Breaking Microscopic Reversibility with Lévy Flights

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Abstract – A system at equilibrium exhibits microscopic reversibility, i.e. any path in phase space is just as often traversed in one direction as that it is traversed in the opposite direction. We show how it is justified to characterize white Gaussian noise as equilibrium noise: when an overdamped particle in a potential is subjected to such noise, microscopic reversibility can be proven for most probable paths that lead from one potential well to another. However, when the overdamped particle is subjected to white Lévy noise, time reversal symmetry is broken and microscopic reversibility is violated, even when the noise is symmetric. We, furthermore, derive how for an overdamped particle inside a parabolic potential microscopic reversibility is violated in the presence of Lévy white noise. Similar to Brownian vortexes, Lévy flights can be associated with the presence of Lévy vortexes in phase space.

Introduction. – Consider an overdamped Brownian particle in a potential $V(x)$. For $|x| \to \infty$ we have $V \to \infty$. The potential landscape has a number of minima, or wells, that we associate with “states” in a chemical space.

In 1925 Gilbert Lewis realized that for Brownian particles in a potential landscape, equilibrium means more than just a stationary probability distribution over a number of states [1]. The system should be invariant under a time reversal transformation, $t \to -t$. Net cyclic flows should thus be forbidden. At the end of his article, Lewis asks us to imagine a movie of a specific particle. He next points out that at equilibrium there is no way to discriminate between a forward played and a backward played movie. Lewis’ realization has the following implication.

Consider a particular phase space trajectory for the particle: $(\dot{x}(t), x(t))$ with $t_i < t < t_f$. Here $t_i$ is the initial time and $t_f$ is the final time. Along any such trajectory there should be just as much flow in the forward direction, from $(\dot{x}(t_i), x(t_i))$ to $(\dot{x}(t_f), x(t_f))$, as there is in the backward direction, from $(\dot{x}(t_f), -x(t_f))$ to $(\dot{x}(t_i), -x(t_i))$.

The terms “detailed balance” and “microscopic reversibility” have been used in different contexts and in occasionally inconsistent ways [2]. Our use [3, 4] is the customary one when the subject is states, rates, and trajectories in a chemical space. The requirement that net flow between any two states is zero is called “detailed balance.” The stricter requirement that net flow along any phase space path is zero is called “microscopic reversibility.” The latter notion is due to Onsager, who, in 1931, derived his reciprocal relationships from it [5,6].

In what follows we first focus on the most probable path between two points. It is obvious that equilibrium demands that the most probable path in the forward time direction runs along the same trajectory as the most probable path in the backward time direction. We will show how Gaussian noise can be associated with microscopic reversibility and how the presence of more general Lévy fluctuations can lead to violation of microscopic reversibility. In our example the Lévy noise itself is symmetric in the sense that each fluctuation in the positive direction is as likely as its negative-direction counterpart. However, following the Langevin formalism for an overdamped particle in a potential, the application of non-Gaussian Lévy noise is found to lead to a breaking of the time reversal symmetry. Microscopic reversibility for most probable paths is violated, so forward and backward kinetics are distinguishable.

The suitably scaled 1D Langevin Equation for a noise-
subjected, overdamped particle on a potential \( V(x) \) is:

\[
\dot{x} = -\frac{dV(x)}{dx} + \xi_\alpha(t).
\] (1)

As a generic example to illustrate the different responses to Gaussian and Lévy noise, we consider a piecewise linear potential \( V(x) \) as drawn in Fig. 1. Piecewise linear setups commonly exhibit unique features due to their sharp corners. However, when noise is present, corners are effectively “smoothed” and piecewise linear systems no longer behave atypically.

Fig. 1: A double-well, symmetric, piecewise linear potential. We consider an overdamped particle in this potential. The particle is subjected to Lévy noise.

