Nonequilibrium physics meets time series analysis: measuring probability currents from data

W. Just[1] (*)(**), H. Kantz[2](***), M. Ragwitz[2] and F. Schmüser[2]

[1] *Dept. of Physics, Chemnitz University of Technology - D–09107 Chemnitz, Germany*
[2] *Max Planck Institute for the Physics of Complex Systems - Nöthnitzer Str. 38, D–01187 Dresden, Germany*

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Abstract. – We present a simple method to estimate probability currents of stochastic systems from a given time series. The method uses results of the theory of stochastic differential equations about conditional averages. Evaluation of the probability current directly aims at detecting the violation of detailed balance and hence yields the proper characterisation of nonequilibrium behaviour. We apply our approach to stochastic resonance and propose a novel resonance criterion which is based on the evaluation of the probability current. It agrees well with other measures, e.g. derived from correlations or signal to noise ratios. Finally we demonstrate on an example of experimental wind data that our approach copes with real experimental data sets as well.

Introduction. – Detailed balance plays an ubiquitous role in equilibrium and near equilibrium physics. While equilibrium conditions imply the absence of macroscopic currents, the underlying microscopic Hamiltonian dynamics enforces in addition the exact balance of currents between different microstates. As a result fluctuation dissipation relations emerge which relate thermodynamic equilibrium fluctuations with macroscopic transport properties [1, 2]. Such a fundamental property holds regardless of the level of description, i.e. detailed balance can be formulated on the level of Boltzmann or master equations as well as for stochastic descriptions. Thus violation of detailed balance is the proper physical characterisation of strong nonequilibrium behaviour. Unfortunately the violation of detailed balance is not easy to measure apart from detecting macroscopic currents.

Over the last decade the development of nonlinear dynamics led to new concepts for analysing data under strong nonequilibrium conditions [3, 4]. Such tools are quite powerful to characterise chaotic behaviour in terms of correlation functions, Lyapunov exponents and generalised dimensions. Although such nonlinear dynamical behaviour is certainly linked

(*) E-mail: wolfram.just@physik.tu-chemnitz.de
(**) permanent address: School of Mathematical Sciences, Queen Mary / Univ. of London, Mile End Road, London E1 4NS, UK
(***) E-mail: kantz@mpipks-dresden.mpg.de

to strong nonequilibrium conditions, most concepts of traditional time series analysis are restricted to low–dimensional deterministic time evolution. There is to our best knowledge still a missing link between time series analysis and fundamental features of nonequilibrium statistical physics. Here we are going to fill this gap to some extent. We present a rather simple scheme which directly aims at detecting the violation of detailed balance but which is solely based on the evaluation of time series data.

As mentioned, violation of detailed balance is typically related to the occurrence of local currents([1]). Thus apart from our general theoretical motivation our considerations will be also quite useful from the practical point of view, since they allow for the computation of local currents. As a nontrivial example we consider the scenario of stochastic resonance, i.e. the increase of a periodic component of a signal by stochastic forcing [5]. The resonance phenomenon comes along with an increase of the current in the system. The details of this will be presented in the third section of this article where we analyse the standard example of the overdamped motion of a particle in a double well potential and subject to a periodic driving force.

To set up the framework of our general theoretical considerations we consider stochastic systems where the dynamics can be described in terms of Langevin equations

$$\dot{x}_t = f(x_t) + g(x_t)\xi_t \quad . \tag{1}$$

Here $f(x)$ denotes the systematic part of the motion, $g(x)$ the coupling coefficient of the stochastic force, and ξ_t a Gaussian white noise with correlation function $\langle \xi_t \xi_{t'} \rangle = 2\delta(t-t')$. Our variables may be vector valued, but to keep the presentation as simple as possible we suppress indices in our notation. The stochastic differential equation (1) induces a corresponding description in terms of probability densities $\rho(x,t)$ which results in the Fokker–Planck equation [6]

$$\partial_t \rho(x,t) = -\partial_x \left[D_1(x)\rho(x,t) - \partial_x D_2(x)\rho(x,t) \right] \quad . \tag{2}$$

