TUR for underdamped dynamics has not been known yet. Even for the case of steady states, a proper way to match underdamped and overdamped TURs has not been found. We derive the TUR for underdamped systems subject to general time-dependent protocols, that covers steady states, by using the celebrating Cramér–Rao inequality. We show the resultant TUR to give rise to the inequality for the product of the variance and entropy production. We prove it to approach to the known overdamped result for large viscosity limit. It is the eventual step to pursue the TUR for Langevin systems. We present three examples to confirm our rigorous result.

1. Introduction

Non-equilibrium fluctuation in thermodynamic quantities produced for periods of time such as work, heat, and entropy production (EP) has been an important subject since the discovery of the fluctuation theorem (FT) for deterministic systems about two decades ago [1–3]. The FT with various forms has been proved to hold for stochastic systems theoretically [4–10] and experimentally [11–18]. Another fundamental property on non-equilibrium fluctuation, the thermodynamic uncertainty relation (TUR), has been discovered [19–21]. The TUR provides a universal trade-off relation between the fluctuation of the time-accumulated production of an arbitrary observable Φ and its dissipation. Φ is written as $\int_0^{\tau} dt\phi$ for production rate ϕ and time τ. For a non-equilibrium steady state (NESS), the TUR for an observable Φ states

$$\frac{\mathrm{Var}\ \Phi}{\langle\Phi\rangle^2} \geqslant \frac{2k_B}{\tau\sigma}, \tag{1}$$

where $\mathrm{Var}\,\Phi$ is the variance of Φ, $\langle\Phi^2\rangle - \langle\Phi\rangle^2$, σ the average EP rate in the system and bath, and k_B the Boltzmann constant.

There have been extensive studies on the TUR for various systems in different dynamics. It has been studied for continuous-time Markov jumping processes for long-time [21] and finite-time [22–24], also for discrete-time jumping process [25], and for linear response systems [26]. It has been studied for general overdamped Langevin systems [27, 28] and heat engines [29, 30]. For systems with time-dependent protocols, it has also been extensively studied for periodically driven systems in the absence of steady states [31–34]. There have been alternative studies to consider a different type of inequality, called the generalized TUR, in use of the detailed FT [35, 36], which typically replaces the right-hand side in equation (1) with $2/(\langle e^{k_B^{-1}\tau\sigma}\rangle - 1)$ and gives a looser bound for long time than the former.

For general time-dependent protocols, the TUR has not been throughly found. For overdamped Langevin systems, the rigorous derivation of the TUR has been found by Koyuk and Seifert [37], which states in terms of our notation

$$\frac{\mathrm{Var}\ \Phi}{\left[(\tau\partial_\tau - \omega\partial_\omega)\langle\Phi\rangle\right]^2} \geqslant \frac{2k_\mathrm{B}}{\langle\Delta S_\mathrm{tot}\rangle}. \tag{2}$$

where ω is the speed of the protocol change in time t, that appears as $\lambda(\omega t)$ for the protocol λ and $\langle\Delta S_\mathrm{tot}\rangle$ is the average EP produced in the system and bath. It holds for any systems prepared in arbitrary initial states and goes to the steady-state TUR in equation (1) in the absence of time-dependent protocol. There have been investigations for underdamped systems including momentum variables with odd-parity in time reversal [38–41], but the recent result for steady states by Vu and Hasegawa [40] has left a controversy that it does not approach to the known overdamped TUR in equation (2) and even gives rise to a looser bound.

In this study, we investigate the TUR for underdamped dynamics subject to general time-dependent protocols which goes to equation (2) for large viscosity. It finalizes the pursuit of the TUR for Langevin systems. First, we will derive the TUR rigorously and show it to go to the proper overdamped limit. We will present a few examples to confirm our results.

2. Derivation of TUR

We consider a particle of mass m in underdamped stochastic dynamics subject to a general time-dependent protocol. The probability distribution function (PDF), $\rho(\mathbf{x}, \mathbf{p}, t)$, for position $\mathbf{x}$ and momentum $\mathbf{p}$ satisfies the Kramers equation

$$\partial_t\rho(\mathbf{x}, \mathbf{p}, t) = -\left[\partial_\mathbf{x}\cdot\frac{\mathbf{p}}{m} - \partial_\mathbf{p}\cdot\left\{\mathbf{H}(\mathbf{x}, \mathbf{p}, t) - D\partial_\mathbf{p}\right\}\right]\rho(\mathbf{x}, \mathbf{p}, t), \tag{3}$$

where ∂_t, $\partial_\mathbf{x}$, and $\partial_\mathbf{p}$ denote partial differentiations with respect to variables in subscript. The drift term $\mathbf{H}$ (non-stochastic force) reads $-(\gamma/m)\mathbf{p} + \mathbf{f}(\mathbf{x}, \omega t)$. The probability currents are defined [45] as

$$\mathbf{j}_\mathbf{x} = (\mathbf{p}/m)\rho, \qquad \mathbf{j}^\mathrm{r}_\mathbf{p} = \mathbf{f}\rho, \qquad \mathbf{j}^\mathrm{irr}_\mathbf{p} = \left(-\gamma\frac{\mathbf{p}}{m} - D\partial_\mathbf{p}\right)\rho \tag{4}$$

where the first is the current density in position space, the second the reversible current density in momentum space, and the third the irreversible current density in momentum space. $\mathbf{j}^\mathrm{irr}_\mathbf{p}$ is known as non-equilibrium measure to be used for the EP. γ and D are viscosity and diffusion coefficients, respectively, satisfying the Einstein relation, $D = \gamma\beta^{-1}$ for the inverse temperature β of the medium (bath) maintained in equilibrium. For simplicity of notation, we consider a single colloidal particle in isotropic medium, which can be extended to a many-particle system in non-isotropic medium with viscosity and diffusion coefficients in matrix form. The time-dependent protocol is included in the force $\mathbf{f}$ and ω is introduced as a parameter to control the speed of protocol change in time [37]; for example, it is the frequency of an oscillating driving force. The force can be given by $\mathbf{f} = -\partial_\mathbf{x}V(\mathbf{x}, \omega t)$ for the time-dependent protocol in potential V or $\mathbf{f} = -\partial_\mathbf{x}V(\mathbf{x}) + \mathbf{f}_\mathrm{nc}(\mathbf{x}, \omega t)$ for the time-dependent protocol in nonconservative external force $\mathbf{f}_\mathrm{nc}$. In the absence of time-dependent protocol, the system reaches a thermal equilibrium with the Boltzmann distribution, $\rho \propto \mathrm{e}^{-\beta E}$ for the energy $E = p^2/(2m) + V(\mathbf{x})$.

