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Rapid Communications

Hyperaccurate currents in stochastic thermodynamics

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Thermodynamic observables of mesoscopic systems can be expressed as integrated empirical currents. Their fluctuations are bound by thermodynamic uncertainty relations. We introduce the hyperaccurate current as the integrated empirical current with the least fluctuations in a given nonequilibrium system. For steady-state systems described by overdamped Langevin equations, we derive an equation for the hyperaccurate current by means of a variational principle. We show that the hyperaccurate current coincides with the entropy production if and only if the latter saturates the thermodynamic uncertainty relation, and it can be substantially more precise otherwise. The hyperaccurate current can be used to improve estimates of entropy production from experimental data.

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Stochastic thermodynamics is a theory describing the nonequilibrium behavior of mesoscopic physical systems, from colloidal particles [1–3] to molecular motors [4–6]. In these systems, thermodynamic observables are stochastic quantities. A vast class of these observables can be expressed as linear functionals of the increments of a stochastic trajectory. Such observables are called *integrated empirical currents*. For continuous systems whose state is specified by a vector $\vec{x}$, an integrated empirical current $R(t)$ (from now on simply "current") evolves according to the dynamics [7]

$$\frac{dR}{dt} = \vec{c} \circ \frac{d\vec{x}}{dt}, \tag{1}$$

where $\vec{c} = \vec{c}(\vec{x})$ is a vector field that determines the current, and $\circ$ indicates the Stratonovich prescription. The total entropy production at steady state and the heat released into a thermal reservoir are examples of thermodynamic observables that can be expressed as currents.

It has been recently observed that, at steady state, all currents must satisfy the so-called *thermodynamic uncertainty relation* [5,8,9]

$$\frac{\sigma_R^2}{\langle R\rangle^2} \geqslant \frac{2}{\langle S\rangle}. \tag{2}$$

The left-hand side of Eq. (2) is the coefficient of variation squared (CV^2) of an arbitrary current R, observed at steady state during a time t. In the right-hand side, $\langle S\rangle$ is the total entropy produced on average in the same time interval. Equation (2) was originally demonstrated for discrete-state systems described by master equations, first in the long-time limit [9] and later for finite times [10]. Continuous-state systems described by Langevin equations also satisfy the same bound [11]. Interestingly, the bound of Eq. (2) does not hold for discrete-time processes [12] and looser bounds have been derived for this case [13,14]. Thermodynamic uncertainty relations have been generalized to periodically driven systems out of steady state [15,16] and to observables other than currents [17]. These results have been recently unified with a geometrical interpretation in the space of observables [18].

Conceptually, the importance of Eq. (2) is that it sets a universal minimum amount of dissipation necessary to achieve currents of a given precision. Equation (2) is also of more practical interest: by seeking for currents approaching the bound, one can estimate the entropy production in a more accurate way than with other methods [19]. To this aim, it is important to know which current R approximates the bound best and how close to saturation it is. It was shown that the only current that can saturate the bound is the entropy production itself [20]. However, it is still unclear what happens when the entropy production does not saturate the bound.

In this Rapid Communication, we introduce the *hyperaccurate current* as the current with the lowest CV^2 in a given stochastic system. For continuous systems described by a set of overdamped Langevin equations, we derive the Euler-Lagrange equations that must be satisfied by the hyperaccurate current, and solve them in concrete examples.

We consider mesoscopic physical systems that can be described by N slow degrees of freedom $\vec{x} = \vec{x}(t) = x_1(t), x_2(t), \dots, x_N(t)$. Such degrees of freedom evolve according to a set of overdamped Langevin equations

$$\frac{d}{dt}\vec{x} = \hat{\mu}\cdot\vec{F} + \vec{\nabla}\cdot\hat{D} + \sqrt{2}\hat{\sigma}\cdot\vec{\xi}, \tag{3}$$