The term \( \xi_\alpha(t) \) in Eq. (1) represents the noise. We assume a low noise limit so barrier crossings are rare events. Upon discretization of Eq. (1) the contributions \( \xi_\alpha(t)\Delta t \equiv \Delta L_\alpha(t) \) are independent increments or “kicks.” In analogy to Gaussian white noise, which is the time derivative of the Wiener process [3], general Lévy white noise can be defined as the time derivative of the alpha-stable free Lévy flight (LF), i.e. \( \xi_\alpha(t) = \dot{L}_\alpha(t) \). For the “kicksizes” distribution \( \tilde{p}_\alpha(k) \) of the symmetric alpha-stable Lévy LF, analytic expression is in terms of the characteristic function \( \tilde{p}_\alpha(k) \equiv \int p_\alpha(\xi) \exp(ik\xi) \, d\xi \) [7–10]:

\[
\tilde{p}_\alpha(k) = \exp\left[-\sigma^\alpha|k|^\alpha\right],
\] (2)

where the parameter \( \alpha (0 < \alpha \leq 2) \) is the stability index and \( \sigma \) is a scale parameter that gives the noise intensity. For \( \alpha = 2 \) the case of Gaussian noise is retrieved where \( \sigma \) represents the standard deviation divided by \( \sqrt{2} \).

With Gaussian noise, tails are rapidly decaying and follow \( p_2(\xi) \propto \exp\left[-\xi^2/4\sigma^2\right] \). For \( \alpha < 2 \) we have a probability density distribution with a “fat” power-law tail, \( p_\alpha(\xi) \propto |\xi|^{-(1+\alpha)}\). Note that such a fat tail results in a diverging variance for the distribution.

A prominent property of LFs and of Gaussian diffusion is the fractal nature of the trajectory. The scaling law that goes with the self-similarity is \( L_\alpha(\sigma t) = \sigma^{1/\alpha}L_\alpha(t) \). The fractality carries over to the kicksizes \( \xi_\alpha(t) \) that feature in Eq. (1). There we have \( \xi_\alpha(\sigma t) = \sigma^{(1-\alpha)/\alpha}\xi_\alpha(t) \). For a discretized representation of Eq. (1), this means that the kicksizes \( \xi_\alpha(t) \) depend on the length of the timestep \( \Delta t \), i.e. \( \xi_\alpha(t_i) = \theta_{n,i}/(\Delta t)^{(\alpha-1)/\alpha} \), where the \( \theta_{n,i} \)'s are drawn from a standard (\( \sigma = 1 \)) alpha-stable distribution. Ultimately, the Wiener process (\( \alpha = 2 \)) looks like a “hairy” trajectory. LFs (\( \alpha < 2 \)), however, exhibit large random jumps [7,10] and superdiffusion [11–13].

The Gaussian distribution is important and ubiquitous. This is because whenever a distribution comes about as the cumulative effect of a large number of stochastic inputs that each have a finite variance, the Central Limit Theorem tells us that this distribution will be Gaussian [3]. In an analogous way the alpha-stable Lévy distributions with \( \alpha < 2 \) “attract” sums of random variables with diverging variance [14]. Hence, LFs occur in the description of fluctuation processes that are characterized by bursts or large outliers. “Noise with pulsatory outbursts” appears to be inherent to phenomena far from equilibrium, such as, e.g., plasma turbulence [15] and financial market dynamics [16, 17]. Lévy noise is also commonly detected in physiology [18] and solar physics [19]. Climate changes have been modelled with LFs and overdamped dynamics as in Eq. (1) [20].

LFs can also emerge in the mathematical description of equilibrium situations [21]. Consider, for instance, a molecule that is diffusively hopping along a flexible polymer from one monomer to a neighboring one. Let the position of the molecule along the polymer chain next be characterized by a chemical coordinate \( x \). If the polymer folds back and touches itself, then the molecule can, when at the “intersection,” hop to a far away part of the chain. The small jump in Euclidian space corresponds in that case to a Lévy jump along \( x \). This process may play a role in protein dynamics on DNA strands [22].