We consider the production Φ of an observable which is produced along the system's path $\mathbf{q}(t) = (\mathbf{x}(t), \mathbf{p}(t))$ in the phase space for $0 \leqslant t \leqslant \tau$ and is mathematically a functional of path written as $\Phi[\mathbf{q}(t)]$. For example, work, heat, and EP are such a path-dependent observable produced continuously in time. It is written as $\int_0^\tau \mathrm{d}t\phi(\mathbf{q}(t), t)$ where $\phi(\mathbf{q}, t)$ is the production rate per time on the system at a specific state $\mathbf{q}$ at time t. We consider the two forms of production rate

$$\phi(\mathbf{x}, \mathbf{p}, t) = \begin{cases} \partial_t\chi(\mathbf{x}, \omega t) & \text{(type I)} \\ \mathbf{g}(\mathbf{x}, \omega t)\cdot\mathbf{p}/m & \text{(type II)}. \end{cases} \tag{5}$$

For example, the work production rate is given by either $\partial_t V(\mathbf{x}, \omega t)$ (type I) or $\mathbf{f}_\mathrm{nc}(\mathbf{x}, \omega t)\cdot\mathbf{p}/m$ (type II). The average production $\langle\Phi[\mathbf{q}(t)]\rangle$ over all paths can be computed in principle by the path integral with the path probability

$$P[\mathbf{q}(t)] \propto \rho_\mathrm{in}(\mathbf{q}_0)\prod_t \delta(\dot{\mathbf{x}} - \mathbf{p}/m)e^{-\int_0^\tau \mathrm{d}t\mathcal{L}}, \tag{6}$$

where $\rho_\mathrm{in}(\mathbf{q}_0)$ is the initial PDF and the Lagrangian density is given by $\mathcal{L} = (1/4)D^{-1}[\dot{\mathbf{p}} - \mathbf{H}]^2 + \epsilon\partial_\mathbf{p}\cdot\mathbf{H}$. The path integral is performed by using the discretization parametrized by $0 \leqslant \epsilon \leqslant 1$ where $\dot{\mathbf{p}} \simeq [\mathbf{p}(t) - \mathbf{p}(t - \mathrm{d}t)]/\mathrm{d}t$ and $\mathbf{H} \simeq \epsilon\mathbf{H}(t) + (1 - \epsilon)\mathbf{H}(t - \mathrm{d}t)$ [48] though the path integral is independent of discretizations; typically, $\epsilon = 0$ (prepoint, Ito), $1/2$ (midpoint, Stratonovich), 1 (postpoint, anti-Ito).

We follow the recent approach via the celebrated Cramér–Rao inequality (CRI) in estimation theory of statistics [42–44] to derive TUR [28, 40]. For probability $P_\theta(X)$ for random variables X, unknown deterministic parameter θ is estimated by an estimator $\Phi(X)$. The CRI expresses a lower bound of the variance of the estimator, given as $\mathrm{Var}_\theta\,\Phi \geqslant [\partial_\theta\psi(\theta)]^2/\langle -\partial_\theta^2 \ln P_\theta(X)\rangle$ for $\psi(\theta) = \langle\Phi\rangle_\theta$ with $\langle\cdot\rangle_\theta$ denoting the average over X by $P_\theta(X)$, where the denominator of the bound is called the Fisher information (FI). $\psi(\theta) = \theta$ is called unbiased, otherwise called biased. The CRI can be applied to stochastic thermodynamics where one considers the adjoint dynamics which differs from the original one by the perturbation parameter θ. A similar idea of virtual perturbation has been used in a recent study [46]. Then, the system's dynamical path $\mathbf{q}(t)$ corresponds to X and the production $\Phi[\mathbf{q}(t)]$ to $\Phi(X)$ for the CRI of estimation theory. There are many choices possible to give rise to different forms of TUR. In this study, we pursue one to lead to the TUR which relates the variance of Φ and the EP in the system and bath and to go to that for overdamped dynamics for large γ recently derived by Koyuk and Seifert [37].

We choose the adjoint dynamics subject to a drift term $\mathbf{H}_\theta$ parametrized by θ starting from the same initial state as in the original one. The drift term reads

$$\mathbf{H}_\theta = -\frac{\gamma}{m(1+\theta)}\mathbf{p} + \alpha\mathbf{f}(\mathbf{x},\omega t) + \left(1 - \frac{1}{1+\theta}\right) D\partial_{\mathbf{p}} \ln \rho_\theta(\mathbf{x},\mathbf{p},t), \tag{7}$$

where ρ_θ is the PDF of the adjoint dynamics. α is introduced for a later use, which is set to be unity for the time being. Recently, we have found an independent study by Lee *et al* of which the resultant adjoint dynamics is equivalent with ours except for the scaling factor $1+\theta$ in stead of $(1+\theta)^{-1}$ while the initial PDF is different from that in the original dynamics [47]. Our approach has an important formal advantage over the previous one by Vu and Hasegawa [40] where the drift term is chosen in terms of our terminology given as

$$\begin{aligned}\mathbf{H}_\theta^{\mathrm{VH}} &= -(1+\theta)\frac{\gamma}{m}\mathbf{p} + (1+\theta)^2\mathbf{f}(\mathbf{x},\omega t)\\ &\quad + \left(1-(1+\theta)^3\right) D\partial_{\mathbf{p}} \ln \rho_\theta(\mathbf{x},\mathbf{p},t).\end{aligned} \tag{8}$$

The probability current in momentum space in equation (4) according to $\mathbf{H}_\theta$ has only modification on the irreversible current, given by $[-\gamma(1+\theta)^{-1}\mathbf{p}/m - \beta\gamma(1+\theta)^{-1}]\rho_\theta$, as similarly with the different scaling in the study by Lee *et al* However, $\mathbf{H}_\theta^{\mathrm{VH}}$ alters both the reversible and irreversible currents. Our choice yields the FI for $\theta = 0$ to be exactly equal to $2k_{\mathrm{B}}$ times EP, only taking the irreversible current as will be shown in the following. It is not possible by using equation (8). The FI from the choice by Lee *et al* is found to have a term depending on initial condition in addition to the EP because they use the initial PDF depending on θ. The Fokker–Planck equation for the adjoint dynamics considered by Koyuk and Seifert [37] is $\partial_t\rho_\theta = -(1+\theta)\partial_{\mathbf{x}}\cdot\left(\mathbf{f}/\gamma - 1/(\gamma\beta)\partial_{\mathbf{x}}\right)\rho_\theta$. Our choice of the scaling $(1+\theta)^{-1}\gamma$ guarantees the desired route to overdamped limit.

For the adjoint dynamics by the drift term $\mathbf{H}_\theta$, the CRI is written as

$$\frac{\mathrm{Var}_\theta\,\Phi}{[\partial_\theta\langle\Phi\rangle_\theta]^2} \geqslant \frac{1}{\mathcal{I}(\theta)}, \tag{9}$$

where $\mathrm{Var}_\theta\,\Phi = \langle\Phi^2\rangle_\theta - \langle\Phi\rangle_\theta^2$ is the variance of the production and $\mathcal{I}(\theta) = -\langle\partial_\theta^2 \ln P_\theta[\mathbf{q}(\mathbf{t})]\rangle_\theta$ is the FI associated with the path probability P_θ in the adjoint θ-dynamics. It goes to a TUR in the limit $\theta \to 0$.

First, $\mathcal{I}(0)$ is found from equation (6). The adjoint dynamics is chosen to start from the same initial condition, so $\rho_{\mathrm{in}}(\mathbf{x}_0,\mathbf{p}_0)$ is independent of θ. Only θ-dependence lies in the Lagrangian density $\mathcal{L}_\theta$, given as

$$\mathcal{L}_\theta = \frac{D^{-1}}{4}(\dot{\mathbf{p}} - \mathbf{H}_\theta)^2 + \epsilon\partial_{\mathbf{p}\cdot\mathbf{H}_\theta}. \tag{10}$$

Using the midpoint (Stratonovich) representation with $\epsilon = 1/2$,

$$\mathcal{I}(0) = \frac{D^{-1}}{2}\int_0^\tau \mathrm{d}t\left\langle(\partial_\theta\mathbf{H}_\theta)^2 - (\dot{\mathbf{p}} - \mathbf{H}_\theta)\cdot\partial_\theta^2\mathbf{H}_\theta + D\partial_\theta^2\partial_{\mathbf{p}}\cdot\mathbf{H}_\theta\right\rangle\Big|_{\theta=0}. \tag{11}$$

