

Direct Route to Thermodynamic Uncertainty Relations

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Thermodynamic uncertainty relations (TURs) bound the dissipation in non-equilibrium 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. By including current-density correlations we, moreover, derive a new sharpened TUR for transient dynamics. Our arguably simplest and most direct proof allows us to systematically determine conditions under which the different TURs saturate and thus allows for a more accurate thermodynamic inference.

A defining characteristic of non-equilibrium systems is a non-vanishing entropy production [1–8] emerging during relaxation [7–12], in the presence of time-dependent (e.g. periodic [13–18]) driving, or in non-equilibrium 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 non-equilibrium 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]

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

with variance $\text{var}(J_t) \equiv \langle J_t^2 \rangle - \langle J_t \rangle^2$ 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 in 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 recently 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, whilst 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. 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.

Setup.—We consider multidimensional time-homogeneous overdamped dynamics (i.e. coefficients do not explicitly depend on time) with (possibly) multiplicative noise [53, 54] described by the thermodynamically consistent [2, 26, 55] anti-Itô (or Hänggi-Klimontovich [56, 57]) stochastic differential (Langevin)

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equation

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

where \circledast is the anti-Itô product [26, 55] and $d\mathbf{W}_\tau$ is the increment of a multidimensional Wiener process with zero mean $\langle d\mathbf{W}_\tau \rangle = \mathbf{0}$ and covariance $\langle dW_{\tau,i}dW_{\tau',j} \rangle = \delta(\tau - \tau')\delta_{ij}d\tau d\tau'$. Due to the latter property, the noise increment $\boldsymbol{\sigma}(\mathbf{x}_\tau)d\mathbf{W}_\tau$ is known as delta-correlated or white noise. The noise amplitude is related to the diffusion coefficient via $\mathbf{D}(\mathbf{x}) \equiv \boldsymbol{\sigma}(\mathbf{x})\boldsymbol{\sigma}(\mathbf{x})^T/2$. Let $P(\mathbf{x}, \tau)$ be the probability density to find \mathbf{x}_τ 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

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

and the Fokker-Planck equation [54, 58] for the time-evolution of $P(\mathbf{x}, \tau)$ follows from Eq. (2) and reads [53]

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

In the special case that $\mathbf{F}(\mathbf{x})$ is sufficiently confining a NESS is eventually reached with invariant density $P_s(\mathbf{x}) \equiv P(\mathbf{x}, \tau \rightarrow \infty)$ and steady-state current $\mathbf{j}_s(\mathbf{x}) \equiv [\mathbf{F}(\mathbf{x}) - \mathbf{D}(\mathbf{x})\nabla]P_s(\mathbf{x})$ with $\nabla \cdot \mathbf{j}_s(\mathbf{x}) = 0$ [54]. The mean total (medium plus system) entropy production in the time interval $[0, t]$ is given by [3, 4]

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

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

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

Note that for any integrand \mathbf{U} this current and its first two moments are readily obtained from measured trajectories $(\mathbf{x}_\tau)_{0 \leq \tau \leq t}$. 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- and $d\tau$ -integrals, $J_t = J_t^I + J_t^{II}$, with [26]

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

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

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

The variance $\text{var}(J_t)$ can in turn be computed from two-point densities [25, 26, 59, 60], but is not required to prove TURs.

We now outline our direct proof of TURs. First, we re-derive the classical TUR Eq. (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 non-stationary dynamics. Finally, we explain how to saturate the various TURs. 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.—First, we require a scalar quantity A_t with zero mean and whose second moment yields the dissipation defined in Eq. (5), i.e. $\langle A_t^2 \rangle = \Sigma_t/2$ [61]. 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"

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

where A_t cannot be inferred from trajectories since only $d\mathbf{x}_\tau$ but not $d\mathbf{W}_\tau$ is observed. Moreover, because $\langle A_t J_t^I \rangle = \langle J_t \rangle$ and $\langle A_t \langle J_t \rangle \rangle = \langle A_t \rangle \langle J_t \rangle = 0$ we have

