Direct Route to Thermodynamic Uncertainty Relations and Their Saturation

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Thermodynamic uncertainty relations (TURs) bound the dissipation in nonequilibrium systems from below by fluctuations of an observed current. Contrasting the elaborate techniques employed in existing proofs, we here prove TURs directly from the Langevin equation. This establishes the TUR as an inherent property of overdamped stochastic equations of motion. In addition, we extend the transient TUR to currents and densities with explicit time dependence. By including current-density correlations we, moreover, derive a new sharpened TUR for transient dynamics. Our arguably simplest and most direct proof, together with the new generalizations, allows us to systematically determine conditions under which the different TURs saturate and thus allows for a more accurate thermodynamic inference. Finally, we outline the direct proof also for Markov jump dynamics.

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A defining characteristic of nonequilibrium systems is a nonvanishing entropy production [1–8] emerging during relaxation [7–12], in the presence of time-dependent (e.g., periodic [13–18]) driving, or in nonequilibrium steady states (NESS) [19–26]. A detailed understanding of the thermodynamics of systems far from equilibrium is in particular required for unraveling the physical principles that sustain active, living matter [27–31]. Notwithstanding its importance, the entropy production within a nonequilibrium system beyond the linear response is virtually impossible to quantify from experimental observations, as it requires detailed knowledge about all dissipative degrees of freedom.

A recent and arguably the most relevant method to infer a lower bound on the entropy production in an experimentally observed complex system is via the so-called thermodynamic uncertainty relation (TUR) [25,26,32–39], which relates the (time-accumulated) dissipation Σ_t to fluctuations of a general time-integrated current J_t. For overdamped systems in a NESS it reads [23,24]

$$\frac{\Sigma_t}{k_B T} \geq 2\frac{\langle J_t\rangle^2}{\mathrm{var}(J_t)}, \tag{1}$$

with variance $\mathrm{var}(J_t) \equiv \langle J_t^2\rangle - \langle J_t\rangle^2$ and thermal energy $k_B T$, which will henceforth be dropped for convenience and replaced by the convention of energies measured in units of $k_B T$. The TUR may be seen as the natural counterpart of the fluctuation-dissipation theorem [40] or a more precise formulation of the second law [41]. Notably, it may also be interpreted as gauging the "thermodynamic cost of precision" [42], and it was found to limit the temporal extent of anomalous diffusion [43].

Since its original discovery [23] and proof [24] for systems in a NESS, a large number of more or less general variants of the TUR were derived. In particular, for paradigmatic overdamped dynamics and Markov jump processes, such generalized TURs have been found for transient systems (i.e., nonstationary dynamics emerging, e.g., from nonsteady-state initial conditions) in the absence [44–46] and presence of time-dependent driving [17,18]. Moreover, an extension to state variables (which we will refer to as "densities") instead of currents has been formulated [18], and recently correlations of densities and currents have been incorporated to significantly sharpen and even saturate the inequality for steady-state systems [41]. Note, however, that the validity of the TUR is generally limited to overdamped dynamics, as it was shown to break down in systems with momenta [47].

Many different techniques have been employed to derive TURs, including large deviation theory [24,33,40,48,49], bounds to the scaled cumulant generating function [18,45,50], as well as martingale [2] and Hilbert-space [51] techniques. Most notably, the TUR has been derived as a consequence of the generalized Cramér-Rao inequality [46,52] which is well known in information theory and statistics. However, while providing valuable insight, the proof via the Cramér-Rao inequality includes quantifying the Fisher information of the Onsager-Machlup path measure [52] and involves a dummy parameter that "tilts" the original dynamics. Thus, it may not be faithfully considered as being direct. In fact, the TUR and its generalizations seem to be an inherent property of overdamped stochastic dynamics and are thus akin to quantum-mechanical uncertainty, expected to follow directly from the equations of motion.

Here, we show that no elaborated concepts beyond the equations of motion are indeed required. Using only stochastic calculus and the well known Cauchy-Schwarz inequality we prove various existing TURs (including the correlation TUR [41]) for time-homogeneous overdamped dynamics in continuous space directly from the Langevin equation. Thereby we both unify and simplify proofs of TURs. Moreover, we derive, for the first time, the sharper correlation TUR for transient dynamics without explicit time dependence. This improved TUR can be saturated arbitrarily far from equilibrium for any initial condition and duration of trajectories, which we illustrate with the example of a displaced harmonic trap. Our simple proof offers several advantages and we therefore believe that it deserves attention even in cases that have already been proven before. Most notably it enables immediate insight into how one can saturate the various TURs and allows for easy generalizations. Beyond the results for overdamped dynamics, we illustrate the analogous direct proof of the steady-state TUR also for Markov jump dynamics.