where $\vec{\xi} = \vec{\xi}(t) = \xi_1(t), \dots, \xi_N(t)$ is a Gaussian white noise with mean $\langle\xi_i(t)\rangle = 0$ and autocorrelation $\langle\xi_i(t)\xi_j(t')\rangle = \delta(t-t')\delta_{ij}$. Here the noise is interpreted in the Ito sense. The symmetric matrix $\hat{\mu} = \hat{\mu}(\vec{x})$ is the motility tensor and the vector $\vec{F} = \vec{F}(\vec{x})$ is the force acting on the system. The matrix $\hat{\sigma} = \hat{\sigma}(\vec{x})$ is related to the symmetric diffusion matrix $\hat{D} = \hat{D}(\vec{x})$ by the relation $\hat{\sigma}^T\hat{\sigma} = \hat{D}$. We assume the Einstein relation $\hat{D} = k_B T\hat{\mu}$ to hold, where k_B is the Boltzmann constant

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and T the temperature. We further assume that the matrices $\hat{\sigma}$, $\hat{D}$, and $\hat{\mu}$ are nondegenerate. We associate to Eqs. (3) the Fokker-Planck equation

$$\partial_t P(\vec{x};t) = \vec{\nabla}\cdot[-\hat{\mu}\cdot\vec{F}P(\vec{x};t) + \hat{D}\cdot\vec{\nabla}P(\vec{x};t)]. \quad (4)$$

We call $P^{\rm st} = P^{\rm st}(\vec{x})$ the stationary solution of Eq. (4), $P(\vec{x};t|\vec{y};t')$ the propagator, $\vec{J} = \vec{J}(\vec{x},t) = \hat{\mu}\cdot\vec{F}P(\vec{x},t) - \hat{D}\cdot\vec{\nabla}P(\vec{x},t)$ the flux, and $\vec{J}^{\rm st} = \vec{J}^{\rm st}(\vec{x}) = \hat{\mu}\cdot\vec{F}P^{\rm st}(\vec{x}) - \hat{D}\cdot\vec{\nabla}P^{\rm st}(\vec{x})$ the stationary flux. We substitute Eqs. (3) and (4) into Eq. (1), finding an explicit evolution equation for a generic current

$$\frac{dR}{dt} = \frac{\vec{c}\cdot\vec{J} + \vec{\nabla}\cdot(\hat{D}\cdot\vec{c}\,P)}{P} + \sqrt{2}\vec{c}\cdot\hat{\sigma}\cdot\vec{\xi}. \quad (5)$$

Equation (5) is interpreted in the Ito sense. Important examples of currents are the heat released in the thermal bath Q, with $\vec{c} = \vec{F}$ [21], and the total entropy production S at steady state, with $\vec{c} = \hat{D}^{-1}\cdot\vec{J}^{\rm st}/P^{\rm st}$. Substituting this latter choice into Eq. (5) directly yields the evolution equation for the entropy production derived in [22].

We consider the evolution a current at steady state and use Eq. (5) to derive the uncertainty bound of Eq. (2) in a straightforward way. We introduce the *bound term*

$$\frac{dR_{\rm bound}}{dt} = \sqrt{2}\frac{\langle R\rangle}{\langle S\rangle}\frac{\vec{J}^{\rm st}}{P^{\rm st}}\cdot(\hat{\sigma}^T)^{-1}\cdot\vec{\xi}. \quad (6)$$

The bound term is defined so that its variance over the mean of the current squared saturates the uncertainty bound of Eq. (2), i.e.,

$$\frac{\sigma^2_{R_{\rm bound}}}{\langle R\rangle^2} = \frac{2}{\langle S\rangle}. \quad (7)$$

We now decompose an arbitrary current $R(t)$ into the sum of the bound term and a deviation term

$$R_{\rm dev}(t) = R(t) - R_{\rm bound}(t). \quad (8)$$

In terms of this decomposition, the left-hand side of the uncertainty bound reads

$$\frac{\sigma^2_R}{\langle R\rangle^2} = \frac{\sigma^2_{R_{\rm bound}}}{\langle R\rangle^2} + \frac{\sigma^2_{R_{\rm dev}}}{\langle R\rangle^2} + 2\frac{\sigma^2_{R_{\rm bound},R_{\rm dev}}}{\langle R\rangle^2}. \quad (9)$$