The second term is written by using the property of midpoint discretization such that $-\langle\partial_\theta^2\mathbf{H}_\theta|_{\theta=0}\cdot(\dot{\mathbf{p}} - \mathbf{H})\rangle = -\langle\partial_\theta^2\mathbf{H}_\theta|_{\theta=0}\cdot(\mathbf{j}_{\mathbf{p}}/\rho - \mathbf{H})\rangle = \langle\partial_\theta^2\mathbf{H}|_{\theta=0}\cdot D\partial_{\mathbf{p}}\rho/\rho\rangle$ that is equal to $-\langle D\partial_{\mathbf{p}}\cdot\partial_\theta^2\mathbf{H}_\theta|_{\theta=0}\rangle$ by integration by parts. It cancels exactly the third term. We find $\partial_\theta\mathbf{H}_\theta|_{\theta=0} = (\gamma/m)\mathbf{p} + D\partial_{\mathbf{p}}\ln\rho = -\mathbf{j}_{\mathbf{p}}^{\mathrm{irr}}/\rho$ where $\mathbf{j}_{\mathbf{p}}^{\mathrm{irr}}$ is the irreversible current density in the momentum space, known as the irreversibility measure for non-equilibrium [45, 49, 50]. Therefore, we have

$$\mathcal{I}(0) = \frac{D^{-1}}{2}\int_0^\tau \mathrm{d}t\left\langle\left(\frac{\mathbf{j}^{\mathrm{irr}}}{\rho}\right)^2\right\rangle = \frac{1}{2k_{\mathrm{B}}}\langle\Delta S_{\mathrm{tot}}\rangle, \tag{12}$$

where $\langle \Delta S_{\text{tot}} \rangle$ is the average EP produced in the system and bath. However, the previous choice in equation (8) is used, $\partial_\theta \mathbf{H}_\theta|_{\theta=0} \neq -\mathbf{j}_{\mathbf{p}}^{\text{irr}}/\rho$, so $2k_{\text{B}}\mathcal{I}(0)$ is not equal to EP, giving a looser TUR bound [40]. In the study by Lee *et al* [47], a different scaling factor $1+\theta$ used instead of $(1+\theta)^{-1}$ only changes the sign of $\partial_\theta \mathbf{H}_\theta|_{\theta=0}$, the square of which gives the same EP. However, the θ-dependent initial PDF, $(\rho_\theta)_{\text{in}}$, gives rise to an addition term, $-\langle \partial_\theta^2 \ln{(\rho_\theta)_{\text{in}}} \rangle_{\theta=0}$, to $\mathcal{I}(0)$ in equation (12).

Next, we find the average production of an observable, basically given by $\langle \Phi \rangle_\theta = \int D[\mathbf{q}]\mathcal{P}_\theta[\mathbf{q}]$ $\int_0^\tau \mathrm{d}t\phi(\mathbf{q},t)$ where $\int D[\mathbf{q}](\cdot)$ stands for the path integration. Note that the production rate ϕ is chosen to be independent of θ, as seen in equation (5). This criterion is based on the perspective that observable is the same as in different adjoint dynamics and has been adopted for all the previous studies. The average production can be found equivalently from

$$\langle \Phi \rangle_\theta = \int_0^\tau \mathrm{d}t \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{p}\ \phi(\mathbf{x},\mathbf{p},t)\rho_\theta(\mathbf{x},\mathbf{p},t), \tag{13}$$

where ρ_θ stands for the PDF for the adjoint dynamics. Substituting $\mathbf{H}_\theta$ for $\mathbf{H}$ in equation (3), we get

$$\partial_t \rho_\theta(\mathbf{x},\mathbf{p},t) = -\left[\partial_{\mathbf{x}} \cdot \frac{\mathbf{p}}{m} \right. \\ \left. + \partial_{\mathbf{p}} \cdot \left\{ -\bar{\gamma}\frac{\mathbf{p}}{m} + \mathbf{f}(\mathbf{x},\omega t) - \bar{\gamma}\beta^{-1}\partial_{\mathbf{p}} \right\} \right] \rho_\theta(\mathbf{x},\mathbf{p},t)\ . \tag{14}$$

ρ_θ satisfies the same form of the Kramers equation with rescaled viscosity coefficient $\bar{\gamma} = \gamma/(1+\theta)$, so we can write

$$\rho_\theta(\mathbf{x},\mathbf{p},t) = \rho(\mathbf{x},\mathbf{p},t;\bar{\gamma}), \tag{15}$$

where ρ stands for the PDF of the original dynamics and only the rescaled parameter $\bar{\gamma}$ is explicitly shown in the argument. If the system is initially prepared in a non-equilibrium state, including NESS, the initial PDF will also depend on the viscosity coefficient which we rename γ_{in} for convenience. It is not rescaled and will take $\gamma_{\text{in}} = \gamma$ at the end of calculation. Then, we find

$$\langle \Phi \rangle_\theta = \int_0^\tau \mathrm{d}t\, \varphi(t;\bar{\gamma}), \tag{16}$$

where $\varphi = \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{p}\phi(\mathbf{x},\mathbf{p},\omega t)\rho(\mathbf{x},\mathbf{p},t;\bar{\gamma})$ is a function of t and $\bar{\gamma}$. Therefore, we get

$$\partial_\theta \langle \Phi \rangle_\theta|_{\theta=0} = \partial_\theta \bar{\gamma} \cdot \partial_{\bar{\gamma}} \langle \Phi \rangle|_{\theta=0} = -\gamma \partial_\gamma \langle \Phi \rangle, \tag{17}$$

The CRI in equation (9) gives the TUR in the limit $\theta \to 0$

$$\frac{\text{Var}\ \Phi}{\left[-\gamma\partial_\gamma\langle\Phi\rangle\right]^2} \geqslant \frac{2k_{\text{B}}}{\langle \Delta S_{\text{tot}} \rangle}. \tag{18}$$

It is a rigorous result, but leaves us a practical problem that γ may not be a relevant protocol parameter in real experiments.

It is desirable to express equation (17) in terms of protocol parameters controlled by external devices such as τ, ω, and β present in the Kramers equation (3). α in equation (7) is designed to control the intensity of the force acting on the system. For many-particle systems in real experiments, interactions on a particle from neighboring particles are basically inherent, so cannot be controlled externally. For low-concentration systems modeled by our single-particle system, such as dilute colloids in a liquid, interaction force can be neglected and α becomes a relevant protocol parameter for remaining force components. For example, the stiffness of an optical trap potential and the strength of an applied force can be controlled accurately with parameter α by using modern experimental technologies. For molecular dynamics, interaction can also be controlled in a model potential, such as the Lenard-Jones potential and α can be regarded as a protocol parameter.

