**Intrinsic ratchets**

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Abstract – We present analytic expressions for the drift behaviour of Brownian particles with intrinsic asymmetry in unbiased time-dependent force fields, derived from a generic formalism. Our findings are supported by molecular dynamics simulations.

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**Introduction.** – In view of their potential applications in bio- and nano-technology, Brownian motors have in recent years been the object of intensive research [1–4]. As is well known, the rectification of the thermal motion of Brownian particles involves the breaking of underlying symmetries. On the one hand, the system has to operate under nonequilibrium conditions to break the microscopic equilibrium symmetry of detailed balance. Spatial symmetry on the other hand is usually broken by applying asymmetric external forcing. The two most cited paradigms in this context are the flashing and rocking ratchets (see, e.g., [3] and references therein), in which an external space-periodic but space-asymmetric forcing using a ratchet-like potential is applied.

Unlike in these “traditional” ratchet models, the spatial asymmetry alternatively may be provided by an internal asymmetry of the Brownian particle itself. This scenario has recently been illustrated by employing an internal degree of freedom that couples asymmetrically to (symmetric) external forcings [5] or that is exposed to asymmetric friction [6–8]. In this letter, we will go one step further and consider the case in which the particle’s asymmetry does not rely on some interaction with the environment but is an inherent property of the Brownian particle. We will refer to such Brownian motors as intrinsic ratchets. We will introduce and solve the equations of motion that generically describe this type of thermal rectification.

Note that the nonlinear rectification of Brownian motion discussed here should be distinguished from work on motility of active Brownian particles which actively create and maintain an asymmetric environment (typically by means of some chemical reaction) in order to drive their directed motion [9,10].

**Generic equations of motion.** – The motion of a Brownian particle (speed \(v\) and mass \(M\)) is usually described by the following Langevin-Newton equation:

\[
M \frac{dv}{dt} = -\gamma v + F + \xi.
\]

Here \(\gamma\) is the friction coefficient, \(F\) is an applied external force and \(\xi\) a Gaussian white noise, whose intensity is determined by the fluctuation-dissipation relation. The above equation can be derived from a microscopic description by assuming that the mass of the Brownian particle is much larger than that of surrounding particles. It forms the starting point for deriving the properties of flashing or rocking ratchets. In fact, since one needs to apply spatially asymmetric forcing in these systems, the analysis is typically carried out at the simpler level of overdamped motion. The latter provides a closed description in terms of the position variable only and is known to be a very good approximation in most situations. As we will see below, we however do not need spatially dependent forcing for the rectification in intrinsic ratchets. This greatly simplifies the analysis, even at the underdamped level. Indeed, when the forcing \(F\) is position independent, the stochastic variable \(v\) is Gaussian, and it suffices to study the equations of motion for the first two moments of the velocity. By choosing as units of time, velocity and force the relaxation time \(\tau_r = M/\gamma\), the thermal speed \(v_T = \sqrt{k_B T/M}\) and \(\gamma v_T\) (where \(k_B\) is Boltzmann’s constant and \(T\) is the...
temperature of the bath particles), the following equations are obtained for the moments $v_1 = \langle v \rangle$ and $v_2 = \langle v^2 \rangle - 1$:

\[
\frac{dv_1}{dt} = -v_1 + f, \\
\frac{dv_2}{dt} = -2v_2 + 2fv_1.
\]  

(2)

We now argue that a minor modification of these equations describes the case of intrinsic ratchets. We first note that the possible asymmetry of the Brownian particle does not appear in the above equations, basically because the relaxation is described by linear response. As a result, the equation for the first moment, which is the central object of interest, is not coupled to the second moment. The asymmetry of the particle will appear at a next order of perturbation, at the level of nonlinear relaxation. Furthermore, the resulting correction appearing in the equation for $v_1$ still has to vanish when operating under equilibrium conditions, i.e., when $v_2 = 0$. The simplest analytical correction is thus a term of the form $\alpha v_2$, where the constant $\alpha$ quantifies the strength of the asymmetry. Since this term acts as a perturbation on the first moment, we can dismiss, to lowest order, the correction that will appear in the equation for $v_2$. The intrinsic ratchet is thus described at lowest order (with $\alpha$ effectively playing the role of a small dimensionless parameter) by the following generic set of equations:

\[
\frac{dv_1}{dt} = -v_1 + \alpha v_2 + f, \\
\frac{dv_2}{dt} = -2v_2 + 2fv_1.
\]  

(3)

In addition to the above handwaving arguments, we note that the equations of motion given in eq. (3) can be derived from microscopic theory of a Brownian particle moving in a bath of an ideal gas, by an expansion in the ratio of the mass of the gas particles ($m$) over the mass of the Brownian particle ($M$) [11–13]. Such a derivation also provides explicit expressions for the open parameters $\alpha$ and $\gamma$ (or $\tau_r$) behind eq. (3) in terms of microscopic quantities. Concrete examples for the cases of translational and rotational motion of an asymmetric object suspended in a thermalized gas will be given below.