An explicit computation shows that the covariance $\sigma^2_{R_{\rm bound},R_{\rm dev}}$ always vanishes (see [23]). This implies

$$\frac{\sigma^2_R}{\langle R\rangle^2} = \frac{2}{\langle S\rangle} + \frac{\sigma^2_{R_{\rm dev}}}{\langle R\rangle^2} \geqslant \frac{2}{\langle S\rangle}. \quad (10)$$

Equation (10) means that the variance of $R_{\rm dev}$ is responsible for the deviation from the bound.

This calculation constitutes a short and direct demonstration of the thermodynamic uncertainty relation for a system governed by Langevin equations [11]. An advantage of this approach is to provide an explicit expression for the deviation from the bound. In particular, a current R saturates the uncertainty bound only when $\sigma^2_{R_{\rm dev}} = 0$. A necessary condition for this to hold is that the noise amplitude of $R_{\rm dev}$ must vanish. Imposing this condition by means of Eqs. (5), (6), and (8) yields

$$\sqrt{2}\left(\vec{c} - \frac{\vec{J}^{\rm st}}{P^{\rm st}}\cdot\hat{D}^{-1}\frac{\langle R\rangle}{\langle S\rangle}\right)\cdot\hat{\sigma} = 0 \quad \Leftrightarrow \quad \vec{c} \propto \frac{\vec{J}^{\rm st}}{P^{\rm st}}\cdot\hat{D}^{-1}. \quad (11)$$

When $\vec{c}$ satisfies the condition in Eq. (11), then $R \propto S$. This means that only the entropy production, or a current proportional to it, can saturate the uncertainty bound [20]. As a corollary, if the entropy production does not saturate the bound, the bound cannot be saturated by any current.

To understand such cases, we define the *hyperaccurate current* $R_{\rm h}$ as the current with the minimum CV^2, among all possible choices of $\vec{c}(\vec{x})$. Since $\sigma^2_R/\langle R\rangle^2 = \langle R^2\rangle/\langle R\rangle^2 - 1$, we seek for the hyperaccurate current by minimizing $\langle R^2\rangle/\langle R\rangle^2$ with respect to the function $\vec{c}(\vec{x})$.

The average value of R reads

$$\langle R\rangle = t\left\langle\frac{dR}{dt}\right\rangle = t\int d\vec{x}\,\vec{c}(\vec{x})\cdot\vec{J}^{\rm st}(\vec{x}), \quad (12)$$

where in the last equality we used Eq. (5). Similarly, we express the second moment as $\langle R^2\rangle = \langle[\int_0^t dt'(dR/dt')]^2\rangle$. We use these expressions to evaluate the first variation of $\langle R^2\rangle/\langle R\rangle^2$ with respect to $\vec{c}(\vec{x})$ and impose that it must vanish (see [23]). This procedure results in the Euler-Lagrange equation

$$\hat{D}^{-1}(\vec{x})\cdot\vec{J}^{\rm st}(\vec{x})\int_0^t dt'\int_0^{t'} dt''\left\langle\frac{\vec{J}^{\rm st}(\vec{y})\cdot\vec{c}_{\rm h}(\vec{y})}{P^{\rm st}(\vec{x})P^{\rm st}(\vec{y})}\right\rangle_y + P^{\rm st}(\vec{x})\vec{\nabla}_{\vec{x}}\left\{\int_0^t dt'\int_0^{t'} dt''\left\langle\frac{\vec{\nabla}_{\vec{y}}\cdot[P^{\rm st}(\vec{y})\hat{D}(\vec{y})\cdot\vec{c}_{\rm h}(\vec{y})]}{P^{\rm st}(\vec{x})P^{\rm st}(\vec{y})}\right\rangle_y\right\}$$
$$= t\hat{D}^{-1}(\vec{x})\cdot\vec{J}^{\rm st}(\vec{x})\frac{\langle R_{\rm h}^2\rangle}{2\langle R_{\rm h}\rangle} - tP^{\rm st}(\vec{x})\vec{c}_{\rm h}(\vec{x}), \quad (13)$$