Let us assume α to be such a protocol parameter. We introduce the change in variables and parameters by rescaling as $\bar{t} = t/(1+\theta)$, $\bar{\omega} = (1+\theta)\omega$, $\bar{\mathbf{p}} = (1+\theta)\mathbf{p}$, $\bar{\alpha} = (1+\theta)^2\alpha$, and $\bar{\beta} = (1+\theta)^{-2}\beta$. In this change, ωt remains having the same form as $\bar{\omega}\bar{t}$. The resultant Kramers equation has an invariant form with these changed variables and parameters, given as

$$\partial_{\bar{t}} \rho_\theta(\mathbf{x},\mathbf{p},t) = -\left[\partial_{\mathbf{x}} \cdot \frac{\bar{\mathbf{p}}}{m} + \partial_{\bar{\mathbf{p}}} \cdot \left\{ -\gamma\frac{\bar{\mathbf{p}}}{m} + \bar{\alpha}\mathbf{f}(\mathbf{x},\bar{\omega}\bar{t}) - \gamma\bar{\beta}^{-1}\partial_{\bar{\mathbf{p}}} \right\} \right] \rho_\theta(\mathbf{x},\mathbf{p},t). \tag{19}$$

The formal solution of this equation is given by $\mathcal{T}_\theta(\mathbf{x},\mathbf{p},t|\mathbf{x}_0,\mathbf{p}_0)\rho_{\text{in}}(\mathbf{x}_0,\mathbf{p}_0)$. The transition probability $\mathcal{T}_\theta$ is a special solution for an initial delta-function PDF with peaks at $(\mathbf{x}_0,\mathbf{p}_0)$. It can be written as

$(1+\theta)^d \mathcal{T}(\mathbf{x}, \bar{\mathbf{p}}, \bar{t}|\mathbf{x}_0, \bar{\mathbf{p}}_0)$ depending on changed parameters, $\{\bar{\omega}, \bar{\alpha}, \bar{\beta}\}$, where $\mathcal{T}$ stands for the transition probability for the original dynamics. The initial PDF common for the adjoint and original dynamics can be written as $\rho_{\rm in}(\mathbf{x}_0, \mathbf{p}_0; \{\lambda_a\})$ with its own set of parameters, $\{\lambda_a\}$ for $a = 1, \ldots, n$, independent of θ. For example, an initial equilibrium distribution $\propto \mathrm{e}^{-\beta(\alpha V(x_0)+p_0^2/(2m))}$ has $n = 2$ with $\lambda_1 = \beta$ and $\lambda_2 = \alpha$. In the following, we express everything in the adjoint dynamics in term of those rescaled variables and parameters, so we get $\rho_{\rm in} = (1+\theta)^d \rho_{\rm in}(\mathbf{x}_0, \bar{\mathbf{p}}_0; \{\bar{\lambda}'_b\})$ for $b = 1, \ldots, m' < n$ where not all but specific part $\{\lambda'_b\}$ out of $\{\lambda_a\}$ are forced to be rescaled as $\{\bar{\lambda}'_b\}$ as initial momentum is rescaled. $(1+\theta)^d$ comes out in the rescaling process and automatically guarantees normalization with respect to $\bar{\mathbf{p}}_0$. For example, $[\beta/(2\pi m)]^{1/2} e^{-\beta p^2/(2m)}$ is rewritten as $(1+\theta)[\bar{\beta}/(2\pi m)]^{1/2} e^{-\bar{\beta}\bar{p}^2/(2m)}$ where $\bar{\lambda}'_1 = \bar{\beta} = (1+\theta)^{-2}\beta$ and $\bar{p} = (1+\theta)p$ for $d = 1$. As a result, we have

$$\rho_\theta(\mathbf{x}, \mathbf{p}, t) = (1+\theta)^d \int \mathrm{d}\mathbf{x}_0 \int \mathrm{d}\bar{\mathbf{p}}_0 \mathcal{T}(\mathbf{x}, \bar{\mathbf{p}}, \bar{t}|\mathbf{x}_0, \bar{\mathbf{p}}_0) \rho_{\rm in}\left(\mathbf{x}_0, \bar{\mathbf{p}}_0; \{\bar{\lambda}'_b\}\right). \tag{20}$$

Then, we conclude

$$\rho_\theta(\mathbf{x}, \mathbf{p}, t) = (1+\theta)^d \rho(\mathbf{x}, \bar{\mathbf{p}}, \bar{t}; \bar{\omega}, \bar{\alpha}, \bar{\beta}, \{\bar{\lambda}'_b\}), \tag{21}$$

which is a different representation for the same PDF in equation (15).

Then, we can find the average production of an observable for the adjoint dynamics by using equation (13). The production rate in equation (5) is expressed in terms of rescaled variables and parameters as $\partial_t \chi(\mathbf{x}, \omega t) = \partial_{\bar{t}} \chi(\mathbf{x}, \bar{\omega}\bar{t})/(1+\theta)$ (type I) and $\mathbf{g}(\mathbf{x}, \omega t) \cdot \mathbf{p}/m = \left(\mathbf{g}\left(\mathbf{x}, \bar{\boldsymbol{\omega}}\bar{\boldsymbol{t}} \cdot \bar{\mathbf{p}}/m\right)/(1+\theta)\right.$ (type II). Both types have a common factor $(1+\theta)^{-1}$, so can be written as $\phi(\mathbf{x}, \bar{\mathbf{p}}, \bar{\omega}\bar{t})/(1+\theta)$. Then, we find

$$\langle \Phi \rangle_\theta = \int_0^{\tau/(1+\theta)} \mathrm{d}\bar{t}\ \bar{\varphi}(\bar{t}; \bar{\omega}, \bar{\alpha}, \bar{\beta}, \{\bar{\lambda}_b\}) \tag{22}$$

where $\bar{\varphi} = \int \mathrm{d}\mathbf{x} \int \mathrm{d}\bar{\mathbf{p}}\ \phi(\mathbf{x}, \bar{\mathbf{p}}, \bar{\omega}\bar{t}) \rho(\mathbf{x}, \bar{\mathbf{p}}, \bar{t}; \bar{\omega}, \bar{\alpha}, \bar{\beta}, \{\bar{\lambda}_b\})$. Finally, we get

$$\partial_\theta \langle \Phi \rangle_\theta|_{\theta=0} = \left(-\tau\partial_\tau + \omega\partial_\omega + 2\alpha\partial_\alpha - 2\beta\partial_\beta + \sum_b \partial_\theta \bar{\lambda}'_b|_{\theta=0} \partial_{\lambda'_b}\right) \langle \Phi \rangle, \tag{23}$$

where $-\beta\partial_\beta$ can be replaced by $T\partial_T$ for the temperature T of the bath. It is an equivalent result with equation (17). There is a similar subtle issue about initial condition. Note that differential parameters except $\{\lambda'_b\}$ are restricted to those in the relaxation process for $t > 0$ and those coexisting in the initial condition should be excluded unless included in $\{\lambda'_b\}$. Some of $\{\lambda'_b\}$ may coincide with protocol parameters, but there is no problem to distinguish them theoretically. Experimentally, however, one should use caution to distinguish them. For example, when one measures the response term corresponding to a derivative term in this expression, one should vary the parameter slightly after initial preparation is completed.

There are special initial PDFs which can be realized in many experiments. One can usually prepare a system in equilibrium or local equilibrium around the average position $\mathbf{a}$ and momentum $m\mathbf{v}$ at a different inverse temperature $\beta' = b\beta$. The initial PDF can be written as

$$\begin{aligned}\rho_{\rm in} &= N\left[\frac{\beta'}{2\pi m}\right]^{d/2} e^{\beta'\alpha V(\mathbf{x}_0-\mathbf{a},0)+\beta'(\mathbf{p}_0-m\mathbf{v})^2/(2m)} \\ &= (1+\theta)^d N\left[\frac{b\bar{\beta}}{2\pi m}\right]^d e^{b[\bar{\beta}\bar{\alpha}V(\mathbf{x}_0-\mathbf{a},0)+\bar{\beta}(\bar{\mathbf{p}}-m\bar{\mathbf{v}})^2/(2m)]},\end{aligned} \tag{24}$$

where $\bar{\mathbf{v}} = (1+\theta)\mathbf{v}$ and $N = [\int \mathrm{d}\mathbf{x}_0 e^{\beta'\alpha V(\mathbf{x}_0-\mathbf{a},0)}]^{-1}$ is the normalization factor remaining invariant in the second line due to the reciprocal scaling $\beta\alpha = \bar{\beta}\bar{\alpha}$. By definition, $\bar{\beta}$, $\bar{\alpha}$, and $\bar{\mathbf{v}}$ belong to $\{\bar{\lambda}'_b\}$. Therefore, the former two parameters release the restriction on the derivatives with respective to α and β in equation (23). $\bar{\mathbf{v}}$ exclusively contributes to the response term to the initial condition. We come up with the most useful result

$$\partial_\theta \langle \Phi \rangle_\theta|_{\theta=0} = \left(-\tau\partial_\tau + \omega\partial_\omega + 2\alpha\partial_\alpha - 2\beta\partial_\beta + \mathbf{v}\cdot\partial_{\mathbf{v}}\right) \langle \Phi \rangle, \tag{25}$$

where there is no restriction on α and β including those in the initial condition.