If the noise, \( \xi_\alpha(t) \), is symmetric, then the resulting stationary probability density for the Brownian particle in the potential of Fig. 1 will be mirror-symmetric around \( x = 1 \). This is because without a symmetry-breaking feature in the setup, Curie’s Principle (a symmetry or asymmetry of a cause is always preserved in its effects [23]) demands a symmetric distribution. This means that for both Gaussian noise and Lévy noise, the probability distribution for the particle will be symmetric around \( x = 1 \). For the two-state system of Fig. 1, stationarity obviously implies detailed balance, i.e. just as much flow from the left to the right well as from the right to the left well.

Microscopic reversibility is a stricter condition than detailed balance. Microscopic reversibility means that any path in phase space is traversed in one direction just as often as in the opposite direction. Microscopic reversibility and time-reversal symmetry are equilibrium characteristics that imply each other. Microscopic reversibility implies detailed balance, but not the other way round [4]. Below we show analytically how, in the case of Lévy noise, microscopic reversibility is broken for the potential depicted in Fig. 1.

Noise-Induced Barrier Crossing. — We first consider white noise with a Gaussian “kicksizes” distribution. This is the \( \alpha = 2 \) case of Eq. (2). The “kicks” \( \xi_\alpha(t_i) \) that occur every \( \Delta t \) are independent, have zero average, and a standard deviation of \( \sqrt{2/\Delta t} \). To go up the barrier from
$x = 0$ to $x = 1$, we need an unlikely sequence of kicks. What we will next calculate is “the most likely such unlikely sequence.”

To calculate the most probable escape path (MPEP) from $x = 0$ to $x = 1$, we write Eq. (1) as $\dot{x} = \xi_2(t)$, where $F$ is the constant force, and we identify the probability that the required sequence of kicks is realized as

$$\mathcal{P} = \prod_{j=1}^{n} \exp \left[-\frac{1}{4} \xi_2^2(t_j) \Delta t \right].$$

Maximal $\mathcal{P}$ occurs when the sum in Eq. (3) is minimal. Suppose we go up the linear slope with a sequence of $n$ kicks that are all of the same magnitude $\kappa$. We then have

$$\mathcal{P} \propto \exp \left[-\frac{n}{4} \kappa^2 \Delta t \right].$$

Next assume a slight variation where one kick has a magnitude $\kappa + \Delta \kappa$ and another kick has a compensating magnitude $\kappa - \Delta \kappa$. The net effect would be the same: you would get up the slope in the same time. However, since $(\kappa + \Delta \kappa)^2 + (\kappa - \Delta \kappa)^2 = 2\kappa^2 + 2(\Delta \kappa)^2$, the sum in Eq. (3) would be larger and the probability $\mathcal{P}$ would be smaller. So equal kicksizes constitute the MPEP because the average of the squares is larger than the square of the average. Essentially, this is a manifestation of Jensen’s Inequality which says that for any concave up function $f(x)$, we have $\langle f(x) \rangle > f(\langle x \rangle)$ [24]. All in all, the MPEP is a smooth upslide with a constant speed $v$.

Next we prove that the upslide with $v = -F$ (where $F = -dV/dx$, i.e. the reverse of the deterministic downslide, is the most probable. Minimizing

$$\sum_{j=1}^{n} \xi_2^2(t_j) \Delta t = \sum (\dot{x} - F)^2 \Delta t,$$

we take the right hand side and treat it as an integral:

$$S = \int_{t=0}^{T} (\dot{x} - F)^2 dt,$$

where $t = 0$ represents the instant at which the trajectory starts and $t = T$ is when the top is reached. Going from $x = 0$ to $x = 1$ we have $\dot{x} = v$ and $v$ needs to be positive. With $T = 1/v$ we now minimize

$$S = \int_{t=0}^{1/v} (v - F)^2 dt = v - 2F + F^2/v.$$

Differentiating w.r.t. $v$ and setting the derivative equal to zero, we find that the minimum for $S$ occurs when $v^2 = F^2$. The positive solution (note that $F$ is negative on (0,1)) is $v = -F$.