where $\vec{c}_{\rm h}(\vec{x})$ is the vector field associated to the hyperaccurate current, and we denoted with $\langle\cdots\rangle_y = \int d\vec{y}\,P(\vec{x};t|\vec{y};t'')P^{\rm st}(\vec{y})$ the average over the initial state. In principle, also the Fano factor $\langle R_{\rm h}^2\rangle/(2\langle R_{\rm h}\rangle)$ on the right-hand side of Eq. (13) implicitly depends on $\vec{c}_{\rm h}(\vec{y})$. However, we can exploit the fact that rescaling $\vec{c}_{\rm h}(\vec{y})$ by an arbitrary multiplicative factor does not change its CV^2. The solution of Eq. (13) is therefore defined up to an arbitrary multiplicative constant. From now on, we shall fix this constant by setting $\sigma^2_{R_{\rm h}}/2\langle R_{\rm h}\rangle = 1$.

In the long-time limit, Eq. (13) reduces to the simpler form [23]

$$\int d\vec{y}\,\hat{K}(\vec{x},\vec{y})\cdot\vec{c}_{\rm h}(\vec{y}) = \vec{J}^{\rm st}(\vec{x}), \quad (14)$$

where we defined the integral kernel

$$\hat{K}(\vec{x},\vec{y}) = \frac{\vec{J}^{st}(\vec{x})}{P^{st}(\vec{x})}\phi(\vec{x},\vec{y})\vec{J}^{st}(\vec{y}) + P^{st}(\vec{x})\hat{D}(\vec{x})\delta(\vec{x}-\vec{y}) - P^{st}(\vec{x})[\hat{D}(\vec{x})\cdot\vec{\nabla}_{\vec{x}}]\cdot\vec{\nabla}_{\vec{y}}\left[\frac{\phi(\vec{x},\vec{y})}{P^{st}(\vec{x})}\right]\cdot\hat{D}(\vec{y})P^{st}(\vec{y}), \tag{15}$$

and the function

$$\phi(\vec{x},\vec{y}) = \int_0^{+\infty} dt[P(\vec{x};t|\vec{y};0) - P^{st}(\vec{x})]. \tag{16}$$

If the kernel $\hat{K}(\vec{x},\vec{y})$ can be inverted, then $\vec{c}_h(\vec{x})$ can be expressed as

$$\vec{c}_h(\vec{x}) = \int d\vec{y}\,\hat{K}^{-1}(\vec{x},\vec{y})\cdot\vec{J}^{st}(\vec{y}), \tag{17}$$

where $\int dz\,\hat{K}^{-1}(\vec{x},\vec{z})\cdot\hat{K}(\vec{z},\vec{y}) = \delta(\vec{x}-\vec{y})$.

We are now in the position to study whether the entropy production can still be hyperaccurate when it does not saturate the bound. To this aim, we assume $R_h \propto S$, i.e., $\vec{c}_h \propto \hat{D}^{-1}\cdot\vec{J}^{st}/P^{st}$ and substitute this choice into Eq. (14), obtaining

$$\int d\vec{y}\,\phi(\vec{x},\vec{y})\frac{\vec{J}^{st}(\vec{y})\cdot\hat{D}^{-1}(\vec{y})\cdot\vec{J}^{st}(\vec{y})}{P^{st}(\vec{y})} \propto P^{st}(\vec{x}). \tag{18}$$