In the remainder of this letter, we focus on the rectification, i.e., the appearance of a nonzero average drift velocity, when the particle is subjected to an unbiased time-periodic force $f(t)$. This scenario is the analogue of the rocking ratchet for particles with intrinsic asymmetry.

**Piecewise constant forcing.** – Equation (3) with time-periodic forcing $f(t)$ has a mathematical structure similar to the Newton equation of motion for a parametric oscillator. It is therefore out of the question to find a general analytical solution. Instead we turn to the case of piecewise constant forcing (square wave profile), viz.,

\[
0 \leq t < \tau/2: \quad f(t) = f_0, \\
t \leq \tau/2 < \tau: \quad f(t) = -f_0.
\]  

(4)

Introducing the vector notation

\[
V(t) = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}(t),
\]  

(5)

one readily finds the solutions in the separate time regimes, with $f = f_0$ and $f = -f_0$, respectively,

\[
V_+(t) = A_+(t)C_+ + B_+,
\]  

(6)

\[
V_-(t) = A_-(t)C_- + B_-.
\]  

(7)

The time propagators $A_\pm$ are given by

\[
A_\pm(t) = \left[ \frac{\pm 1 + d_{\pm} - e^{-3(3\pm d_{\pm})\tau/2}}{2} \right],
\]  

(8)

with $d_{\pm} = \sqrt{1 \pm 8\alpha f_0}$. $B_\pm$ are the steady-state solutions:

\[
B_\pm = \frac{f_0/\pm(1 \pm \alpha f_0)}{f_0^2/\pm(1 \pm \alpha f_0)}.
\]  

(9)

The vector constants $C_\pm$ are specified by the assumption that we operate in the steady-state regime, hence the velocity moments in eqs. (6) and (7) satisfy time-periodic boundary conditions, $V_+(0) = V_-(\tau)$. This, together with continuity at $t = \tau/2$, $V_+(\tau/2) = V_-(\tau/2)$, leads to a solution,

\[
C_+ = \left( A_2^{-1} A_1 - A_4^{-1} A_3 \right)^{-1} \left( A_2^{-1} - A_4^{-1} \right) (B_+ - B_-),
\]  

(10)

\[
C_- = \left( A_2^{-1} A_1 - A_3^{-1} A_4 \right)^{-1} \left( A_1^{-1} - A_3^{-1} \right) (B_+ - B_-),
\]  

(11)

with $A_1 = A_+(\tau/2)$, $A_2 = A_-(\tau/2)$, $A_3 = A_+(0)$, $A_4 = A_-(\tau)$. We will not reproduce here the resulting expression for the time-dependent average speed $v_1$. It is extremely cumbersome, and, strictly speaking, only valid to the lowest order in the asymmetry contribution $\alpha$. For an illustration of the typical time dependence of $v_1$, we refer to fig. 1.

We remark that our theory yields accurate results when $\alpha f_0 \ll 1$. Under the described ratchet operation, the speed $v_1$ and second moment $v_2$ are then of order $f_0$ and $f_0^2$, respectively. This means that the nonlinear correction term $\alpha v_2$ in the equations of motion (eq. (3)) is a factor $\alpha f_0$ smaller than the linear $v_1$ term.

The quantity of central interest is the resulting time-average net speed, being the average net displacement over a period $\tau$ divided by this period:

\[
v_{\text{net}} = \tau^{-1} \int_0^\tau v_1(t) dt.
\]  

(12)

Again, the exact expression for $v_{\text{net}}$ is extremely long. In any case, our approach is limited to small $\alpha$, so it suffices
the particle’s mass.