Setup.—We consider d-dimensional [53] time-homogeneous (i.e., coefficients do not explicitly depend on time) overdamped dynamics described by the stochastic differential (Langevin) equation [54,55]

$$d\mathbf{x}_\tau = \mathbf{F}(\mathbf{x}_\tau)d\tau + \boldsymbol{\sigma}(\mathbf{x}_\tau) \circledast d\mathbf{W}_\tau, \tag{2}$$

where the anti-Itô product $\circledast$ assures thermodynamical consistency in the case of multiplicative noise [i.e., space dependent $\boldsymbol{\sigma}(\mathbf{x}_\tau)$] [2,26,56–58]. The choice of the product is irrelevant in the case of additive noise $\boldsymbol{\sigma}(\mathbf{x}_\tau) = \boldsymbol{\sigma}$. The increment $d\mathbf{W}_\tau$ of the Wiener process has zero mean $\langle d\mathbf{W}_\tau \rangle = \mathbf{0}$ and is due to its covariance $\langle dW_{\tau,i} dW_{\tau',j} \rangle = \delta(\tau - \tau')\delta_{ij} d\tau d\tau'$ known as delta correlated or white noise. The noise amplitude is related to the diffusion coefficient via $\mathbf{D}(\mathbf{x}) \equiv \boldsymbol{\sigma}(\mathbf{x})\boldsymbol{\sigma}(\mathbf{x})^T/2$ where $\boldsymbol{\sigma}$ and $\mathbf{D}$ are $d \times d$ matrices. Let $P(\mathbf{x}, \tau)$ be the probability density to find $\mathbf{x}_\tau$ at a point $\mathbf{x}$ given some initial condition $P(\mathbf{x}, 0)$. Then the instantaneous probability density current $\mathbf{j}(\mathbf{x}, \tau)$ is given by

$$\mathbf{j}(\mathbf{x}, \tau) = [\mathbf{F}(\mathbf{x}) - \mathbf{D}(\mathbf{x})\nabla]P(\mathbf{x}, \tau), \tag{3}$$

and the Fokker-Planck equation [55,59] for the time evolution of $P(\mathbf{x}, \tau)$ follows from Eq. (2) and reads [54]

$$\partial_\tau P(\mathbf{x}, \tau) = -\nabla \cdot \mathbf{j}(\mathbf{x}, \tau). \tag{4}$$

In the special case that $\mathbf{F}(\mathbf{x})$ is sufficiently confining a NESS is eventually reached with invariant density $P_s(\mathbf{x}) \equiv P(\mathbf{x}, \tau \to \infty)$ and steady-state current $\mathbf{j}_s(\mathbf{x}) \equiv [\mathbf{F}(\mathbf{x}) - \mathbf{D}(\mathbf{x})\nabla]P_s(\mathbf{x})$ with $\nabla \cdot \mathbf{j}_s(\mathbf{x}) = 0$ [55]. The mean total (medium plus system) entropy production in the time interval $[0, t]$ is given by [3,4]

$$\Sigma_t = \int d\mathbf{x} \int_0^t \frac{\mathbf{j}^T(\mathbf{x}, \tau)\mathbf{D}^{-1}(\mathbf{x})\mathbf{j}(\mathbf{x}, \tau)}{P(\mathbf{x}, \tau)} d\tau. \tag{5}$$

Let J_t be a generalized time-integrated current with some vector-valued $\mathbf{U}(\mathbf{x}, \tau)$ defined via the Stratonovich stochastic integral (only for $\mathbf{x}$-dependent $\mathbf{U}$ the convention matters)

$$J_t \equiv \int_{\tau=0}^{\tau=t} \mathbf{U}(\mathbf{x}_\tau, \tau) \cdot \circ d\mathbf{x}_\tau. \tag{6}$$

Note that for any integrand $\mathbf{U}$ this current and its first two moments are readily obtained from measured trajectories $(\mathbf{x}_\tau)_{0 \le \tau \le t}$. Therefore, a TUR involving such J_t is "operationally accessible." For dynamics in Eq. (2) the current may be equivalently written as the sum of Itô integrals and $d\tau$ integrals, $J_t = J_t^{\mathrm{I}} + J_t^{\mathrm{II}}$, with [26]

$$\begin{aligned} J_t^{\mathrm{I}} &\equiv \int_{\tau=0}^{\tau=t} \mathbf{U}(\mathbf{x}_\tau, \tau) \cdot \boldsymbol{\sigma}(\mathbf{x}_\tau) d\mathbf{W}_\tau, \\ J_t^{\mathrm{II}} &\equiv \int_0^t [\mathbf{U}(\mathbf{x}_\tau, \tau) \cdot \mathbf{F}(\mathbf{x}_\tau) + \nabla \cdot [\mathbf{D}(\mathbf{x}_\tau)\mathbf{U}(\mathbf{x}_\tau, \tau)]] d\tau \\ &\equiv \int_0^t \mathcal{U}(\mathbf{x}_\tau, \tau) d\tau. \end{aligned} \tag{7}$$