3. Overdamped limit

We can show that the found TUR for large γ goes to that recently derived by Koyuk and Seifert for overdamped dynamics. We will take the limit of large γ for the two equivalent equations (17) and (23). The rigorous proof is possible by using the PDF form found by the perturbation expansion for small γ^{-1} in the previous work [51], given as

$$\rho(\mathbf{x},\mathbf{p},t) \propto \exp\left[-\frac{\beta}{2m}(\mathbf{p}-m\mathbf{u})^2 - \mathcal{V}(\mathbf{x},t)\right]. \tag{26}$$

where

$$\mathbf{u} = \gamma^{-1}[\alpha\mathbf{f}(\mathbf{x},\omega t) + \beta^{-1}\partial_{\mathbf{x}\mathcal{V}}]. \tag{27}$$

Here, $\mathcal{V}$ is the leading-order potential landscape, $-\ln\rho(\mathbf{x},t)$, for the PDF in the position space given by $\rho(\mathbf{x},t) = \int \mathrm{d}\mathbf{p}\rho(\mathbf{x},\mathbf{p},t)$. $\mathbf{u}$ is the velocity field of the probability current in the position space, $\mathbf{j}_\mathbf{x} = \mathbf{u}\rho(\mathbf{x},t)$. In this derivation, the relaxation time for momentum of $\mathcal{O}(\gamma^{-1})$ is negligible, so any initial memory of momentum distribution is assumed to decay exponentially as $e^{-c_1\gamma t}$. As a consequence, the PDF in overdamped limit has no dependence on initial parameters $\{\lambda_b'\}$. This equation manifests our expectation that fast-varying momentum variable maintains a local equilibrium distribution around an instantaneous average momentum $m\mathbf{u}$ along the trajectory of slowly varying position variable.

Integrating the Kramers equation (3) over momentum, we get

$$\begin{aligned}\partial_t\rho(\mathbf{x},t) &= -\partial_\mathbf{x}\cdot\frac{\langle\mathbf{p}\rangle_\mathbf{p}}{m}\rho(\mathbf{x},t) - \partial_\mathbf{x}\mathcal{V}\cdot\frac{\langle\mathbf{p}-m\mathbf{u}\rangle_\mathbf{p}}{m}\rho(\mathbf{x},t)\\ &= -\gamma^{-1}\partial_\mathbf{x}\cdot\left[\alpha\mathbf{f}(\mathbf{x},\omega t) - \beta^{-1}\partial_\mathbf{x}\right]\rho(\mathbf{x},t)\ ,\end{aligned} \tag{28}$$

where $\langle\cdot\rangle_\mathbf{p}$ denotes the average over $\mathbf{p}$ with the PDF in equation (26) and we use $\langle\mathbf{p}\rangle_\mathbf{p} = m\mathbf{u}$ to get the final line. The result leads to the desired Fokker–Planck equation. Changing time variable as $s = t\alpha/\gamma$, the above Fokker–Planck equation becomes

$$\partial_s\rho(\mathbf{x},t) = -\partial_\mathbf{x}\cdot[\mathbf{f}(\mathbf{x},\omega\gamma\alpha^{-1}s) - (\alpha\beta)^{-1}\partial_\mathbf{x}]\rho(\mathbf{x},t) \tag{29}$$

and hence we can write

$$\rho(\mathbf{x},t) = \rho(\mathbf{x},s;(\alpha\beta)^{-1},\omega\gamma\alpha^{-1}). \tag{30}$$

We find

$$\langle\phi(\mathbf{x},\mathbf{p},t)\rangle_\mathbf{p} = \begin{cases}\alpha\gamma^{-1}\partial_s\chi(\mathbf{x},\omega\gamma\alpha^{-1}s) & \text{(type I)}\\ \alpha\gamma^{-1}\mathbf{g}(\mathbf{x},\omega\gamma\alpha^{-1}s)\cdot\left\{\mathbf{f}(\mathbf{x},\omega\gamma\alpha^{-1}s) + (\alpha\beta)^{-1}\partial_{\mathbf{x}\mathcal{V}}\right\} & \text{(type II)}\end{cases} \tag{31}$$

Then, we can write $\langle\phi(\mathbf{x},\mathbf{p},t)\rangle_\mathbf{p} = \alpha\gamma^{-1}\phi^{\mathrm{OD}}(\mathbf{x},(\omega\gamma\alpha^{-1})s)$. The average production of an observable is equal to $\int_0^\tau \mathrm{d}t\int \mathrm{d}\mathbf{x}\langle\phi(\mathbf{x},\mathbf{p},t)\rangle_\mathbf{p}\rho(\mathbf{x},t)$, given as

$$\begin{aligned}\langle\Phi\rangle &= \int_0^\tau \mathrm{d}t\alpha\gamma^{-1}\int \mathrm{d}\mathbf{x}\,\phi^{\mathrm{OD}}(\mathbf{x},(\omega\gamma\alpha^{-1})s)\rho(\mathbf{x},s;(\alpha\beta)^{-1},\omega\gamma\alpha^{-1})\\ &= \int_0^{\tau\alpha\gamma^{-1}} \mathrm{d}s\,\varphi^{\mathrm{OD}}(s;(\alpha\beta)^{-1},\omega\gamma\alpha^{-1}),\end{aligned} \tag{32}$$

where $\varphi^{\mathrm{OD}} = \int \mathrm{d}\mathbf{x}\phi^{\mathrm{OD}}(\mathbf{x},(\omega\gamma\alpha^{-1})s)\rho(\mathbf{x},s;(\alpha\beta)^{-1},\omega\gamma\alpha^{-1})$.

Differentiating equation (32) with respect to γ, we find the overdamped limit of equation (17) as

$$-\gamma\partial_\gamma\langle\Phi\rangle = (\tau\alpha\gamma^{-1}\partial_{\tau\alpha\gamma^{-1}} - \gamma\omega\alpha^{-1}\partial_{\omega\gamma\alpha^{-1}})\langle\Phi\rangle = (\tau\partial_\tau - \omega\partial_\omega)\langle\Phi\rangle. \tag{33}$$

For consistency check, we similarly find the overdamped limit of equation (23) as

$$\begin{aligned}&\left(-\tau\partial_\tau + \omega\partial_\omega + 2\alpha\partial_\alpha - 2\beta\partial_\beta\right)\langle\Phi\rangle\\ &\quad= \left\{-\tau\partial_\tau + \omega\partial_\omega + 2\alpha\left(\tau\gamma^{-1}\partial_{\tau\alpha\gamma^{-1}} + \beta\partial_{\alpha\beta} - \omega\gamma\alpha^{-2}\partial_{\omega\gamma\alpha^{-1}}\right) - 2\beta\alpha\partial_{\alpha\beta}\right\}\langle\Phi\rangle\\ &\quad= (\tau\partial_\tau - \omega\partial_\omega)\langle\Phi\rangle.\end{aligned} \tag{34}$$

It comes up with the TUR for the overdamped case derived by Koyuk and Seifert, as seen in equation (2).