We interpret the left-hand side of Eq. (18) as the integral operator $\int d\vec{y}\,\phi(\vec{x},\vec{y})$ acting on the function $g(\vec{y}) = \vec{J}^{st}(\vec{y})\cdot\hat{D}^{-1}(\vec{y})\cdot\vec{J}^{st}(\vec{y})/P^{st}(\vec{y})$. Such integral operator shares the same eigenfunctions of the Fokker-Planck equation (4). In particular, the stationary solution in the right-hand side of Eq. (18) is a right eigenfunction associated to a nondegenerate eigenvalue equal to zero. Therefore, Eq. (18) can be satisfied only if $g(y) \propto P^{st}(\vec{y})$, i.e., if the quantity $\vec{J}^{st}\cdot\hat{D}^{-1}\cdot\vec{J}^{st}/(P^{st})^2$ is constant. But this is precisely the condition for the entropy production to saturate the uncertainty bound [22]. We therefore conclude that, when the entropy production does not saturate the bound, it cannot be identified as the hyperaccurate current.

By definition, the CV^2 of the hyperaccurate current provides the tightest possible bound on the CV^2 of a current, the *hyperaccurate bound* $\mathcal{B}_h$. Since we set $\sigma^2_{R_h}/2\langle R_h\rangle = 1$, $\mathcal{B}_h$ depends solely on the average of R_h

$$\frac{\sigma_R^2}{\langle R\rangle^2} \geqslant \mathcal{B}_h = \frac{\sigma_{R_h}^2}{\langle R_h\rangle^2} = \frac{2}{\langle R_h\rangle}. \tag{19}$$

By using Eqs. (12) and (17) to express the average of the hyperaccurate current, we obtain

$$\mathcal{B}_h = \frac{2}{t}\left(\int d\vec{x}\,d\vec{y}\,\vec{J}^{st}(\vec{y})\cdot\hat{K}^{-1}(\vec{y},\vec{x})\cdot\vec{J}^{st}(\vec{x})\right)^{-1}. \tag{20}$$

We now study the hyperaccurate current in two concrete models, where we take $\hat{\mu} = \hat{D} = \hat{I}$ for simplicity, with $\hat{I}$ the identity matrix. Our first example is a molecular motor in a one-dimensional periodic potential $U(x) = \sin(2\pi x)$ subject to a constant nonconservative force f. The system is described by the Langevin equation

$$\frac{dx}{dt} = f - \frac{dU(x)}{dx} + \sqrt{2}\xi. \tag{21}$$

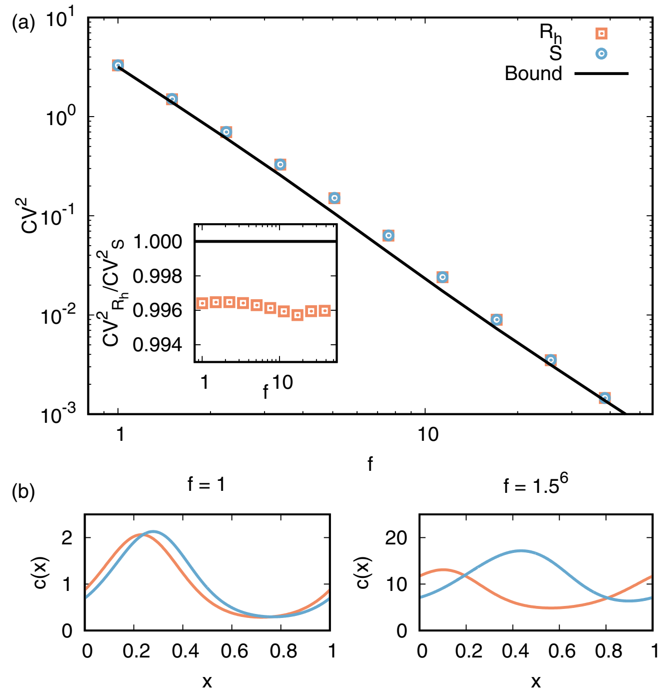

FIG. 1. Hyperaccurate current of a molecular motor model, Eq. (21). (a) CV^2 of the hyperaccurate current and the entropy production as a function of the force f. The continuous line is the uncertainty bound of Eq. (2). Inset: Ratio between the CV^2 of the hyperaccurate current and that of the entropy production as a function of f. (b) Comparison of $c(x)$ for the hyperaccurate current in red (lighter gray) and for the entropy production in blue (darker gray) for two different values of the force f, shown in the figures.