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

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

$$\frac{\Sigma_t}{2} \text{var}(J_t) \geq [\langle J_t \rangle + \langle A_t J_t^{II} \rangle]^2. \quad (11)$$

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

To obtain the TUR we are left with evaluating $\langle A_t J_t^{II} \rangle$, which involves the two-time correlation of $d\mathbf{W}_\tau$ and $d\tau'$ integrals in Eq. (9) and Eq. (7), respectively. Therefore, we must evaluate $\langle \mathbf{g}(\mathbf{x}_\tau, \tau) \cdot \boldsymbol{\sigma}(\mathbf{x}_{\tau'}) d\mathbf{W}_\tau \mathcal{U}(\mathbf{x}_{\tau'}, \tau') \rangle$ where $\mathbf{g}(\mathbf{x}_\tau, \tau) \equiv \mathbf{j}(\mathbf{x}_\tau, \tau) \cdot [2P(\mathbf{x}_\tau, \tau)\mathbf{D}(\mathbf{x}_\tau)]^{-1}$. For times $\tau \geq \tau'$ this correlation vanishes due to the independence property of the Wiener process. However, non-trivial correlations occur for $\tau < \tau'$ because the probability density of $\mathbf{x}_{\tau'}$ depends on $d\mathbf{W}_\tau$. Nevertheless, all necessary information is contained in the equation of motion (2).

Following [26, 60], for a given point $\mathbf{x}_\tau = \mathbf{x}$ we set $\boldsymbol{\varepsilon} \equiv \boldsymbol{\sigma}(\mathbf{x})d\mathbf{W}_\tau = \mathcal{O}(\sqrt{d\tau})$ and write Eq. (2) in Itô form as $d\mathbf{x}_\tau(\mathbf{x}, \tau, \boldsymbol{\varepsilon}) = [\mathbf{F}(\mathbf{x}) + \nabla \cdot \mathbf{D}(\mathbf{x})]d\tau + \boldsymbol{\varepsilon}$. The average $\langle \mathbf{g}(\mathbf{x}_\tau, \tau) \cdot \boldsymbol{\varepsilon} \mathcal{U}(\mathbf{x}_{\tau'}, \tau') \rangle$ is evaluated over the joint density to be at points $\mathbf{x}, \mathbf{x} + d\mathbf{x}_\tau, \mathbf{x}'$ at times $\tau < \tau + d\tau < \tau'$, respectively, i.e. over $P(\boldsymbol{\varepsilon})P(\mathbf{x}', \tau' | \mathbf{x} + d\mathbf{x}_\tau(\mathbf{x}, \tau, \boldsymbol{\varepsilon}), \tau + d\tau)P(\mathbf{x}, \tau)$ where $P(\boldsymbol{\varepsilon})$ is Gaussian with zero mean and covariance matrix $2\mathbf{D}(\mathbf{x})d\tau$. Moreover, by expanding in $d\tau$ we find [26, 60]

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

By symmetry only the term of even power $\sim \varepsilon^2$ in $\varepsilon d\mathbf{x}_\tau(\mathbf{x}, \tau, \varepsilon) \cdot \nabla_{\mathbf{x}} P(\mathbf{x}', \tau' | \mathbf{x}, \tau)$ survives the integration over $P(\varepsilon)$. Evaluating this integral, using the explicit form of $\mathbf{g}(\mathbf{x}_\tau, \tau)$, and integrating by parts, we arrive at

$$\langle A_t J_t^{\text{II}} \rangle = - \int_0^t d\tau' \int d\mathbf{x}' \mathcal{U}(\mathbf{x}', \tau') \int_0^t d\tau \mathbb{1}_{\tau < \tau'} \int d\mathbf{x} \times P(\mathbf{x}', \tau' | \mathbf{x}, \tau) \nabla_{\mathbf{x}} \cdot \mathbf{j}(\mathbf{x}, \tau). \quad (13)$$

The above integral may be formulated as a general calculation rule (see [26, 60]) that can alternatively be derived via Doob conditioning [2, 62, 63] as in [39].