It is pedagogically interesting to see $\langle\Delta S_{\mathrm{tot}}\rangle$ approach to that for the overdamped limit. The irreversible current is found as $\mathbf{j}_\mathbf{p}^{\mathrm{irr}} = (-\gamma\mathbf{p}/m - D\partial_\mathbf{p})\rho = -\gamma\mathbf{u}\rho(\mathbf{x},\mathbf{p},t)$ by using equation (26). Then, the average EP rate is given in the leading order as

$$D^{-1}\left\langle\left(\mathbf{j}_\mathbf{p}^{\mathrm{irr}}\rho^{-1}\right)^2\right\rangle \simeq \gamma^{-1}\beta\langle(\gamma\mathbf{u})^2\rangle = D_{\mathrm{OD}}^{-1}\left\langle\left(\mathbf{j}_\mathbf{x}\rho(\mathbf{x},t)^{-1}\right)^2\right\rangle, \tag{35}$$

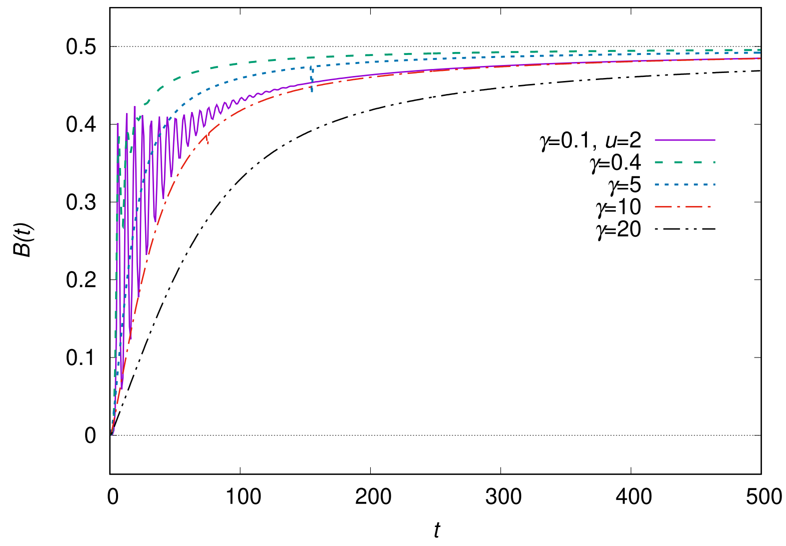

Figure 1. $B(t)$ versus time t in unit of ω_0^{-1} for the pulled harmonic oscillator with the angular frequency $\omega_0 = \sqrt{k/m}$. The system is considered to start from the equilibrium state for the initial center of the harmonic potential, $a(0) = 0$. Graphs are drawn from the analytic calculations for various values of γ in unit of $\sqrt{km}$ and pulling speed $u = 2$ in unit of $\omega_0(\beta k)^{-1/2}$. All graphs meet the TUR, $B(t) \leqslant 1/2$. Graphs for $\gamma = 0.1, 0.4$ present oscillation, which belong to the underdamped regime of damped harmonic oscillator, $\gamma < 2$. For small t, $B(t)$ sales as t^3 due to the scaling:Var $W \sim t^2$, EP $\sim t$, and DW $\sim t^3$. For large t, $B(t)$ is analytically shown to converge asymptotically to 1/2, i.e. corresponding to the TUR bound $2k_\mathrm{B}$.

where $D_\mathrm{OD} = (\beta\gamma)^{-1}$ is the diffusion coefficient for the overdamped dynamics. Hence we get

$$\mathcal{I}(0) = \frac{D_\mathrm{OD}^{-1}}{2}\int_0^\tau \mathrm{d}t \int \mathrm{d}\mathbf{x}\, \frac{\mathbf{j}_\mathbf{x}(\mathbf{x},t)\cdot\mathbf{j}_\mathbf{x}(\mathbf{x},t)}{\rho(\mathbf{x},t)}. \tag{36}$$

It is indeed equal to $(2k_\mathrm{B})^{-1}\langle\Delta S_\mathrm{tot}\rangle$ for the overdamped system.

4. Examples

We investigate the non-equilibrium motion of a single particle in a harmonic trap potential which is perturbed in time by an external device. There are two cases for the change of potential protocols, center and stiffness. We check the inequality in equation (18) for the work production W by plotting the reciprocal form of TUR

$$B(t) = \frac{\mathrm{DW}^2}{\mathrm{Var}\ W\cdot\mathrm{EP}}, \tag{37}$$

where $\mathrm{EP} = k_\mathrm{B}^{-1}\langle\Delta S_\mathrm{tot}\rangle$ and $DW = -\gamma\partial_\gamma\langle W\rangle$. The TUR states $B(t) \leqslant 1/2$.

We examine the case where the center of the potential varies in time. In this case, the potential is given by $V(x,t) = k(x - a(t))^2/2$ for stiffness k. We consider the two examples: (i) $a(t) = ut$ for a constant pulling velocity u playing the role of ω (ii) $a(t) = A\sin\omega t$. We investigate the TUR for work production W given by $\int_0^\tau \mathrm{d}t\partial_t V$ and the production rate $\phi(x,t) = \partial_t V = -ku(x - ut)$ for (i) and $\phi(x,\omega t) = -kA\omega\cos\omega t$ $(x - A\sin\omega t)$ for (ii). An initial local-equilibrium-state in equation (24) can be considered by using the PDF

$$\rho_\mathrm{in}(x,p,t) = \left[\frac{\beta'^2 k}{(2\pi)^2 m}\right]^{1/2} e^{-(\beta'/2)(k(x-a)^2+(p-mv)^2/m)}, \tag{38}$$

where a and v are the average values of position and velocity at $t = 0$, respectively, and $\beta' \neq \beta$ in general. We note $\mathbf{v} = v$ in equation (23) for this one dimensional problem. This initial condition is explicitly applied to example (ii). The problem is simplified as we separate stochastic and deterministic variables such that $(x,p) = (z_x, z_p) + (X,P)$ for mean variables $X = \langle x\rangle$ and $P = \langle p\rangle$, equivalently written as $\mathbf{q} = \mathbf{z} + \bar{\mathbf{q}}$. Using $P = m\dot{X}$, X satisfies $m\ddot{X} + \gamma\dot{X} + \alpha kX = \alpha ka(t)$, that is well-known as driven damped harmonic oscillator, and $\bar{\mathbf{q}}(t)$ can be found easily. It turns out that the stochastic part $\mathbf{z}$ evolves through the equilibration process around the deterministic part $\bar{\mathbf{q}}(t)$. Then, the PDF for $\mathbf{q}$ is written as

$$P(\mathbf{q},t) = \frac{1}{Z(t)}\exp\left[-\frac{1}{2}[\mathbf{q} - \bar{\mathbf{q}}(\mathbf{t})]^\mathrm{t}\cdot\mathsf{A}(t)\cdot[\mathbf{q} - \bar{\mathbf{q}}(\mathbf{t})]\right], \tag{39}$$