In this case, Eq. (15) is one dimensional. We numerically solve it by discretizing the interval [0,1] with a mesh Δ, so that the integral in Eq. (14) becomes a linear system of equations and the integral kernel in Eq. (15) becomes a matrix. We estimate this matrix by solving the Fokker-Planck equation numerically with the same spatial mesh Δ (see [23] for details).

In this model, both R_h and S are quite close to the bound, Fig. 1(a), with appreciable differences only for intermediate values of f (see also [22]). The CV^2 of R_h is lower than that of S as predicted, but their difference is rather small [less than 1% in the range of f we considered; inset of Fig. 1(a)]. Inspecting $c_h(x)$, we find that it is rather similar to the one characterizing the entropy production for low values of the force and substantially different at larger values of the force, Fig. 1(b).

As a second example, we consider the two-dimensional Langevin dynamics on a torus $[0, 1] \times [0, 1]$:

$$\frac{dx_1}{dt} = F(x_2) + \sqrt{2}\xi_1, \quad \frac{dx_2}{dt} = \sqrt{2}\xi_2 \tag{22}$$

with the nonconservative force $F(x_2) = f\cos(2\pi x_2)$. The stationary probability distribution is homogeneous, $P^{st}(x_1,x_2) = 1$, and the steady state flux is $\vec{J}^{st}(x_1,x_2) = F(x_2), 0$.

Since the dynamics is invariant under translations along the x_1 axis, then $\vec{c}_h(x_1, x_2) = c_{h,1}(x_1, x_2), c_{h,2}(x_1, x_2)$ cannot depend on x_1. Writing Eq. (14) by components, we find that $c_{h,2}(x_2) = 0$ (see [23]). Consequently, Eq. (14) reduces to the one-dimensional equation in the unknown $c_{h,1}(x_2)$,

$$\int dy_2 K(x_2, y_2) c_{h,1}(y_2) = f \cos(2\pi x_2), \tag{23}$$

where the kernel is

$$K(x_2, y_2) = f^2 \cos(2\pi x_2)\phi(x_2, y_2)\cos(2\pi y_2) + \delta(x_2 - y_2). \tag{24}$$

Since the coordinate x_2 evolves according to a simple diffusion process with periodic boundary conditions, the function $\phi(x_2, y_2)$ can be explicitly expressed as

$$\phi(x_2, y_2) = \sum_{n=0}^{+\infty} \frac{1}{2\pi^2 n^2} \cos[2\pi n(x_2 - y_2)]. \tag{25}$$

Expanding the solution $c_{h,1}(x_2)$ in a Fourier basis and substituting into Eq. (23), the Fourier coefficients can be analytically calculated at any order (see [23]).

In this case the CV^2 of the hyperaccurate current is much lower than that of the entropy production far from equilibrium, i.e., when $f \gg 1$ [see Fig. 2(a)]. The hyperaccurate current converges to the entropy production when the system is near equilibrium and the bound tends to be saturated. Farther from equilibrium, the hyperaccurate current is markedly different from the entropy production, Fig. 2(b).

In this Rapid Communication, we introduced the hyperaccurate current for systems described by overdamped Langevin equations. We have shown with examples that the hyperaccurate current can be substantially more accurate than the entropy production, in cases where the latter significantly departs from the uncertainty bound. By its definition, the hyperaccurate current provides the tightest possible uncertainty bound to the CV^2 of an arbitrary current. Our theory can be extended to discrete-state or discrete-time systems and possibly employed to study nonintegrated currents or nonstationary dynamics. We leave these investigations for future work.