Fig. 1: (Colour on-line) Time evolution of (a) the first moment of the velocity $v_1$ (in thermal speed $v_T$ units) for the periodic forcings in (b) (correspondence by line style). For harmonic and symmetric sawtooth profiles, the first-order approximation (eq. (14)) is used. For square modulation, the full analytical solution is shown. In all three cases, a numerical solution of the dynamic equation is indistinguishable from the analytical results in the graph. Parameter values are period $\tau = 4$, force amplitude $f_0 = 0.4$ and asymmetry $\alpha = 0.3$. Unit of time is the particle’s relaxation time $\tau_r$, unit of force is $Mv_T/\tau_r$, with $M$ the particle’s mass.

to reproduce the lowest-order term in $\alpha$:

$$v_{\text{net}} \simeq \alpha f_0^2 \left(1 - \frac{4}{\tau} \tanh \frac{\tau}{4}\right). \tag{13}$$

We note that the next term in the expansion in $\alpha$ is an order of magnitude $(\alpha f_0)^2$ smaller.

We make the following observations. First, there is no directed motion, $v_{\text{net}} = 0$, in the absence of forcings, $f_0 = 0$, or when the particle has intrinsic symmetry, $\alpha = 0$. Second, $v_{\text{net}}$ is an uneven function of $\alpha$, hence an inversion of the asymmetry, $\alpha \rightarrow -\alpha$, results in an inversion of the speed of net motion. We represent $v_{\text{net}}$ as a function of the asymmetry, $\alpha$, the amplitude of the force, $f_0$, and the period, $\tau$, in fig. 2 (solid curves). In all three cases, the lowest-order approximation, eq. (13), is in fact indistinguishable from the exact result for the chosen range of values of $\alpha$ and $f_0$. Finally, we note that the maximum speed $v_{\text{net}}^{\text{max}} \simeq \alpha f_0^2$ is reached in the limit of very slow modulation, $\tau \rightarrow \infty$. Since this speed is expressed in units of thermal velocity, we conclude that one can reach high net drift speeds, comparable to thermal speeds, by applying unbiased periodic forcing of small to moderate intensity to intrinsic ratchets.

Other periodic forcings. – To investigate the effect of other types of periodic forcing, such as harmonic or symmetric sawtooth (cf. fig. 1(b)), we resort to a perturbational solution of eq. (3). As the contribution due to the intrinsic asymmetry $\alpha$ is considered small, we can make the following first-order ansatz for the velocity moments:

$$v_1 = v_{1,0} + \alpha v_{1,1}, \tag{14}$$
$$v_2 = v_{2,0} + \alpha v_{2,1}. \tag{15}$$

With this ansatz, eq. (3) can be solved to first order in $\alpha$ for arbitrary periodic force fields $f(t)$, yielding the

steady-state solutions

$$v_{1,0}(t) = \int_{-\infty}^{t} dt' e^{-(t-t')} f(t'), \tag{16}$$
$$v_{2,0}(t) = \int_{-\infty}^{t} dt' e^{-(2(t-t'))} 2 f(t') v_{1,0}(t'), \tag{17}$$
$$v_{1,1}(t) = \int_{-\infty}^{t} dt' e^{-(t-t')} v_{2,0}(t'), \tag{18}$$
$$v_{2,1}(t) = \int_{-\infty}^{t} dt' e^{-(2(t-t'))} 2 f(t') v_{1,1}(t'). \tag{19}$$

Using $f(t + \tau) = f(t)$, it is easy to show that these expressions are indeed periodic with periodicity $\tau$. The results for the time evolution of the first moment $v_1$ under harmonic or sawtooth forcing are reproduced in fig. 1(a); they are indistinguishable from numerically integrated solutions of the original eq. (3). For comparison, the results for the square wave profile are also included.
With regard to the net velocity $v_{\text{net}}$ as defined in eq. (12), we observe that for unbiased symmetric forcings $f(t + \pi/2) = -f(t)$, and thus $\int_0^\tau dt' v_{1,0}(t') = 0$ (see eq. (16)), so that $v_{\text{net}}$ is given by

$$v_{\text{net}} = \alpha \tau^{-1} \int_0^\tau dt' v_{1,1}(t').$$

(20)

Again, $v_{\text{net}}$ is zero when $\alpha = 0$, consistent with the notion that no directed motion occurs for symmetrical particles.