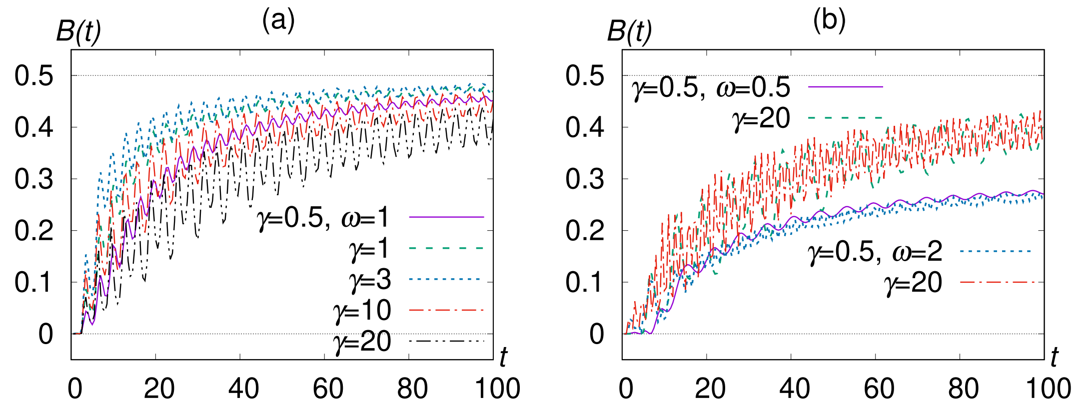

Figure 2. $B(t)$ versus time t in unit of ω_0^{-1} for the harmonic oscillator with the oscillating center. The system is considered to start from the local-equilibrium state given in equation (38). Graphs are drawn from the analytical calculations for various values of γ and ω in the same units as in figure 1. We use the amplitude of driving $A = 1$ and the initial root-mean-square (rms) distance $a = 0.1$ in unit of $(\beta k)^{-1/2}$, and the initial rms velocity $v = 0.1$ in unit of $(m\beta)^{-1/2}$. We use an initial inverse temperature $\beta' = 0.5\beta$. The panel (a) is for $\omega = 1$ and (b) for $\omega = 0.5, 2$. For small t, $B(t) \sim t^3$ because Var $W \sim t^2$, EP $\sim t$, and DW $\sim t^3$, which shows the same scaling behavior as in figure 1. All graphs are shown to increase with oscillation due to driven oscillation. Graphs for low driving frequency, $\omega = 0.5$ in panel (b), are shown to touch $B(t) = 0$ line again at small times. It is not shown for non-oscillatory driving in figure 1. For large t, all graphs approach to the analytically found asymptote $B_\infty = (1/2)[\left((1-\omega^2)^2 - \gamma^2\omega^2\right) / \left((1-\omega^2)^2 + \gamma^2\omega^2\right)]^2$.

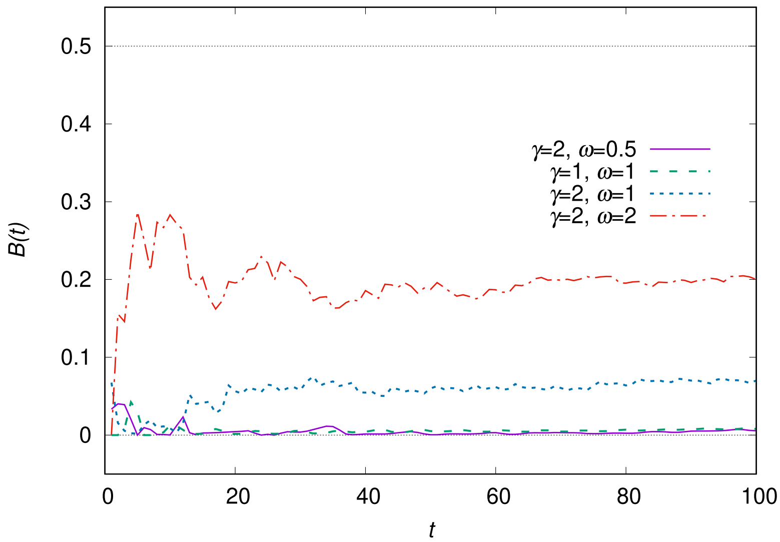

Figure 3. $B(t)$ versus time t in unit of ω_0^{-1} for the harmonic potential with the time-varying stiffness. Graphs are drawn from the computer simulations for various values of γ and ω in the same units as in the previous figures. We use $b = 1/2$ for $k(t) = k(1 + b \sin \omega t)$. Due to non-equilibrium fluctuation the large number of samples, 3.93216×10^9, are used. Obtained graphs show $B(t) < 1/2$, as expected. The asymptotic behavior for large time requires further simulations for huge computing time, though $B(t)$ approaches to smaller value than 1/2.

where $Z(t) = \sqrt{(2\pi)^2/\det \mathsf{A}(t)}$. It is in fact the Gaussian distribution for $\mathbf{z} = \mathbf{q} - \bar{\mathbf{q}}$. From the previous study [52], the covariance matrix of the Gaussian distribution is given by $\mathsf{A}(t)^{-1} = \mathsf{A}_{\mathrm{eq}}^{-1} - e^{-\mathsf{F}t}\left[\mathsf{A}_{\mathrm{eq}}^{-1} - \mathsf{A}(0)^{-1}\right] e^{-\mathsf{F}^{\mathrm{t}}t}$, where $\mathsf{A}_{\mathrm{eq}} = \beta \begin{pmatrix} k & 0 \\ 0 & 1/m \end{pmatrix}$ and $\mathsf{F} = \begin{pmatrix} 0 & 1/m \\ k & \gamma/m \end{pmatrix}$. The two examples can be studied analytically. Example (i) has been studied extensively in theory and experiment for overdamped dynamics [16, 53–55]. For the underdamped dynamics, we use the results from our recent studies [56, 57]. Example (ii) has also been studied recently by our group [58]. Figures 1 and 2 shows that all $B(t)$ graphs for various values of parameters for γ and ω (u) are below the horizontal line $B(t) = 1/2$. In figure 1, all graphs of $B(t)$ converge to the asymptote $B_\infty = 1/2$, which can be shown analytically. The asymptote for example (ii) can be found analytically as $B_\infty = (1/2)[\left((1-\omega^2)^2 - \gamma^2\omega^2\right) / \left((1-\omega^2)^2 + \gamma^2\omega^2\right)]^2$ for ω in unit of $\omega_0 = \sqrt{k/m}$ and γ in unit of $\sqrt{mk}$, which agrees with the graphs in figure 2. It is interesting that $B_\infty(t) = 1/2$ only for $\omega = 1$, as well observed in figure 2(a).

We can examine another case of time-varying stiffness, for which we consider a third example (iii): $V = k(t)x^2/2$ with $k(t) = k(1 + b\sin\omega t)$. The work production rate is equal to $\phi(x, \omega t) = \partial_t V(x, \omega t) = (kb\omega\cos\omega t)x^2/2$. This problem is investigated by using the computer simulation. Figure 3 shows that $B(t) < 1/2$ for various values of γ and ω, though the asymptotic behavior for large t needs further investigation with huge computing time and samples. From present simulations, $B(t)$ is found to approach to a smaller value than 1/2 for large t.

5. Summary

We derive the TUR for the time-accumulated production for time period τ for an arbitrary observable in underdamped dynamics subject to general time-dependent protocols by exploiting the CRI. We show it to approach to the known TUR in overdamped dynamics for large viscosity limit. Any scaling function $s(\theta)$ with $s(0) = 1$ and non-zero $s'(0)$ for the place of $(1 + \theta)^{-1}$ in equation (7) leads to the unique TUR in the limit $\theta \to 0$, since $\mathcal{I}(\theta)$ and $(\partial_\theta\langle\Phi\rangle_\theta)^2$ will have the same factor $s'(0)^2$, which can be seen from the detail limiting step $\theta \to 0$ in equations (11) and (17). The TUR derived in our study is shown to give universal bound for the product of the variance and EP, for which we provide the two equivalent representations: one in terms of response function for γ only and the other in terms of response functions for various protocol parameters other than γ used in experiments. Formulation for general N-particle system in non-isotropic medium is straightforward by writing the ith component of force on lth particle as $-\gamma_{ij}\sum_j p_{lj}/m + f_{li} - \sum_j D_{ij}\partial_{p_{lj}} \ln\rho$ with $f_{li} = -\partial_{x_{li}}(V + V_{\mathrm{int}}) + f_{li}^{\mathrm{nc}}$ for $l = 1, \ldots, N$ and $i, j = 1, \ldots, d$ where V and V_{int} are respectively a confining potential as a function of individual particle positions and an interaction potential as a function of inter-particle distances among particles. Then, we can find a similar TUR to equation (18) with derivatives with respect to many γ_{ij}'s and also that using equation (23). However, as pointed out, for high particle concentration the equivalent form of TUR in use of equation (23) loses its practicability in experiments due to the uncontrollable α parameter. Interestingly, in the overdamped limit α-dependence of the TUR disappears as shown in our study and hence no practicability issue arises.