It is worthwhile discussing how the results presented here can help in estimating entropy production in experiments. Naive estimators of entropy production often require very large sample size and/or observation times to provide accurate results. Reference [19] proposes to use Eq. (2) as a tool to estimate entropy production, or at least bound it. This strategy relies on the fact that, empirically, the CV^2 of a current is much easier to estimate than the entropy production. One crucial ingredient of this strategy is to identify a current whose CV^2 is sufficiently close to the bound. Reference [19] tackles this problem by means of a Monte Carlo scheme. This approach is relatively simple to implement, but has the disadvantages of being computationally costly and prone to overfitting, especially in high-dimensional systems. These difficulties are circumvented by the theory developed in this Rapid Communication. One possible strategy is therefore to build an approximate model of the physical system at hand, evaluate its hyperaccurate current using the theory developed in this Rapid Communication, and then measure the CV^2 of the hyperaccurate current in experiments. To pursue this strategy, it will be key to develop efficient numerical schemes [24] to solve the integral equation (14) and therefore compute the hyperaccurate current in systems more complex than the simple examples considered in this Rapid Communication. The results of Fig. 2(a) show that, even perturbing the hyperaccurate current, one can obtain currents that are substantially more accurate than the entropy production. This supports the idea that the hyperaccurate current computed in an approximate model of a physical system can be sufficiently close to the bound to provide a reliable estimate of entropy production, if measured in an experiment.

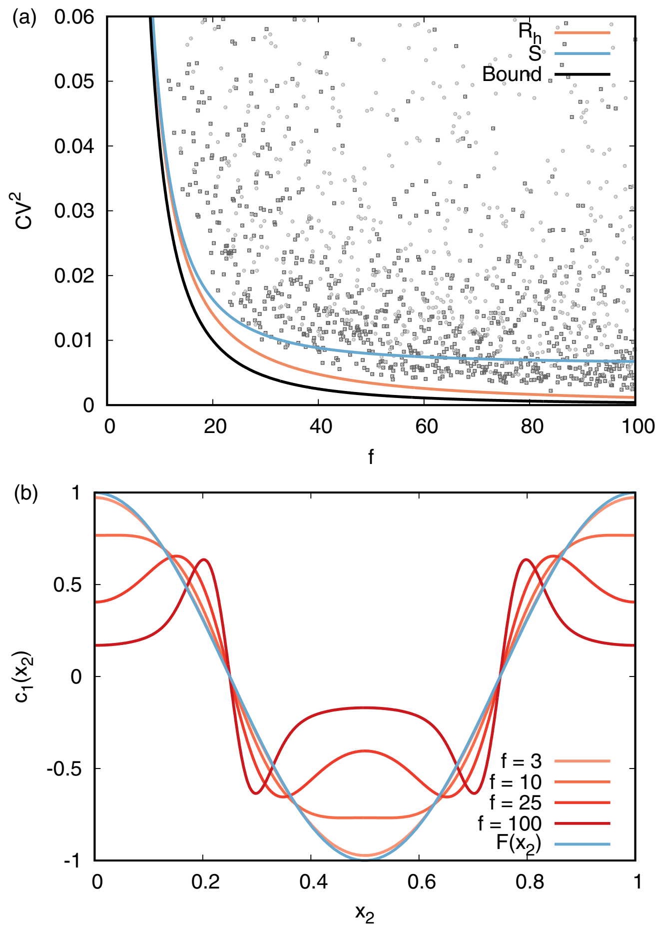

FIG. 2. Hyperaccurate current in a two-dimensional model, Eq. (22). (a) The black line is the thermodynamic uncertainty bound. The blue (top gray) line is the CV^2 of the hyperaccurate current. The red (middle gray) line is the CV^2 of the entropy production. All curves are plotted as a function of the nonconservative force f. The points represent random currents generated by adding to the coefficients $\kappa_{h,n}$ Gaussian random variables with mean zero and variance equal to f (dark-gray points) and $4f$ (light-gray points). (b) Red (dark-gray) lines represent $c_{h,1}(x_2)$ for different values of f. The blue line (dark-gray) represents $c_1(x_2) = F(x_2)$, whose associated current is the entropy production.

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