By the zero-mean and independence properties of the Wiener process $\langle J_t^{\mathrm{I}} \rangle = 0$ and thus $\langle J_t \rangle = \langle J_t^{\mathrm{II}} \rangle = \int_0^t d\tau \int d\mathbf{x} \mathcal{U}(\mathbf{x}, \tau) P(\mathbf{x}, \tau)$. Integrating by parts and using Eq. (3) we obtain (see also [26])

$$\langle J_t \rangle = \int_0^t d\tau \int d\mathbf{x} \mathbf{U}(\mathbf{x}, \tau) \cdot \mathbf{j}(\mathbf{x}, \tau). \tag{8}$$

The variance $\mathrm{var}(J_t)$ can in turn be computed from two-point densities [25,26,60,61], but is not required to prove TURs.

We now outline our direct proof of TURs. First, we rederive the classical TUR (1) and its generalization to transients [45], whereby we find a novel correction term that extends the validity of the transient TUR. Next, we prove the TUR for densities [18] and thereafter the correlation-improved TUR [41], for the first time also for nonstationary dynamics. Finally, we explain how to saturate the various TURs and illustrate our findings with an example. The proof relies solely on the equation of motion Eq. (2) and implied Fokker-Planck equation (4), which is why we call the proof "direct."

Direct proof of TURs.—The essence of the direct proof is fully contained in the following equations (9)–(11). First, we require a scalar quantity A_t with zero mean and whose second moment yields the dissipation defined in Eq. (5), i.e., $\langle A_t^2 \rangle = \Sigma_t/2$ [62]. Considering the "delta-correlated" property of $d\mathbf{W}_\tau$ and $\mathbf{D} = \mathbf{D}^T = \boldsymbol{\sigma}(\mathbf{x})\boldsymbol{\sigma}(\mathbf{x})^T/2$ leads to the "educated guess" (see [63])

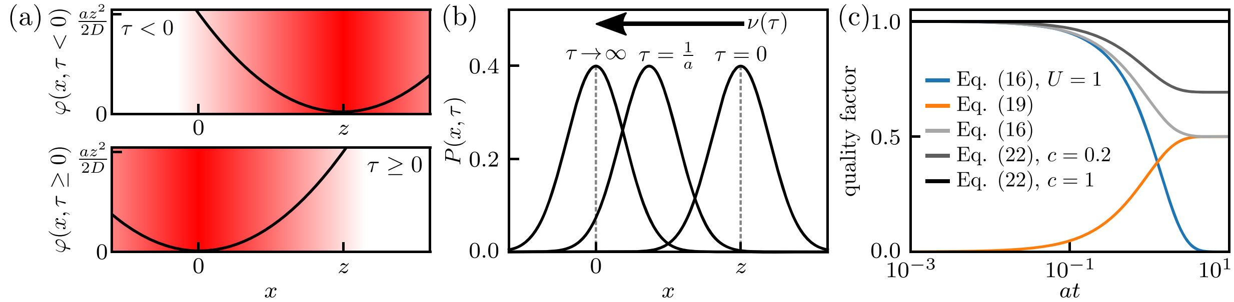

FIG. 1. (a) Brownian particle in a one-dimensional harmonic trap with stiffness a, $\varphi(x,\tau)=a(x-x_\tau^0)^2/2D$ displaced from $x^0_{\tau<0}=z$ to $x^0_{\tau\geq 0}=0$. Upon being initially equilibrated in $\varphi(x,\tau<0)=a(x-z)^2/2D$ (i.e., from the initial condition $p_0(x)\propto\exp[-a(x-z)^2/2D]$) the particle evolves for $\tau\geq 0$ due to $D\partial_x\varphi(x,\tau\geq 0)=ax$ according to $dx_\tau=-ax_\tau d\tau+\sqrt{2D}dW_\tau$ toward an equilibrium $p_{\tau\to\infty}(x)\propto\exp(-ax^2/2D)$. (b) Illustration of the evolution of $P(x,\tau)$ for $z=5\sqrt{D/a}$. (c) Quality factors defined as the ratio of right- and left-hand side of the TURs as a function of the dimensionless quantity at. All quality factors turn out to be independent of z, D and only depend on a, t through at; explicit analytic expressions are given in [63]. Except for $J_t=\int 1\circ dx_\tau=x_t-x_0$ (blue line) we always choose the current defined with $U(\tau)=\nu(\tau)$ and density defined with $V(x,\tau)=-x\nu(\tau)$.