For steady-state systems we have $\nabla \cdot \mathbf{j}(\mathbf{x}, \tau) = \nabla \cdot \mathbf{j}_s(\mathbf{x}) = 0$ and due to Eq. (13) thus $\langle A_t J_t^{\text{II}} \rangle = 0$, such that Eq. (11) immediately implies the original TUR in Eq. (1).

To generalize to transients we use Eq. (4) $\nabla_{\mathbf{x}} \cdot \mathbf{j}(\mathbf{x}, \tau) = -\partial_\tau P(\mathbf{x}, \tau)$. An integration by parts in τ with the boundary term $-\int d\mathbf{x} P(\mathbf{x}', \tau' | \mathbf{x}, 0) P(\mathbf{x}, 0) = -P(\mathbf{x}', \tau')$ yields

$$\langle A_t J_t^{\text{II}} \rangle = \int_0^t d\tau' \int d\mathbf{x}' \mathcal{U}(\mathbf{x}', \tau') \left(-P(\mathbf{x}', \tau') - \int d\mathbf{x} \int_0^t d\tau P(\mathbf{x}, \tau) \partial_\tau [\mathbb{1}_{\tau < \tau'} P(\mathbf{x}', \tau' | \mathbf{x}, \tau)] \right). \quad (14)$$

Note that the first line is $-\langle J_t^{\text{II}} \rangle$. Since we consider Markovian systems without *explicit* time-dependence of \mathbf{F} and $\boldsymbol{\sigma}$, we have $\partial_\tau P(\mathbf{x}', \tau' | \mathbf{x}, \tau) = \partial_\tau P(\mathbf{x}', \tau' - \tau | \mathbf{x}) = -\partial_{\tau'} P(\mathbf{x}', \tau' - \tau | \mathbf{x}) = -\partial_{\tau'} P(\mathbf{x}', \tau' | \mathbf{x}, \tau)$. Using moreover $\int d\mathbf{x} P(\mathbf{x}', \tau' | \mathbf{x}, \tau) P(\mathbf{x}, \tau) = P(\mathbf{x}', \tau')$ and $\int_0^t d\tau \mathbb{1}_{\tau < \tau'} = \tau'$ we obtain, upon integrating by parts with the boundary term entering at $\tau' = t$, and recalling $\langle J_t^{\text{II}} \rangle = \langle J_t \rangle$,

$$\begin{aligned} \langle A_t J_t^{\text{II}} \rangle &= -\langle J_t^{\text{II}} \rangle + \int d\mathbf{x}' \int_0^t d\tau' \mathcal{U}(\mathbf{x}', \tau') \partial_{\tau'} [\tau' P(\mathbf{x}', \tau')] \\ &= (t\partial_t - 1) \langle J_t \rangle - \int d\mathbf{x}' \int_0^t d\tau' P(\mathbf{x}', \tau') \tau' \partial_{\tau'} \mathcal{U}(\mathbf{x}', \tau'). \end{aligned} \quad (15)$$

In order to make Eq. (15) operationally accessible we define a second current

$$\tilde{J}_t \equiv \int_{\tau=0}^{\tau=t} \tau \partial_\tau \mathbf{U}(\mathbf{x}_\tau, \tau) \cdot \circ d\mathbf{x}_\tau, \quad (16)$$

where $\langle \tilde{J}_t \rangle$ is analogously to Eqs. (7) and (8) obtained via $\tau \partial_\tau \mathcal{U}$ such that Eq. (15) becomes

$$\langle A_t J_t^{\text{II}} \rangle = (t\partial_t - 1) \langle J_t \rangle - \langle \tilde{J}_t \rangle. \quad (17)$$

Thus, we have expressed the correlation $\langle A_t J_t^{\text{II}} \rangle$ 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

$$\Sigma_t \text{var}(J_t) \geq 2 \left[t\partial_t \langle J_t \rangle - \langle \tilde{J}_t \rangle \right]^2. \quad (18)$$

The fact that the TUR for transient dynamics (18) follows from the original TUR (1) upon replacing $\langle J_t \rangle \rightarrow$

$t\partial_t \langle J_t \rangle$ is well known [44, 46] and was first derived in continuous space in Ref. [45]. However, the 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 that this additional freedom in choosing \mathbf{U} is crucial for saturating the transient TUR under general conditions. To highlight that the correction term $\langle \tilde{J}_t \rangle$ is strictly necessary we provide an explicit counterexample against the TUR in Eq. (18) without the correction term (see [64]).