Figure 2a shows this most probable path in phase space. For microscopic reversibility to be true, there should be just as much traffic at speed $v = -F$ from $x = 0$ to $x = 1$ as that there is from $x = 1$ to $x = 0$. It is obvious that the most probable downslide is the deterministic one. After all, $\xi = 0$ is the most likely Brownian kick size. The downward $v = F$ (the green dotted arrow) and the upward $v = -F$ (red arrow) thus form a “microscopic reversibility pair.”

Next we determine the MPEP for Lévy noise, i.e. when $\alpha < 2$ in Eqs. (1) and (2). Moving up the barrier is a rare event that requires kicks from the power-law tail, $p_\alpha(\xi) \propto (1/|\xi|)^{1+\alpha}$, of the distribution. For the probability of moving up the barrier with a certain sequence of $n$ kicks, we next write down

$$\mathcal{P} \propto \prod_{j=1}^{n} \frac{1}{|\xi_\alpha(t_j)|}.$$
for any shape potential. However, presently there are no meaningful Lévy-noise-equivalents of Eqs. (5-7).

For symmetric Lévy noise the most probable kicksize is given by the modal value of the corresponding probability density function, i.e. \( \xi_0 = 0 \). In this it does not differ from the Gaussian-noise case. This implies that, for both Gaussian noise and for Lévy noise, the most probable path down the slopes in Fig. 1 is a deterministic downslide, i.e. a trajectory described by \( \dot{x} = -dv/dx \).

Putting together all the results that we have obtained above, we find, first of all, that microscopic reversibility applies for Gaussian noise. Figure 2a shows how the most probable 0-to-2 path is the exact time reverse of the most probable 2-to-0 path.

For Lévy noise, however, microscopic reversibility is broken. The most likely trajectory over the barrier is one where the upside has a speed \( v = 1/\Delta t \) as the unit interval is traversed in one single timestep. The downslide is again a deterministic one with a speed \( v = |F| \). Figure 2b shows how the two most probable paths do not fall along the same curve!

Lewis’ idea of forward and backward played movies is instructive here. With Gaussian noise it is obvious that a backward-played movie of the most probably path leading from 0 to 2 is indistinguishable from a forward-played movie of the most probable path from 2 to 0. The same constant speed is observed. With Lévy noise, on the other hand, the 0-to-2, backward-played movie looks very different from the 2-to-0 forward-played movie. The forward played movie has the fast part first and the slow part second. For the backward played movie it is the other way round.

Different authors have observed, discussed and studied how, for Brownian motion, nonequilibrium can give rise to rotational flows or “Brownian vortexes” [5, 29-31]. Such cycling implies a production of entropy. Figure 2b shows how, in our case, LFs lead to the presence of Lévy vortexes in the phase plane. The divergence-free flow in our phase plane could, in principle, be associated with the curl of a vector potential \( \mathbf{A} \), i.e. \( \mathbf{J} = \nabla \times \mathbf{A} \). It is a future research challenge to more explicitly relate LFs to cyclic phase-space flow and a vector potential \( \mathbf{A} \) that describes Lévy vortexes.

Lévy Noise Inside a Parabolic Potential. – The example in this section is to illustrate that it is not just in piecewise linear potentials that Lévy noise leads to breaking of microscopic reversibility and formation of Lévy vortexes. With a different mathematical formalism we show below how, within a quadratic potential \( V(x) = x^2/2 \), the same phenomena occur. A quadratic potential can be considered generic as it generally describes the lowest order behavior around a minimum in a continuous potential.

For the Brownian particle inside the quadratic potential we have after appropriate scaling:

\[
\dot{x} = -x + \xi_\alpha(t). \tag{11}
\]