$$A_t\equiv\int_{\tau=0}^{\tau=t}\frac{\mathbf{j}(\mathbf{x}_\tau,\tau)}{P(\mathbf{x}_\tau,\tau)}\cdot[2\mathbf{D}(\mathbf{x}_\tau)]^{-1}\boldsymbol{\sigma}(\mathbf{x}_\tau)d\mathbf{W}_\tau,\tag{9}$$

where A_t cannot be inferred from trajectories since only $d\mathbf{x}_\tau$ but not $d\mathbf{W}_\tau$ is observed. A_t can be understood as the "purely random" part $\boldsymbol{\sigma}(\mathbf{x}_\tau)d\mathbf{W}_\tau$ of the increment $d\mathbf{x}_\tau$ weighted by the local velocity and inverse diffusion coefficient. Because $\langle A_tJ_t^{\mathrm{I}}\rangle=\langle J_t\rangle$ and $\langle A_t\langle J_t\rangle\rangle=\langle A_t\rangle\langle J_t\rangle=0$ we have

$$\langle A_t(J_t-\langle J_t\rangle)\rangle=\langle J_t\rangle+\langle A_tJ_t^{\mathrm{II}}\rangle,\tag{10}$$

and the Cauchy-Schwarz inequality $\langle A_t(J_t-\langle J_t\rangle)\rangle^2\leq\langle A_t^2\rangle\mathrm{var}(J_t)$ further yields

$$\frac{\Sigma_t}{2}\mathrm{var}(J_t)\geq[\langle J_t\rangle+\langle A_tJ_t^{\mathrm{II}}\rangle]^2.\tag{11}$$

Compared to Eq. (10) the inequality (11) has the advantage that $\mathrm{var}(J_t)$ is operationally accessible and Σ_t (unlike A_t) has a clear physical interpretation.

To obtain the TUR we are left with evaluating $\langle A_tJ_t^{\mathrm{II}}\rangle$, which involves the two-time correlation of $d\mathbf{W}_\tau$ and $d\tau'$ integrals in Eqs. (9) and Eq. (7), respectively. For times $\tau\geq\tau'$ this correlation vanishes due to the independence property of the Wiener process. However, nontrivial correlations occur for $\tau<\tau'$ because the probability density of $\mathbf{x}_{\tau'}$ depends on $d\mathbf{W}_\tau$. We quantify these correlations including $d\mathbf{W}_\tau$ by writing $\langle A_tJ_t^{\mathrm{II}}\rangle$ as an average over the joint density to be at points $\mathbf{x},\mathbf{x}+d\mathbf{x},\mathbf{x}'$ at times $\tau<\tau+d\tau<\tau'$, respectively, and expanding

$$\begin{aligned}&P(\mathbf{x}',\tau'|\mathbf{x}+d\mathbf{x},\tau+d\tau)\\&\quad=P(\mathbf{x}',\tau'|\mathbf{x},\tau)+d\mathbf{x}\cdot\nabla_{\mathbf{x}}P(\mathbf{x}',\tau'|\mathbf{x},\tau)+\mathcal{O}(d\tau).\end{aligned}\tag{12}$$

Following this approach [26,61] (or alternatively via Doob conditioning [2,66,67] as in Ref. [39]) one can formulate a general calculation rule that in this case reads (for details, see [63])

$$\begin{aligned}\langle A_tJ_t^{\mathrm{II}}\rangle=&-\int_0^t d\tau'\int d\mathbf{x}'\mathcal{U}(\mathbf{x}',\tau')\int_0^{\tau'}d\tau\int d\mathbf{x}\\&\times P(\mathbf{x}',\tau'|\mathbf{x},\tau)\nabla_{\mathbf{x}}\cdot\mathbf{j}(\mathbf{x},\tau).\end{aligned}\tag{13}$$

For steady-state systems we have $\nabla\cdot\mathbf{j}(\mathbf{x},\tau)=\nabla\cdot\mathbf{j}_s(\mathbf{x})=0$ and thus $\langle A_tJ_t^{\mathrm{II}}\rangle=0$, such that Eq. (11) immediately implies the original TUR in Eq. (1).