Drift and diffusion coefficients are of course related to the coefficients of the stochastic description, e.g $D_1(x) = f(x) + g(x)\partial_x g(x)$ and $D_2(x) = g(x)g(x)$ holds if we adopt the Stratonovich interpretation of Eq.(1). The Fokker–Planck equation has the form of a conservation law involving the probability current

$$j(x,t) = D_1(x)\rho(x,t) - \partial_x[D_2(x)\rho(x,t)] \quad . \tag{3}$$

In a time independent state the current has vanishing divergence according to Eq.(2). Detailed balance implies that in addition the current vanishes identically. The computation of the probability current from Eq.(3) requires the knowledge of the invariant density as well as its spatial derivatives. Furthermore the drift and diffusion coefficients are needed. Thus the determination of the current from observed data suffers from many inaccuracies, in particular in phase spaces of higher dimension. We propose a quite robust estimate of the probability current which is solely based on trajectories of a Langevin equation.

Estimation of the probability current. – Recalling the Kramers Moyal expansion [6], drift and diffusion coefficients can be obtained through conditional averages of stochastic trajectories

$$\langle x_{t+\tau} - x_t \rangle|_{x_t = x} \;=\; \tau D_1(x) + \mathcal{O}(\tau^2)\ , \tag{4}$$

$$\langle (x_{t+\tau} - x_t)^2 \rangle|_{x_t = x} \;=\; \tau D_2(x) + \mathcal{O}(\tau^2) \quad . \tag{5}$$

([1])To be more precise: irreversible currents. In what follows we neglect reversible currents. We think a generalisation of our considerations is straightforward.

Relations of this type have in fact been used to extract drift and diffusion coefficients from data (cf. e.g. [7–9]) in order to establish effective stochastic models for the underlying dynamics. But one has to be careful in order to avoid several numerical traps which are intimately related to the limit of small delay τ [10]. Eq.(4) resembles the usual finite difference for estimating the first order derivative. From such a naive point of view one would guess that the estimate $\langle x_t - x_{t-\tau}\rangle|_{x_t=x}$ yields the same drift coefficient. But a simple consideration for the case of detailed balance (i.e. $j(x,t) \equiv 0$) already shows that the relation

$$\langle x_t - x_{t-\tau}\rangle|_{x_t=x} = -\langle x_{t+\tau} - x_t\rangle|_{x_t=x} \tag{6}$$

follows from the time reversal symmetry of equilibrium dynamics (see e. g. [11]). In the general case this 'acausal' estimate where the value of the trajectory is fixed at the later time yields an expression which involves the negative drift and the probability current

$$\langle x_t - x_{t-\tau}\rangle|_{x_t=x} = \tau[-D_1(x) + 2j(x,t)/\rho(x,t)] + \mathcal{O}(\tau^2) \quad . \tag{7}$$

The expression (7) is in fact not new. It has been obtained earlier in the context of 'stochastic mechanics' [12, 13], i.e. a reformulation of quantum mechanics in terms of classical particles which are subjected to stochastic forces. However, these concepts were not applied to discuss probability currents and detailed balance. Thus in order to keep our presentation self–contained we redo here an appropriate derivation of Eq.(7). Let $\rho(x,t;x',t')$ denote the joint probability for events x and x' at time t and t', respectively. Then

$$p(x',t-\tau|x,t) = \rho(x,t;x',t-\tau)/\rho(x,t) \tag{8}$$

denotes the conditional probability density and the left hand side of Eq.(7) can be written as

$$\begin{aligned}\langle x_t - x_{t-\tau}\rangle|_{x_t=x} &= \int dx'(x-x')p(x',t-\tau|x,t) \\ &= \int dx'(x-x')p(x,t|x',t-\tau)\rho(x',t-\tau)/\rho(x,t) \quad .\end{aligned} \tag{9}$$