The corresponding Fractional Fokker-Planck Equation [32] reads:

\[
\partial_t p(x,t|x_0) = \partial_x^\alpha p(x,t|x_0) + \partial_x (xp(x,t|x_0)), \tag{12}
\]

where \( x(t = 0) = x_0 \) and the time evolution after \( t \) is considered. The function \( p(x,t|x_0) \) represents the probability density for a particle to be at position \( x \) at time \( t \), given that it is at \( x = x_0 \) at \( t = 0 \). In Eq. (12) the superscript \( \alpha \) denotes the taking of a fractional Riesz derivative. Equation (12) is readily solved in Fourier space:

\[
\hat{p}(k,t|x_0) = \exp[ik\mu(t) - |k|^\alpha \sigma(t)], \tag{13}
\]

where \( \mu(t) = x_0e^{-t} \) and \( \sigma(t) = [(1 - e^{-\alpha t})]/\alpha \). From there we find for the solution of Eq. (12):

\[
p(x,t|x_0) = \frac{1}{\Gamma(\alpha)} \rho_{\alpha} \left( \frac{x - \mu(t)}{\sigma(t)} \right). \tag{14}
\]

We denote the stationary state as \( p_s(x) = \lim_{t \to \infty} p(x,t|x_0) \).

We next focus on \( \alpha = 1 \). In that case the alpha-stable distribution is the simple and well-known Cauchy distribution: \( p_1(x) = [\pi (1 + x^2)]^{-1/2} \). We define three regions on the parabolic potential as in Fig. 3. Region A is a small neighborhood around \( x = 0 \): \( A = [-a,a] \). Region C constitutes the outer edges of the parabola: \( C = (-\infty,-c) \cup [c,\infty) \). Region B is made up of the intervals in between: \( B = \mathbb{R} \setminus (A \cup C) \). For the net amount of probability that flows from region A to region C in time \( \Delta t \) we have:

\[
\Delta P_{A \to C}(\Delta t) = P(X_{\Delta t} \in C; X_0 \in A) - P(X_{\Delta t} \in A; X_0 \in C). \tag{15}
\]

Here \( X_0 \) is taken from the stationary distribution. With the expression for the Cauchy distribution, the joint probability is readily evaluated:

\[
P(X_{\Delta t} \in C; X_0 \in A) = \int_C \int_A p(x,\Delta t|x_0)p_s(x_0)dx_0dx
\]
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Fig. 3: We consider a particle subjected to Lévy noise inside this parabolic potential, cf. Eqs. (11-13). We define the three regions A (solid), B (dashed), and C (dotted). In the text it is derived how microscopic reversibility is violated and how vortex behavior emerges: particles “shoot up” from A to C in a short time and take a longer time to slide back to A.

\[
= \int_{x \in C} dx \int_{y \in A} dy \frac{1}{(1 - e^{-\Delta t})^2 + (x - ye^{-\Delta t})^2} \frac{1}{1 + y^2}.
\]

It is now straightforward to derive that we have at first order in \(\Delta t\):

\[
\Delta P_{A \rightarrow C}(\Delta t) \approx \frac{4}{\pi^2} \left( \int_0^a dy \frac{a}{1 + y^2} \frac{c}{c^2 - y^2} - \int_0^\infty dy \frac{a}{1 + y^2} \frac{1}{a^2 - y^2} \right) \Delta t.
\]

Expanding for small \(a\), a concise expression is found:

\[
\Delta P_{A \rightarrow C}(\Delta t) = \frac{4a\Delta t}{\pi^2} \arctan \left( \frac{1}{c} \right) + \text{higher order in } a, \Delta t.
\]

For a stationary state, i.e. \(t \rightarrow \infty\), there should be constant probabilities, \(p(A)\), \(p(B)\), and \(p(C)\), to be in the regions A, B, and C, respectively. What the above derivation shows is the following. Consider traffic between region A and C and look at how fast the intermediate segment B is traversed. It appears that microscopic reversibility is broken as the segment B is traversed faster on the way up than on the way down. For a small \(\Delta t\), upward trajectories that are completed within \(\Delta t\) are more common than downward trajectories. Had there been microscopic reversibility, the expression for \(\Delta P_{A \rightarrow C}(\Delta t)\) (cf. Eqs. 15 and 16) would have yielded zero at all orders.

In other words, particles in a parabolic potential that are subjected to alpha-distributed noise “shoot up and slide down.” Lewis explained flow on an energy landscape by comparing it to traffic between cities [1]. Carrying on this analogy, we can compare the flow in the parabolic potential with traffic from A to C being by airplane and traffic from C to A by car.