We note that Eq. (18) 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, 59, 65])

$$\begin{aligned} \rho_t &= \int_0^t V(\mathbf{x}_\tau, \tau) d\tau, \\ \tilde{\rho}_t &\equiv \int_{\tau=0}^{\tau=t} \tau \partial_\tau V(\mathbf{x}_\tau, \tau) d\tau. \end{aligned} \quad (19)$$

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 $\mathcal{U} \rightarrow V$ and omitting the J_t^{II} -term. Analogously to Eqs. (10) and (17) we thus obtain

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

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

$$\Sigma_t \text{var}(\rho_t) \geq 2 \left[(t\partial_t - 1) \langle \rho_t \rangle - \langle \tilde{\rho}_t \rangle \right]^2. \quad (20)$$

Note that due to the absence of the J_t^{II} -term, the right-hand side vanishes in steady-state systems. As in the discussion of Eq. (18) above, Eq. (20) is in some sense contained in the results of [18]. However, Eq. (20) allows for multidimensional spaces 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. (19). To re-derive 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)

$$\frac{\Sigma_t}{2} \text{var}(J_t - c\rho_t) \geq [\langle J_t \rangle + \langle A_t(J_t^{\text{II}} - c\rho_t) \rangle]^2. \quad (21)$$

Note that $\text{var}(J_t - c\rho_t) = \text{var}(J_t) + c^2 \text{var}(\rho_t) - 2c \text{cov}(J_t, \rho_t)$, where cov denotes the covariance. Using the optimal choice $c = \text{cov}(J_t, \rho_t) / \text{var}(\rho_t)$ and recalling that for steady-state systems $\langle A_t(J_t^{\text{II}} - c\rho_t) \rangle = 0$, Eq. (21) becomes the NESS correlation-TUR in [41]

$$\begin{aligned} \Sigma_t \text{var}(J_t) [1 - \chi_{J\rho}^2] &\geq 2\langle J_t \rangle^2, \\ \chi_{J\rho}^2 &\equiv \frac{\text{cov}^2(J_t, \rho_t)}{\text{var}(J_t) \text{var}(\rho_t)}. \end{aligned} \quad (22)$$

Since $\chi_{J\rho}^2 \in [0, 1]$, Eq. (22) 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 $\langle A_t(J_t^{\text{II}} - c\rho_t) \rangle$ as in Eq. (17) to obtain from Eq. (21) the *generalized correlation-TUR*

$$\begin{aligned} \Sigma_t \text{var}(J_t - c\rho_t) &\geq \\ 2 \left(t\partial_t \langle J_t \rangle - \langle \tilde{J}_t \rangle - c [(t\partial_t - 1)\langle \rho_t \rangle - \langle \tilde{\rho}_t \rangle] \right)^2. \end{aligned} \quad (23)$$

One could again optimize the left-hand side over c to obtain $\text{var}(J_t - c\rho_t) = \text{var}(J_t) [1 - \chi_{J\rho}^2]$. 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 (23) represents a *novel result* that sharpens the transient TUR in Eq. (18), and, as we show below, even allows 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 $\text{var}(J_t)$ [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.