Using the Taylor series expansion for the ratio of the densities

$$\rho(x',t-\tau)/\rho(x,t) = 1 + (x'-x)\partial_x\rho(x,t)/\rho(x,t) + \mathcal{O}(\tau,(x-x')^2) \tag{10}$$

and employing the usual short time expansion for the conditional probability density using the backward Fokker Planck operator [6]

$$p(x,t|x',t-\tau) = \delta(x-x') + \tau\left[D_1(x')\partial_{x'}\delta(x-x') + D_2(x')\partial^2_{x'}\delta(x-x')\right] + \mathcal{O}(\tau^2) \tag{11}$$

we obtain

$$\langle x_t - x_{t-\tau}\rangle|_{x_t=x} = \tau[D_1(x) - 2\partial_x D_2(x) - 2D_2(x)\partial_x\rho(x,t)/\rho(x,t)] + \mathcal{O}(\tau^2) \quad . \tag{12}$$

If we finally take the definition Eq.(3) of the probability current into account we end up with Eq.(7). We should stress that the derivation does not require the stationarity of the density. We note that according to Eq.(7) both the drift and the probability current contribute to the 'acausal' difference $\langle x_t - x_{t-\tau}\rangle|_{x_t=x}$.

Combining Eqs.(4) and (7) we arrive at the expression

$$\langle x_{t+\tau} - x_{t-\tau}\rangle|_{x_t=x} = 2\tau j(x,t)/\rho(x,t) + \mathcal{O}(\tau^2) \quad . \tag{13}$$

Thus the symmetric estimator for the temporal derivative of x yields directly the current in the stochastic system. These theoretical results can be used to obtain the probability current from a time series. Here the case of a stationary processes is of most interest. If $z_n = x_{n\tau}$ denotes a time series of length N with sampling rate $1/\tau$, then Eq.(13) yields the following estimator for the current

$$j(x) = \frac{1}{4\tau N\varepsilon} \sum_{|z_n - x|<\varepsilon} (z_{n+1} - z_{n-1}) \quad . \tag{14}$$

This expression takes the density $\rho(x)$ at the point x implicitly into account (cf. Eq.(13)).

Stochastic resonance. – To illustrate our method with a nontrivial example we consider the classic stochastic resonance scenario [14]. The equations of motion describe an overdamped particle in a double well potential with a low amplitude slow periodic and a stochastic forcing

$$\dot{x}_t = x_t - x_t^3 + a \sin \omega t + \sigma \xi_t \quad . \tag{15}$$

For a suitable noise amplitude σ, which is approximately such that the Kramers tunnelling time equals half the period $T = 2\pi/\omega$, the hopping of the particle from one well to the other is synchronised with the periodic driving term. For both lower and higher noise levels this synchronisation disappears. The two limits, without noise and large noise amplitudes, are of course trivial, since in the first case no hopping can occur due to the smallness of a, whereas in the latter case hopping is completely unrelated to the periodic driving. Meanwhile, a much better understanding of stochastic resonance has led to several refined resonance conditions [5, 15].

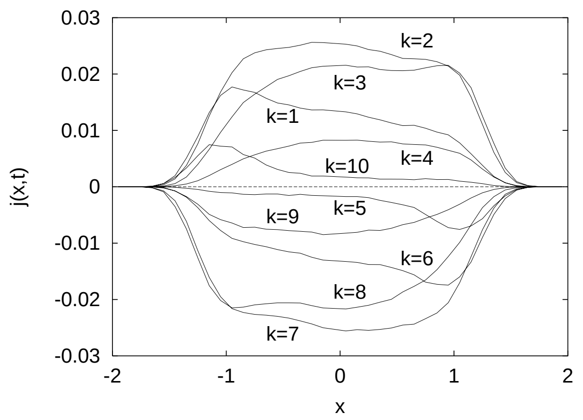

Fig. 1 – The probability current estimated numerically by Eq.(14) ($\tau = 0.1$) for the system Eq.(15) ($a = 0.2$, $\omega = 2\pi/100$, $\sigma = 0.5$). Different phase angles $\phi_k = 2\pi k/10$ of the driving term are indicated by $k = 1, \ldots, 10$, .