**Thermodynamic Consequences.** – For a two-state system, steady state and detailed balance are the same thing. But with three states they may be different. To explore possible steady-state circular flow, we thus consider the setup in Fig. 4, where A, B, and C indicate three states along a circular track. If the slopes are not symmetric, then we have a ratchet potential. It has been shown that net flow occurs for an overdamped particle in such a ratchet potential if Lévy noise with \(\alpha \neq 2\) is present [33–35]. Both microscopic reversibility and detailed balance are violated in that case. However, when the slopes are symmetric, there is no way to geometrically discriminate between the two directions. If the applied Lévy noise is also symmetric, then Curie’s Principle forbids net rotation. This implies that detailed balance is maintained among the states A, B, and C in Fig. 4. But following the analysis associated with Figs. 1 and 2, we see that microscopic reversibility is violated! Imagine again a movie of the system. In a forward played movie it is observed that the most likely trajectory that brings the particle from one state to another covers the first half of that trajectory fast and the second half slow. For a backward played movie it is the other way round. Of course, for Gaussian white noise the most likely state-transition-trajectories have constant speed again. Time-reversal symmetry and microscopic reversibility are preserved in the Gaussian case. But this example shows how, with LFs, it is possible to break microscopic reversibility (and thereby time reversal symmetry), while preserving detailed balance.

Fig. 4: Three states along a circular track. The two spatial directions are indistinguishable. The applied Lévy noise is also symmetric. In the text it is explained how detailed balance is preserved while time reversal symmetry and microscopic reversibility are violated for the most likely trajectories going from one state to another.

Biophysicists have long been curious about to what extent microscopic reversibility applies to the activities of biomolecules. With the development of the patch clamp technique, about three decades ago, researchers acquired the ability to follow the opening and closing of an individual ion channel. From there it is relatively straightforward to compare forward and backward open-and-closed records and see whether they follow the same statistics. Doing such analyses, both compliance with microscopic reversibility and detailed balance are violated in that case. However, when the slopes are symmetric, there is no way to geometrically discriminate between the two directions. If the applied Lévy noise is also symmetric, then Curie’s Principle forbids net rotation. This implies that detailed balance is maintained among the states A, B, and C in Fig. 4. But following the analysis associated with Figs. 1 and 2, we see that microscopic reversibility is violated! Imagine again a movie of the system. In a forward played movie it is observed that the most likely trajectory that brings the particle from one state to another covers the first half of that trajectory fast and the second half slow. For a backward played movie it is the other way round. Of course, for Gaussian white noise the most likely state-transition-trajectories have constant speed again. Time-reversal symmetry and microscopic reversibility are preserved in the Gaussian case. But this example shows how, with LFs, it is possible to break microscopic reversibility (and thereby time reversal symmetry), while preserving detailed balance.
intense as the thermal, equilibrium part [39]. The mechanisms pointed out in this Letter may therefore be relevant for the behavior of ion channels.

Mechanical noise in a living cell has only recently become experimentally accessible. But it has quickly become obvious that cytoplasmic mechanical activity is far from equilibrium and that the total noise intensity far exceeds the basic thermal kT-level [40, 41]. With small probes it has furthermore been found that the large fluctuations that are typical for Lévy statistics occur in both cytoskeletal networks and surrounding cytoplasmic fluid [42, 43].

All in all, we may conclude that when microscopic reversibility is turned into a central principle for molecular machines [44], phenomena may remain unexplained and nanoengineering opportunities may be passed up [45].

With LFs the concepts of thermalization and equilibrium need be addressed with much care [46, 47]. Langevin equations driven by Lévy white noises lead to non-Gibbsian distributions. Furthermore, Lévy noise has infinite variance and so there is no fluctuation-dissipation relation to connect the variance of the noise to the strength of the friction. In this Letter an analytic connection was made between the noise statistics and the ensuing statistical mechanics in a nonequilibrium regime. Our results are for simple potentials, but further extension and generalization should be possible.

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