To generalize to transients we use Eq. (4) $\nabla_{\mathbf{x}}\cdot\mathbf{j}(\mathbf{x},\tau)=-\partial_\tau P(\mathbf{x},\tau)$, integrate by parts twice (see [63] for details), and define a second operationally accessible current

$$\tilde{J}_t\equiv\int_{\tau=0}^{\tau=t}\tau\partial_\tau\mathbf{U}(\mathbf{x}_\tau,\tau)\cdot\circ d\mathbf{x}_\tau,\tag{14}$$

to obtain

$$\langle A_tJ_t^{\mathrm{II}}\rangle=(t\partial_t-1)\langle J_t\rangle-\langle\tilde{J}_t\rangle.\tag{15}$$

Thus, we have expressed the correlation $\langle A_tJ_t^{\mathrm{II}}\rangle$ in terms of operationally accessible quantities. From this and Eq. (11), the TUR for general initial conditions and general time-homogeneous Langevin dynamics Eq. (2) reads

$$\Sigma_t\mathrm{var}(J_t)\geq 2[t\partial_t\langle J_t\rangle-\langle\tilde{J}_t\rangle]^2.\tag{16}$$

The fact that the TUR for transient dynamics (16) follows from the original TUR (1) upon replacing $\langle J_t\rangle\to t\partial_t\langle J_t\rangle$ is well known [44,46] and was first derived in continuous space in Ref. [45]. However, the novel correction term $\langle\tilde{J}_t\rangle$ extends the validity of the TUR to currents with an explicit time dependence $\mathbf{U}(\mathbf{x},\tau)$. We show below and in Fig. 1 that this additional freedom in choosing $\mathbf{U}$ is crucial for saturating the transient TUR under general conditions. To highlight that end-point derivative $t\partial_t$ and the correction term $\langle \tilde{J}_t \rangle$ are strictly necessary we provide explicit counter-examples (see [63]).

We note that Eq. (16) in one-dimensional space and for additive noise can be deduced from restricting the result in [18], where an explicit time dependence was introduced via a speed parameter v, to a time-homogeneous drift, translated to time-integrated currents, and noting that $v\partial_v U(x, v\tau) = \tau\partial_\tau U(x, v\tau)$. The form without the speed parameter has the advantage that the correction term $\langle \tilde{J}_t \rangle$ is accessible from a single experiment while the ∂_v correction requires perturbing the speed of the experiment. However, the result in [18] even holds for an explicitly time-dependent drift.

Notably, generalizing this proof to explicitly time-dependent drift or diffusion, although probably possible, is *not* straightforward because it requires perturbing the dynamics (see [18]), and therefore all relevant information is no longer contained in a single equation of motion.

TUR for densities.—We define general, operationally accessible densities (the term "density" is motivated by the analogy to "current" as, e.g., in [25,26,60,68])

$$\rho_t = \int_0^t V(\mathbf{x}_\tau, \tau) d\tau,$$
$$\tilde{\rho}_t \equiv \int_0^t \tau\partial_\tau V(\mathbf{x}_\tau, \tau) d\tau. \tag{17}$$

Since in the proof above we did not use the explicit form of $\mathcal{U}$, the density can be treated analogously to J_t in Eq. (7) by replacing $\mathcal{U} \to V$ and omitting the J_t^{I} term. Analogously to Eqs. (10) and (15) we thus obtain

$$\langle A_t(\rho_t - \langle \rho_t \rangle) \rangle = \langle A_t \rho_t \rangle = (t\partial_t - 1)\langle \rho_t \rangle - \langle \tilde{\rho}_t \rangle, \tag{18}$$

and analogously to Eq. (11) the transient density-TUR

$$\Sigma_t \mathrm{var}(\rho_t) \geq 2[(t\partial_t - 1)\langle \rho_t \rangle - \langle \tilde{\rho}_t \rangle]^2. \tag{19}$$

Note that due to the absence of the J_t^{I} term, the right-hand side vanishes in steady-state systems. As in the discussion of Eq. (16) above, Eq. (19) is in some sense contained in the results of [18]. However, Eq. (19) allows for multidimensional space and multiplicative noise, and does not require a variation in protocol speed.