Theoretical approaches to stochastic resonance may be based on a Fokker–Planck description. Due to the periodic driving, the Fokker–Planck equation of this problem is periodic in time. The dynamical features are thus governed by the corresponding Floquet problem (cf. [16]) and the asymptotic state becomes periodically time dependent. When the system is close to the resonance condition the asymptotic distribution alternates between two states that have their maximum in the one or the other well, respectively. Of course the probability current oscillates, too. With our approach we can easily determine the time periodic probability current for different noise levels from a simple time series of Eq.(15). Fig. 1 displays the result for parameter values in the vicinity of the resonance. For a given phase angle $\phi = \omega t$ of the driving term, the current seems to have a given sign in the whole range of x. Hence, the dynamics of the current clearly reflects the synchronised motion in the stochastic system.

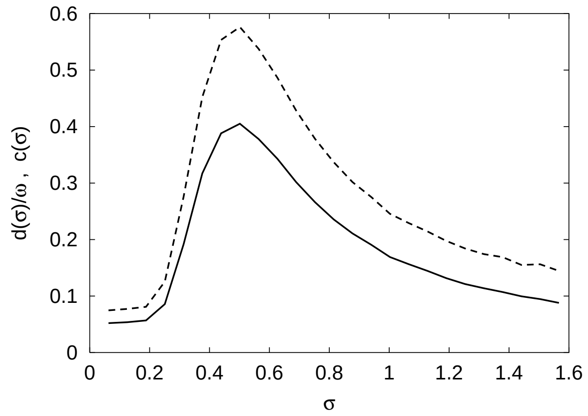

Fig. 2 – The dispersion of the probability current (broken line: $d(\sigma)/\omega$) and the coherence index (full line: $c(\sigma)$) as a function of the noise level σ for $a = 0.2$ and $\omega = 2\pi/100$.

To quantify the stochastic resonance phenomenon the amplitude of the current seems to be an adequate quantity. We measure such an amplitude in terms of the dispersion of the current

$$d^2(\sigma) = \int_0^T dt\, [\bar{j}(t)]^2 \tag{16}$$

where

$$\bar{j}(t) := \int_{-\infty}^{\infty} dx\, j(x,t) \tag{17}$$

denotes the integrated current. Fig. 2 nicely demonstrates that the dispersion reflects the resonance phenomenon. In fact the quantity coincides almost perfectly with the coherence index between the particle position and the driving term

$$c^2(\sigma) = \left(\int_0^T dt\, \langle x\rangle(t)\cos(\omega t)\right)^2 + \left(\int_0^T dt\, \langle x\rangle(t)\sin(\omega t)\right)^2 \tag{18}$$

when a simple rescaling is performed (cf. Fig. 2). Such a coincidence can be understood also analytically. Calculating the time derivative of the mean value $\langle x\rangle(t)$ from the Fokker–Planck equation (2) we find $d\langle x\rangle/dt = \bar{j}(t)$, taking the definition of the current (3) into account. Then performing an integration by parts the coherence index (18) reads

$$c^2(\sigma) = \left(\int_0^T dt\, \bar{j}(t)\frac{\sin(\omega t)}{\omega}\right)^2 + \left(\int_0^T dt\, \bar{j}(t)\frac{\cos(\omega t)}{\omega}\right)^2 \quad . \tag{19}$$