It is straightforward to recover the net velocity for square forcing to lowest order in $\alpha$, eq. (13), from (20). Similarly, for harmonic driving, $f(t) = f_0 \sin(2\pi t/\tau)$, we find a time-average net velocity

$$v_{\text{net}} = \frac{\alpha f_0^2}{2} \frac{\tau^2}{4\pi^2 + \tau^2}.$$  

(21)

For sawtooth forcing,

$$0 \leq t < \tau/2 : \quad f(t) = f_0 (t - \tau/4)/(\tau/4),$$

$$t \leq \tau/2 \leq \tau : \quad f(t) = f_0 (3\tau/4 - t)/(\tau/4),$$

(22)

a net speed

$$v_{\text{net}} = \frac{\alpha f_0^2}{3} \left[ 1 - 3 \left( \frac{4}{\tau} \right)^2 + 3 \left( \frac{4}{\tau} \right)^3 \tanh \frac{\tau}{4} \right]$$

(23)

is obtained. These first-order results for the net velocity $v_{\text{net}}$ are compared with the analytical solution for square forcing in fig. 2 (dashed curves). We conclude that the resulting drift behaviour is very similar in all three cases. In fact, comparing eqs. (13), (21) and (23), we see that the differences become very small, and even vanish for slow forcing $\tau \to \infty$, if, instead of using the same amplitude for the three modulations, one considers the same average quadratic amplitude, i.e., if one replaces $f_0/\sqrt{2} \to f_0$ in eq. (21) and $f_0/\sqrt{3} \to f_0$ in eq. (23).

**Microscopic models.** As already mentioned, the structure of eq. (3) can be obtained from kinetic theory of microscopic models, that describe a small, nontrivially shaped object (mass $M$) moving under the influence of collisions with a surrounding bath of gas particles (mass $m$), by an expansion in the mass ratio $\varepsilon = \sqrt{m/M}$ [11–13]. Such a procedure also provides explicit expressions for the parameters $\tau_r$ and $\alpha$ of the intrinsic ratchet.

For a three-dimensional asymmetric object of arbitrary convex shape, that is confined to move along a fixed $z$-axis (translational motion), one obtains [13]

$$\tau_r = \varepsilon^{-2} \sigma_2^{-1},$$

(24)

$$\alpha = \sqrt{\pi/8} \varepsilon^3 \tau_r \sigma_3,$$

(25)

where the geometry-dependent moments $\sigma_n$ are given by

$$\sigma_n = \rho \sqrt{\frac{8k_B T}{\pi m}} \int_S dS \langle -\vec{e}_\perp | z \rangle^n,$$

(26)

with $\rho$ being the particle density of the gas, and where the integral is over the surface of the asymmetric object. $\vec{e}_\perp | z$ is the component in the free direction of motion ($z$) of the outward unit normal vector $\vec{e}_\perp$ at its surface. A similar shape-dependent parameter was discussed in [9] for the self-driven motility of active Brownian particles.

To get an idea of the actual net velocity that a realistic setup of an intrinsic ratchet can attain, we use eqs. (13), (24)–(26) to calculate the speed for a cone-shaped silica ($\text{SiO}_2$) Brownian particle with half opening angle $30^\circ$ and $10\text{nm}$ base diameter (see fig. 3(a) for a schematic representation). The cone’s axis is along the free direction of motion. In air, the ratio $M/m$ is about 10000 and the asymmetry parameter is $\alpha = 0.003$. At temperature $T = 300\text{K}$, the relaxation time is $\tau_r = 7.5\text{ns}$. An amplitude $f_0 = 10\text{ of unbiased square forcing then corresponds to 1.9}\text{pN}$ in real units and is well within the accuracy range of our theory: $\alpha f_0 = 0.03$. These conditions produce a maximum speed of $v_{\text{lim}} = 0.88\text{m/s}$ or $30\%$ of the thermal speed of the particle. Note that the direction of the particle’s motion is towards the apex of the cone.

**Rotational Brownian motion.** For simplicity of presentation, we started with the generic equations of motion for one-dimensional translational Brownian motion of an asymmetric particle. In practice, this supposes that the particle is constrained to move on a track. The so-far presented discussion of the intrinsic ratchet can however be repeated, with minor modifications, for the rotational Brownian motion of chiral objects, with angular velocity $\omega$ and moment of inertia $I$.