Acknowledgments

We thank Professor Hyunggyu Park and Dr. Jongmin Park at Korean Institute of Advanced Studies for stimulating and helpful discussions. This work was supported by Basic Science Research Program of the National Research Foundation(NRF) funded by the Ministry of Education with Grant Nos. 2020R1A2C100976111 (CK) and 2018R1D1A1B07049254 (HKL).

ORCID iDs

Chulan Kwon https://orcid.org/0000-0003-0011-4385

References

[1] Evans D J, Cohen E G D and Morriss G P 1993 *Phys. Rev. Lett.* **71** 2401
[2] Evans D J and Searles D J 1994 *Phys. Rev.* E **50** 1645
[3] Gallavotti G and Cohen E G D 1995 *Phys. Rev. Lett.* **74** 2694
Gallavotti G and Cohen E G D 1995 *J. Stat. Phys.* **80** 931
[4] Jarzynski C 1997 *Phys. Rev. Lett.* **78** 2690
[5] Jarzynski C 1997 *Phys. Rev.* E **56** 5018
[6] Crooks G E 1999 *Phys. Rev.* E **60** 2721
[7] Kurchan J 1998 *J. Phys. A: Math. Gen.* **31** 3719
[8] Lebowitz J L and Spohn H 1999 *J. Stat. Phys.* **95** 333
[9] Speck T and Seifert U 2005 *J. Phys. A: Math. Gen.* **38** L581
Seifert U 2005 *Phys. Rev. Lett.* **95** 040602
[10] Esposito M and Van den Broeck C 2010 *Phys. Rev. Lett.* **104** 090601
[11] Wang G M, Sevick E M, Mittag E, Searles D J and Evans D J 2002 *Phys. Rev. Lett.* **89** 050601
[12] Hummer G and Szabo A 2001 *Proc. Natl Acad. Sci.* **98** 3658
[13] Liphardt J, Dumont S, Smith S B, Tinoco I and Bustamante C J 2002 *Science* **296** 1832
[14] Trepagnier E H, Jarzynski C, Ritort F, Crooks G E, Bustamante C J and Liphardt J 2004 *Proc. Natl Acad. Sci.* **101** 15038
[15] Collin D, Ritort F, Jarzynski C, Smith S B, Tinoco I and Bustamante C 2005 *Nature* **437** 231
[16] Garnier N and Ciliberto S 2005 *Phys. Rev.* E **71** 060101
[17] Hayashi K, Ueno H, Iino R and Noji H 2010 *Phys. Rev. Lett.* **104** 218103
[18] Lee D Y, Kwon C and Pak H K 2015 *Phys. Rev. Lett.* **114** 060603

[19] Uffink J and van Lith J 1999 *Found. Phys.* **29** 655
[20] Barato A C and Seifert U 2015 *Phys. Rev. Lett.* **114** 158101
[21] Gingrich T R, Horowitz J M, Perunov N and England J L 2016 *Phys. Rev. Lett.* **116** 120601
[22] Horowitz M and Gingrich T R 2017 *Phys. Rev.* E **96** 020103(R)
[23] Gingrich T R, Rotskoff G M and Horowitz J M 2017 *J. Phys. A: Math. Theor.* **50** 184004
[24] Pietzonka P, Ritort F and Seifert U 2017 *Phys. Rev.* E **96** 012101
[25] Proesmans K and Van den Broeck C 2017 *Europhys. Lett.* **119** 20001
[26] Macieszczak K, Brandner K and Garrahan J P 2018 *Phys. Rev. Lett.* **121** 130601
[27] Dechant A and Sasa S-i 2018 *J. Stat. Mech.* 063209
[28] Hasegawa Y and Vu T V 2019 *Phys. Rev.* E **99** 062126
[29] Pietzonka P and Seifert U 2018 *Phys. Rev. Lett.* **120** 190602
[30] Holubec V and Ryabov A 2018 *Phys. Rev. Lett.* **121** 120601
[31] Barato A C and Seifert U 2016 *Phys. Rev.* X **6** 041053
[32] Barato A C, Chetrite R, Faggionato A and Gabrielli D 2018 *New J. Phys.* **20** 103023
[33] Koyuk T, Seifert U and Pietzonka P 2019 *J. Phys. A: Math. Theor.* **52** 02LT02
[34] Koyuk T and Seifert U 2019 *Phys. Rev. Lett.* **122** 230601
[35] Hasegawa Y and Van Vu T 2019 *Phys. Rev. Lett.* **123** 110602
[36] Potts P P and Samuelsson P 2019 *Phys. Rev.* E **100** 052137
[37] Koyuk T and Seifert U 2020 *Phys. Rev. Lett.* **125** 260604
[38] Fischer L P, Pietzonka P and Seifert U 2018 *Phys. Rev.* E **97** 022143
[39] Chun H-M, Fischer L P and Seifert U 2019 *Phys. Rev.* E **99** 042128
[40] Vu T V and Hasegawa Y 2019 *Phys. Rev.* E **100** 032130
[41] Lee J S, Park J-M and Park H 2019 *Phys. Rev.* E **100** 062132
[42] Rao C R 1945 *Bull. Calcutta Math. Soc.* **37** 81
[43] Cremér H 1946 *Mathematecal Methods of Statistics* (Princeton, NJ: Princeton University Press)
[44] Casella G and Berger R L 2001 *Statistical Inference* ed C Crockett (Pacific Grove, CA: Duxbury-Thomson Learning)
[45] Risken H 1989 *The Fokker–Planck Equation: Methods of Solution and Applications* 2nd edn (Berlin: Springer)
[46] Dechant A and Sasa S-i 2020 *Proc. Natl Acad. Sci. USA* **117** 6430
[47] Lee J S, Park J-M and Park H 2021 arXiv:2106.01599
[48] Kwon C 2015 *J. Korean Phys. Soc.* **67** 785
[49] Spinney R E and Ford I J 2012 *Phys. Rev. Lett.* **108** 170603
Spinney R E and Ford I J Phys. Rev. E 85 051113.
Spinney R E and Ford I J Phys. Rev. E 86 021127.
[50] Yeo J, Kwon C, Lee H K and Park H 2016 *J. Stat. Mech.* 093205
[51] Ao P, Kwon C and Qian H 2007 *Complexity* **12** 19
[52] Kwon C, Noh J D and Park H 2011 *Phys. Rev.* E **83** 061145
[53] van Zon R and Cohen E G D 2003 *Phys. Rev.* E **67** 046102
[54] van Zon R and Cohen E G D 2003 *Phys. Rev. Lett.* **91** 110601
[55] Kim K, Kwon C and Park H 2014 *Phys. Rev.* E **90** 032117
[56] Kwon C 2018 *J. Korean Phys. Soc.* **73** 866
[57] Kwon C, Um J, Yeo J and Park H 2019 *Phys. Rev.* E **100** 052127
[58] Kwon C, Kwon Y and Lee H private note.