Due to the simplicity and directness of our proof, we can very well discuss the tightness of the bound based on the step from Eq. (10) to Eq. (11) where we applied the Cauchy-Schwarz inequality $\langle A_t(J_t - \langle J_t \rangle) \rangle^2 \leq \langle A_t^2 \rangle \text{var}(J_t)$ to the exact Eq. (10). Thus, the closer A_t and $J_t - \langle J_t \rangle$ are to being linearly dependent [66], 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 $\mathbf{U}(\mathbf{x}, \tau) = c' [\mathbf{j}(\mathbf{x}_\tau, \tau) / P(\mathbf{x}_\tau, \tau)] \cdot [2\mathbf{D}(\mathbf{x}_\tau)]^{-1}$ for which $J_t^{\text{I}} = c' A_t$ (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 $J_t = J_t^{\text{I}} + J_t^{\text{II}}$ 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 $t \rightarrow 0$ [35, 36]. This result is in turn reproduced with our approach by noting that $J_t^{\text{I}} = c' A_t$ and $\langle A_t J_t^{\text{II}} \rangle = 0$ give $\langle A_t(J_t - \langle J_t \rangle) \rangle^2 = \langle A_t J_t^{\text{I}} \rangle^2 = \langle A_t^2 \rangle \langle J_t^{\text{I}2} \rangle$, and in the limit $t \rightarrow 0$ the integrals in Eq. (7) asymptotically scale like a single time-step, such that $\langle J_t^{\text{I}2} \rangle \sim (\mathbf{W}_t - \mathbf{W}_0)^2 \sim t$ dominates all $\sim t^{3/2}$, $\sim t^2$ contributions in $\text{var}(J_t)$. In turn, $\langle J_t^{\text{I}2} \rangle \xrightarrow{t \rightarrow 0} \text{var}(J_t)$ which yields $\langle A_t(J_t - \langle J_t \rangle) \rangle^2 \xrightarrow{t \rightarrow 0} \langle A_t^2 \rangle \text{var}(J_t)$. Thus, the Cauchy-Schwarz step from the equality (10) to the inequality (11) saturates as $t \rightarrow 0$, in turn implying that the TUR saturates.

More recently it was also found that including correlations (see Eq. (22) and Ref. [41]) allows 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 re-derivation of the NESS correlation-TUR in Eq. (22) applied the Cauchy-Schwarz inequality to A_t and $J_t - c\rho_t$ we see that choosing $c\rho_t = J_t^{\text{II}}$ yields $J_t - c\rho_t = J_t^{\text{I}} = c' A_t$, such that the application of the Cauchy-Schwarz inequality becomes an equality. That is, the correlation-TUR (22) 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. (23) for transient systems even 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). 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. (18), (20) and (23)).

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 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.

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**Supplementary Material for:
Direct Route to Thermodynamic Uncertainty Relations**

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Recall the definitions

$$\begin{aligned} J_t &\equiv \int_{\tau=0}^{\tau=t} \mathbf{U}(\mathbf{x}_\tau, \tau) \cdot \circ d\mathbf{x}_\tau, \\ \tilde{J}_t &\equiv \int_{\tau=0}^{\tau=t} \tau \partial_\tau \mathbf{U}(\mathbf{x}_\tau, \tau) \cdot \circ d\mathbf{x}_\tau, \end{aligned} \quad (\text{S1})$$

and the thermodynamic uncertainty relation (TUR) for transient/non-steady-state dynamics [Eq. (18) in the Letter],

$$2 \left[t \partial_t \langle J_t \rangle - \langle \tilde{J}_t \rangle \right]^2 \leq \Sigma_t \text{var}(J_t). \quad (\text{S2})$$

We here give an explicit example that would violate the above inequality if the correction term $-\langle \tilde{J}_t \rangle$ was missing, i.e. we choose a process $(\mathbf{x}_\tau)_{0 \leq \tau \leq t}$ and a function $\mathbf{U}(\mathbf{x}_\tau, \tau)$ for which for some parameters $2 [t \partial_t \langle J_t \rangle]^2 > \Sigma_t \text{var}(J_t)$. This shows that the correction term $-\langle \tilde{J}_t \rangle$ is indeed necessary, and that the result (S2) [Eq. (18) in the Letter] is valid for a broader class of systems than existing literature [1] by allowing explicit time-dependence in $\mathbf{U}(\mathbf{x}_\tau, \tau)$.