Improving TURs using correlations.—It has been recently found [41] that the steady-state TUR can be eminently improved, and even saturated arbitrarily far from equilibrium, by considering correlations between currents and densities as defined in Eq. (17). To rederive this sharper version we rewrite Eq. (11) for the observable $J_t - c\rho_t$ (the constant c is in fact technically redundant since it can be absorbed in the definition of ρ_t)

$$\frac{\Sigma_t}{2} \mathrm{var}(J_t - c\rho_t) \geq [\langle J_t \rangle + \langle A_t(J_t^{\mathrm{II}} - c\rho_t) \rangle]^2. \tag{20}$$

Note that $\mathrm{var}(J_t - c\rho_t) = \mathrm{var}(J_t) + c^2 \mathrm{var}(\rho_t) - 2c\,\mathrm{cov}(J_t, \rho_t)$, where cov denotes the covariance. Using the optimal choice $c = \mathrm{cov}(J_t, \rho_t)/\mathrm{var}(\rho_t)$ and recalling that for steady-state systems $\langle A_t(J_t^{\mathrm{II}} - c\rho_t) \rangle = 0$, Eq. (20) becomes the NESS correlation TUR in [41]

$$\Sigma_t \mathrm{var}(J_t)[1 - \chi_{J\rho}^2] \geq 2\langle J_t \rangle^2,$$
$$\chi_{J\rho}^2 \equiv \frac{\mathrm{cov}^2(J_t, \rho_t)}{\mathrm{var}(J_t)\mathrm{var}(\rho_t)}. \tag{21}$$

Since $\chi_{J\rho}^2 \in [0, 1]$, Eq. (21) is sharper than Eq. (1) and, as proven in [41] and discussed below, for any steady-state system there exist J_t, ρ_t that saturate this inequality.

Our approach allows to generalize this result to transient dynamics by computing $\langle A_t(J_t^{\mathrm{II}} - c\rho_t) \rangle$ as in Eq. (15) to obtain from Eq. (20) the generalized correlation TUR

$$\Sigma_t \mathrm{var}(J_t - c\rho_t)$$
$$\geq 2(t\partial_t \langle J_t \rangle - \langle \tilde{J}_t \rangle - c[(t\partial_t - 1)\langle \rho_t \rangle - \langle \tilde{\rho}_t \rangle])^2. \tag{22}$$

One could again optimize the left-hand side over c to obtain $\mathrm{var}(J_t - c\rho_t) = \mathrm{var}(J_t)[1 - \chi_{J\rho}^2]$. However, since here the right-hand side also involves c this may not be the optimal choice. Thus, it is instead practical to keep c general (or absorb it into ρ_t). The generalized correlation TUR (22) represents a novel result that sharpens the transient TUR in Eq. (16), and, as we show below and illustrate in Fig. 1, even allows us to generally saturate the TUR arbitrarily far from equilibrium.

Saturation of TURs.—For any choice $\mathbf{U}$ in the definition of J_t in Eq. (6), the TUR allows to infer a lower bound on the time-accumulated dissipation Σ_t from $\langle J_t \rangle$ and $\mathrm{var}(J_t)$ [25,26,32–38]. The tighter the inequality, the more precise is the lower bound on Σ_t. It is therefore important to understand when the inequality becomes tight or even saturates, i.e., gives equality.

Because of the simplicity and directness of our proof, we can very well discuss the tightness of the bound based on the single application of the Cauchy-Schwarz inequality. As elaborated in the Appendix, this approach reproduces, and extends beyond, numerous existing results on asymptotic and exact saturation of TURs. Most importantly, choosing $\mathbf{U}(\mathbf{x}, \tau) = c'[\mathbf{j}(\mathbf{x}, \tau)/P(\mathbf{x}, \tau)] \cdot [2\mathbf{D}(\mathbf{x})]^{-1}$ with arbitrary c' and $c\rho_t = J_t^{\mathrm{II}}$ [see Eq. (7)] gives $J_t - c\rho_t = J_t^{\mathrm{I}} = c' A_t$ which in turn implies equality in the Cauchy-Schwarz argument leading to the correlation TURs Eqs. (21) and (22). This directly implies exact saturation of the correlation TURs which was so far achieved only in the steady-state case [41]. Our generalization of the correlation TUR in Eq. (22) for transient systems therefore allows to saturate a TUR arbitrarily far from equilibrium for any t and for general initial conditions and general time-homogeneous dynamics in Eq. (2).

Example.—To illustrate the novel results in Eqs. (16), (19), and (22) and the new insight into the saturation, we provide an explicit example of transient dynamics in Fig. 1, that of a Brownian particle in a one-dimensional harmonic potential $\varphi(x,t) = a(x - x_t^0)^2/2D$ displaced from $x_{\tau<0}^0 = z$ to $x_{\tau\geq 0}^0 = 0$, see Fig. 1(a). This setting, illustrated by the color gradient in Fig. 1(a), can easily be realized experimentally using optical tweezers [69–71]. The process features a Gaussian probability density $P(x,\tau)$ with constant variance D/a that moves with a space-independent velocity $\nu(\tau) = j(x,\tau)/P(x,\tau) = -az\exp(-a\tau)$ toward the equilibrium $\propto \exp(-ax^2/2D)$, see Fig. 1(b).