If the T–periodicity of the integrated current $\bar{j}(t)$ were strictly harmonic, Parseval's theorem predicts that $c(\sigma) = d(\sigma)/\omega$. Since there is some power of the current contained in higher harmonics of the driving frequency ω, the inequality $\omega c(\sigma) \leq d(\sigma)$ holds in general. However, the maximum occurs at the same noise level (cf. Fig. 2). Hence, the resonance comes along with the maximal deviation of the system from detailed balance, which, in turn, states that the effects of the external driving have the maximal macroscopic effect. We argue therefore that the maximisation of the probability current is a theoretically much better justified criterion for stochastic resonance than others. In addition to this novel definition of the resonance condition and new insight into the phenomenon of stochastic resonance, this also could open up a new way to detect the presence or absence of stochastic resonance in natural phenomena.

Analysis of experimental data. – In order to demonstrate that our method can be applied successfully to real experiments we evaluate a time series of experimentally measured surface wind velocities $v(t)$, obtained by an ultrasonic anemometer positioned about 40m above ground and recorded with 16Hz. We are not going into the details of the experiment (cf. [17]) but just focus on the evaluation of Eqs.(4) and (13) for the particular time series.

Within our approach we assume that the velocity can be described in terms of a simple stochastic model. Whether such an assumption is valid is beyond the scope of our presentation, but we refer the reader to [7] for a similar discussion of such a question in a different context. In particular, the analysis of [7] and [10] shows that velocity increments and the turbulent cascade can be modelled in some range by a Fokker–Planck equation. However, such results cannot be extrapolated in a simple way to the stochastic motion of the velocity itself. Nevertheless, if this approach is possible, the current has to vanish as it is computed for a stationary stationary state of a one–dimensional Fokker–Planck equation on an infinite domain.

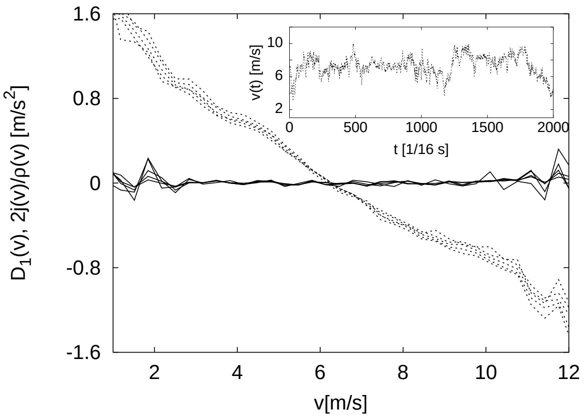

Fig. 3 – Probability current (full line) and effective drift (dotted line) computed by Eqs.(4) and (13), for $\tau = 1/16\text{s}, \ldots, 5/16\text{s}$, respectively. Inset: Segment of the wind speed time series.

Evaluation of Eqs.(4) and (13) is straightforward, and results for different values of τ are displayed in Fig. 3. We clearly see convergence already for $\tau \leq 5/16\text{s}$. Such a convergence supports the conjecture that a stochastic model in terms of the velocity is valid, although a thorough analysis requires the computation of higher order moments. Here we stress that the effective drift and the current behave differently. While the drift is an important ingredient which enters the correlation properties of the velocity the vanishing current is in accordance with the assumption that the wind data can be described in terms of a simple stochastic model.

Altogether our simple demonstration shows that our novel way of estimating probability currents is robust enough to be applied to experimental data. The proper physical interpretation depends on the additional issue of whether the observable really is subject to a Fokker–Planck equation.

Summary. – We have presented a simple method which allows the computation of the probability current. Our approach just requires the evaluation of a conditional average from a plain time series. For simplicity we have assumed from the very beginning that the underlying dynamics is governed by a simple Langevin equation with Gaussian white noise. Formulation of detailed balance becomes more intricate if variables behave differently with respect to time reversal or if the noise is non–Gaussian so that one needs a full master equation to describe the dynamics properly. We think that our approach can be extended to cope with such cases so that time series analysis becomes possible in quite general situations. But the details are beyond the scope of the present contribution and will be published elsewhere.

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