Consider one-dimensional Brownian motion in a parabolic potential (i.e. a Langevin equation with linear force; known as the Ornstein-Uhlenbeck process) [2] with a Gaussian initial condition x_0 [we denote a normal distribution by $\mathcal{N}(\text{mean}, \text{variance})$],

$$\begin{aligned} dx_\tau &= -ax_\tau d\tau + \sqrt{2D} dW_\tau, \\ x_0 &\sim \mathcal{N}(z, \sigma_0^2). \end{aligned} \quad (\text{S3})$$

Even though this process approaches an equilibrium steady-state, for finite times it features transient dynamics if x_0 is not sampled from the steady-state distribution. For any Gaussian initial condition this process is Gaussian [2]. Therefore, the mean and the variance completely determine the distribution of x_τ . The mean, variance and covariance are simply obtained as (see e.g. Appendix F in Ref. [3])

$$\begin{aligned} \langle x_\tau \rangle &= ze^{-a\tau}, \\ \text{var}(x_\tau) &\equiv \langle x_\tau^2 \rangle - \langle x_\tau \rangle^2 = \frac{D}{a} (1 - e^{-2a\tau}) + \sigma_0^2 e^{-2a\tau}, \\ \text{For } \tau \geq \tau': \quad \text{cov}(x_\tau, x_{\tau'}) &\equiv \langle x_\tau x_{\tau'} \rangle - \langle x_\tau \rangle \langle x_{\tau'} \rangle = e^{-a(\tau-\tau')} \text{var}(x_{\tau'}). \end{aligned} \quad (\text{S4})$$

The Gaussian probability density $P(x, \tau)$ given the initial condition in Eq. (S3) accordingly reads

$$P(x, \tau) = \sqrt{\frac{1}{2\pi \text{var}(x_\tau)}} \exp \left[-\frac{(x - ze^{-a\tau})^2}{2\text{var}(x_\tau)} \right]. \quad (\text{S5})$$

The local mean velocity $\nu(x, \tau) \equiv j(x, \tau)/P(x, \tau)$ with current $j(x, \tau) \equiv (-ax - D\partial_x)P(x, \tau)$ reads

$$\nu(x, \tau) = -ax + D(x - ze^{-a\tau})/\text{var}(x_\tau). \quad (\text{S6})$$

For this example we consider the simple case $\sigma_0^2 = D/a$, i.e. we start in the steady-state variance (but as long as $z \neq 0$ not in the steady-state distribution), for which we obtain the simplified expressions

$$\begin{aligned} \text{var}(x_\tau) &= D/a, \\ \text{For } \tau \geq \tau': \quad \text{cov}(x_\tau, x_{\tau'}) &= e^{-a(\tau-\tau')} D/a, \\ \nu(x, \tau) &= -aze^{-a\tau}. \end{aligned} \quad (\text{S7})$$

For this initial condition, $P(x, \tau)$ corresponds to a Gaussian distribution of constant variance with mean value $ze^{-a\tau}$ drifting from z to 0. Since only the mean changes (but the distribution around the mean remains invariant), the local

mean velocity $\nu(x, \tau)$ is independent of x [and in fact given by the velocity of the mean $\nu(x, \tau) = \partial_\tau \langle x_\tau \rangle$]. This easily allows to compute the time-accumulated dissipation

$$\Sigma_t = D^{-1} \int_0^t d\tau \int dx \langle \nu(x_\tau, \tau) \rangle^2 = \frac{a^2 z^2}{D} \int_0^t d\tau e^{-2a\tau} = \frac{az^2}{2D} (1 - e^{-2at}). \quad (\text{S8})$$

To show that the inequality (S2) without the correction term can be violated, i.e. to find an example for which $2[t\partial_t \langle J_t \rangle]^2 > \Sigma_t \text{var}(J_t)$, we note [recalling Eq. (8) in the Letter, $\langle J_t \rangle = \int_0^t d\tau \int d\mathbf{x} \mathbf{U}(\mathbf{x}, \tau) \cdot \mathbf{j}(\mathbf{x}, \tau)$] that the term $t\partial_t \langle J_t \rangle = t \int d\mathbf{x} \mathbf{U}(\mathbf{x}, t) \cdot \mathbf{j}(\mathbf{x}, t)$ only involves $\mathbf{U}(\mathbf{x}, t)$ at the final time but not at any $\tau < t$. In contrast, Σ_t is independent of the choice of \mathbf{U} and $\text{var}(J_t)$ involves $\mathbf{U}(\mathbf{x}, \tau)$ at all times. Therefore, examples for $2[t\partial_t \langle J_t \rangle]^2 > \Sigma_t \text{var}(J_t)$ can be found by making $\mathbf{U}(\mathbf{x}, t)$ large compared to $\mathbf{U}(\mathbf{x}, \tau)$ at $\tau < t$.