To quantify the tightness of the respective TURs we inspect quality factors—the ratio of the right- and left-hand side of the TUR—shown in Fig. 1(c) as a function of the dimensionless quantity at. The blue line represents the transient TUR (16) for the current $J_t = x_t - x_0$ where $U(x,\tau) = 1$. Since this U does not feature explicit time dependence the correction term $\tilde{J}_t$ does not contribute and the transient TUR from the existing literature [45] applies. The existing (as well as our) results allow varying the spatial dependence of U but we refrain from considering this for simplicity and since it is not necessary for saturation (i.e., ν, D have no spatial dependence in our example). Because of the novel correction term in Eq. (16) we may choose a time-dependent U, and following our discussion of the saturation we choose for all following examples J_t with $U(\tau) = c'\nu(\tau)/2D = \nu(\tau)$ (the prefactor c' is arbitrary as it cancels in quality factor) and the corresponding $\rho_t = J_t^{\mathrm{II}}$, i.e., with $V(x,\tau) = \mathcal{U}(x,\tau) = -axU(\tau)$, see Eq. (7). For this choice we evaluate the transient current [Eq. (16)] and density-TUR [Eq. (19)], see light gray and orange line in Fig. 1(c). Moreover, we evaluate the novel generalized correlation TUR (22) for $c = 0.2$ (dark gray line), where we find that the current TUR is improved by considering correlations with the a density, and for $c = 1$ (black line), where we find the expected saturation. This saturation means that the lower bound obtained for Σ_t from this TUR is exactly Σ_t. Note that this exact saturation requires the knowledge of the details of the dynamics for the choice of U, V. However, even with very limited knowledge one can simply consider different guesses or approximations of the optimal U, V and each guess will give a valid lower bound (given sufficient statistics).

Direct route for Markov jump processes.—Beyond overdamped dynamics, one may employ the above direct approach for deriving TURs to Markov jump dynamics on a discrete state-space $\mathcal{N}$ with jump-rates $(r_{xy})_{x,y\in\mathcal{N}}$ and steady-state distribution $(p_x)_{x\in\mathcal{N}}$. To illustrate this generalization, we here provide the proof of the steady-state TUR (1). Let $\hat{\tau}_x$ denote the (random) time spent in state x and $\hat{n}_{xy}$ the (random) number of jumps from x to y in the time interval $[0,t]$. A general time-accumulated current in a jump process is defined with antisymmetric prefactors $d_{xy} = -d_{yx}$ as the double sum $J \equiv \sum_{x\neq y} d_{xy}\hat{n}_{xy}$. The steady-state dissipation in turn reads $\Sigma \equiv t\sum_{x\neq y} p_x r_{xy}\ln[p_x r_{xy}/p_y r_{yx}]$. Analogously to A_t in Eq. (9) define

$$A \equiv \sum_{x\neq y} \frac{p_x r_{xy} - p_y r_{yx}}{p_x r_{xy} + p_y r_{yx}}(\hat{n}_{xy} - \hat{\tau}_x r_{xy}). \tag{23}$$

For this choice of A one can check that $\langle A\rangle = 0$, $\langle A^2\rangle \leq \Sigma/2$, and $\langle AJ\rangle = \langle J\rangle$ (a "direct" proof as above follows by analogy of covariance properties of $\partial_t(\hat{n}_{xy} - \hat{\tau}_x r_{xy})$ and $\boldsymbol{\sigma}(\mathbf{x}_t)d\mathbf{W}_t$, see [63] for details) which imply, via the Cauchy-Schwarz inequality, equivalently to Eqs. (10) and (11) the steady-state TUR for Markov jump processes

$$\langle A(J - \langle J\rangle)\rangle = \langle J\rangle \Rightarrow \frac{\Sigma}{2}\mathrm{var}(J) \geq \langle J\rangle^2. \tag{24}$$

A discussion of possible generalizations of this proof beyond steady-state dynamics is given in [63].

Conclusion.—Using only stochastic calculus and the well known Cauchy-Schwarz inequality we proved various existing TURs directly from the Langevin equation. This underscores the TUR as an inherent property of overdamped stochastic equations of motion, analogous to quantum-mechanical uncertainty relations. Moreover, by including current-density correlations we derived a new sharpened TUR for transient dynamics. Based on our simple and more direct proof we were able to systematically explore conditions under which TURs saturate. The new equality (10) is mathematically even stronger than TUR (11). Therefore, it allows us to derive further bounds, e.g., by applying Hölder's instead of the Cauchy-Schwarz inequality which, however, may not yield operationally accessible quantities. Our approach may allow for generalizations to systems with time-dependent driving (see, e.g., [18]) which, however, are not expected to follow anymore directly from a single equation of motion. The novel correction term for currents with explicit time dependence as well as the new transient correlation TUR and its saturation are expected to equally apply to Markov jump processes by generalizing the approach illustrated in Eqs. (23) and (24).

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Appendix: Saturation of TURs.—Thanks to the directness of our proof, we only need to discuss the tightness based on the step from Eqs. (10) to (11), where we applied the Cauchy-Schwarz inequality $\langle A_t(J_t - \langle J_t\rangle)\rangle^2 \leq \langle A_t^2\rangle\mathrm{var}(J_t)$ to the exact Eq. (10). Thus, the closer A_t and $J_t - \langle J_t\rangle$ are to being linearly dependent (recall that the Cauchy-Schwarz inequality measures the angle φ between two vectors $(\vec{x}\cdot\vec{y})^2 = \vec{x}^2\vec{y}^2\cos^2(\varphi) \le \vec{x}^2\vec{y}^2$), the tighter the TUR, with saturation for $J_t - \langle J_t \rangle = c' A_t$ for some constant c'. Therefore, the TUR is expected to be tightest for the choice $\mathbf{U}(\mathbf{x},\tau) = c'[\mathbf{j}(\mathbf{x},\tau)/P(\mathbf{x},\tau)]\cdot[2\mathbf{D}(\mathbf{x})]^{-1}$ for which $J_t^{\mathrm{I}} = c' A_t$ [see Eq. (7)]. Note that for NESS this $\mathbf{U}$ becomes time independent with $\mathbf{j}_s(\mathbf{x})/P_s(\mathbf{x})$. This choice is known to saturate the original TUR in Eq. (1) in the near-equilibrium limit [2]. However, since the full $J_t = J_t^{\mathrm{I}} + J_t^{\mathrm{II}}$ current cannot be chosen to exactly agree with $c' A_t$, equality is generally not reached.

The original TUR (1) with this choice of $\mathbf{U}(\mathbf{x},\tau)$ was also found to saturate in the short-time limit $t \to 0$ [35,36]. This result is in turn reproduced with our approach by noting that $J_t^{\mathrm{I}} = c' A_t$ and $\langle A_t J_t^{\mathrm{II}} \rangle = 0$ give $\langle A_t (J_t - \langle J_t \rangle)\rangle^2 = \langle A_t J_t^{\mathrm{I}} \rangle^2 = \langle A_t^2 \rangle \langle J_t^{\mathrm{I}2} \rangle$, and in the limit $t \to 0$ the integrals in Eq. (7) asymptotically scale like a single time step, such that $\langle J_t^{\mathrm{I}2} \rangle \sim (\mathbf{W}_t - \mathbf{W}_0)^2 \sim t$ dominates all $\sim t^{3/2}, \sim t^2$ contributions in $\mathrm{var}(J_t)$. In turn, $\langle J_t^{\mathrm{I}2} \rangle \overset{t\to 0}{\to} \mathrm{var}(J_t)$ which yields $\langle A_t (J_t - \langle J_t \rangle)\rangle^2 \overset{t\to 0}{\to} \langle A_t^2 \rangle \mathrm{var}(J_t)$. Thus, the Cauchy-Schwarz step from the equality (10) to the inequality (11) saturates as $t \to 0$, in turn implying that the TUR saturates.

More recently it was also found that including correlations [see Eq. (21) and Ref. [41]] allows us to saturate a sharpened TUR for steady-state systems arbitrarily far from equilibrium for any t, again for the same choice $\mathbf{U}(\mathbf{x},\tau)$ as above. Since our rederivation of the NESS correlation TUR in Eq. (21) applied the Cauchy-Schwarz inequality to A_t and $J_t - c\rho_t$ we see that choosing $c\rho_t = J_t^{\mathrm{II}}$ yields $J_t - c\rho_t = J_t^{\mathrm{I}} = c' A_t$, such that the application of the Cauchy-Schwarz inequality becomes an equality. That is, the correlation TUR (21) for this choice of J_t and ρ_t is generally saturated. Notably, this powerful result follows very naturally from the direct proof presented here.

Our generalization of the correlation TUR in Eq. (22) for transient systems even allows us to saturate a TUR (arbitrarily far from equilibrium for any t and) for general initial conditions and general time-homogeneous dynamics in Eq. (2). This result is strong but obvious, since as for the NESS correlation TUR we can choose J_t and ρ_t such that $J_t - c\rho_t = c' A_t$. Note that it is here crucial that we allowed for an explicit time dependence in $\mathbf{U}$ and V, i.e., that we found new correction terms [terms with tilde in Eqs. (16), (19), and (22)].

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