We now give an explicit example by choosing a linear time-dependence $U(x, \tau) = \tau$ (here one-dimensional),

$$J_t \equiv \int_{\tau=0}^{\tau=t} \tau \circ dx_\tau. \quad (\text{S9})$$

Note that due to $\partial_x U(x, \tau) = 0$ there is no difference between Stratonovich and Itô integration. We calculate

$$\begin{aligned} \langle J_t \rangle &= \int_0^t \tau \langle -ax_\tau \rangle d\tau = -az \int_0^t \tau e^{-a\tau} d\tau = -\frac{z}{a} [1 - e^{-at}(1 + at)], \\ t\partial_t \langle J_t \rangle &= \frac{zt}{a} [-a(1 + at) + a] e^{-at} = -zat^2 e^{-at}. \end{aligned} \quad (\text{S10})$$

For the variance write

$$\text{var}(J_t) = \langle [J_t - \langle J_t \rangle]^2 \rangle = \left\langle \left(\int_0^t v\tau [-a(\mathbf{x}_\tau - \langle \mathbf{x}_\tau \rangle)] d\tau + \sqrt{2D} dW_\tau \right)^2 \right\rangle. \quad (\text{S11})$$

Here, cross terms $d\tau dW_\tau$ can be computed according to the "Lemma" in Refs. [4, 5] or as outlined in the Letter in Eqs. (12) and (13), but one then immediately sees that such terms vanish here due to $\partial_x DU(x, \tau) = 0$. Thus we get (using cov from Eq. (S7))

$$\begin{aligned} \text{var}(J_t) &= a^2 \int_0^t d\tau \int_0^t d\tau' \tau\tau' \text{cov}(x_\tau, x_{\tau'}) + 2D \int_0^t d\tau \tau^2 \\ &= 2D \left(\frac{t^3}{3} + \frac{1}{6a^5} [a^2 t^2 (2at - 3) - 6e^{-at}(1 + at) + 6] \right). \end{aligned} \quad (\text{S12})$$

Since the dissipation Σ_t does not depend on the choice of J_t, U , it is still given by Eq. (S8).

We now have evaluated all relevant expressions. Set $a = D = z = 1$ such that t is the only remaining parameter. The TUR $2[t\partial_t \langle J_t \rangle]^2 \leq \Sigma_t \text{var}(J_t)$ that would hold in the absence of explicit time-dependence in U [see Ref. [1] or Eq. (S2) where $\tilde{J}_t = 0$ in the absence of explicit time-dependence in U], is now broken e.g. for $t = 0.1$ where $2[t\partial_t \langle J_t \rangle]^2 = 1.6 \times 10^{-4} > \Sigma_t \text{var}(J_t) = 6.3 \times 10^{-5}$. One also obtains a counterexample to $2[t\partial_t \langle J_t \rangle]^2 \leq \Sigma_t \text{var}(J_t)$ by taking the limit $t \rightarrow 0$ since asymptotically $2[t\partial_t \langle J_t \rangle]^2 \stackrel{t \rightarrow 0}{\approx} 2t^4$, $\Sigma_t \stackrel{t \rightarrow 0}{\approx} t$ and $\text{var}(J_t) \stackrel{t \rightarrow 0}{\approx} 2t^3/3$, i.e. $2[t\partial_t \langle J_t \rangle]^2 \stackrel{t \rightarrow 0}{\approx} \Sigma_t \text{var}(J_t)/3$. Thus, the inequality $2[t\partial_t \langle J_t \rangle]^2 \leq \Sigma_t \text{var}(J_t)$ is violated by a factor of 3 for $t \rightarrow 0$.

This example shows that the correction term $-\langle \tilde{J}_t \rangle$ in the TUR (S2) is necessary for general validity for currents with explicitly time-dependent \mathbf{U} .

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