With an adaptation of the expressions for the relaxation time $\tau_r = I/\gamma$ and the thermal velocity $v_T = \sqrt{k_B T/I}$ as units of time and angular velocity, respectively, and now signifying a torque, this leads to the same generic equations of motion (eq. (3)) for the moments $\omega_1 = \langle \omega \rangle$ and $\omega_2 = \langle \omega^2 \rangle - 1$. Microscopic theory [14] yields the same expressions for the relaxation time $\tau_r$ (eq. (24)) and asymmetry coefficient (eq. (25)), but now with geometrical moments given by

$$\sigma_n = \rho \sqrt{\frac{8k_B T}{\pi m}} \int_S dS \langle (\vec{e}_\perp \times \vec{e}_\perp) | z \rangle^n,$$

(27)
where the axis of rotation is taken to be parallel to the $z$-axis. Again, the integral is over the surface of the object and $\vec{e}_\perp$ is the outward unit normal vector on the surface. $\vec{r}$ is given by $\vec{r}/r_0$, with $\vec{r}$ denoting the position of a surface element measured from the axis of rotation (the $z$-component in $\vec{r}$ is irrelevant), and $r_0 = \sqrt{I/M}$ being the radius of gyration of the object.

Due to the chosen orientation of the rotation axis, only the $z$-component of $\vec{e}_\perp \times \vec{e}_\parallel$ appears in the expression for $\sigma_n$. With these new notations and units, the previous results, in particular the expressions for the time-average net velocity (eqs. (13), (21), (23)), remain valid.

In view of the technological potential of the rotational setup, and in order to get an idea of the order of magnitudes involved, we again consider a realistic physical realization. A silica triangular prism of height 10 nm and with right triangular top and bottom surfaces (sides: 10 nm, 10 nm, 14 nm) is connected with a rotation axis at one of its vertical edges, cf. fig. 3(b). Operating in air, the ratio $M/m$ is about 23000. If the axis is connected to the 90° corner edge, $\alpha=0$ and no rectification or net rotation will occur. Connected to the 45° corner edges, $\alpha = \pm 0.0016$ and relaxation time is $\tau_r = 8.1$ ns, at air temperature $T = 300$ K. A torque amplitude (for square forcing) of $f_0 = 10$ corresponds to $2.2 \times 10^{-20}$ Nm and produces a maximum net rotation frequency of 6 MHz, 16% of the thermal frequency.

**Molecular-dynamics simulations.** – In the following, we verify our generic theory for the intrinsic ratchet with molecular-dynamics simulations. As concrete microscopic system, we consider the prism from fig. 3(b) surrounded by a thermalized bath of ideal gas particles, and perform event-driven simulations of its rotational Brownian motion. The rotation axis is chosen to be located slightly (4 nm in the units of fig. 3(b)) outside the prism in the plane given by one of the prism surfaces merging at the 90° edge, and is oriented parallel to this edge.

Exploiting the homogeneity of the prism along the direction of the rotation axis, the simulations are carried out in a (projected) two-dimensional space, where the ratchet object is given by the right triangular top (or bottom) surface of the prism, and where the rotation axis is reduced to a point-like centre of rotation. The rotation centre is positioned at the centre of a quadratic box, containing an ideal gas of point particles (mass $m$). The box walls “absorb” gas particles upon collision, but also randomly “emit” new particles (into the box’ interior) such that the gas properties, in particular density $\rho$ and Maxwellian equilibrium distribution, are preserved. In this way, an infinitely large reservoir of gas particles is realized.

Collisions between gas particles and the triangle are detected by numerically solving the exact equations of motion for the point in time of the impact. At each collision, the speed of the gas particle and the rotational velocity of the triangle are changed according to the rules for elastic collisions, neglecting tangential forces [14]. In between collisions, the triangle is accelerated by an external periodically switching torque (square profile).

In fig. 4, the net rotational speed of the triangle under the action of a periodically switching torque is shown for different values of the modulation period $\tau$. The agreement between simulation results for the time-average net velocity $v_{\text{net}}$ and theory, eq. (13), is excellent. We also compared the asymptotic rotation of the triangle under constant but opposite torques (“infinite” driving period $\tau$) with the theoretical result, eq. (9), and again found excellent agreement.

**Stop-and-go motor.** – We finally discuss an alternative approach to intrinsic ratchets, anticipated in [15] and further worked out in more detail in [16]. The so-called stop-and-go motor consists of an asymmetric particle which is periodically stopped, for example by an array of traps or binding sites that can be activated or deactivated at will. The basic assumption is that the (thermal) energy of the Brownian particle is changed when it is subjected to the trapping mechanism. This energy exchange results in a specific value of the second velocity moment at the stopping sites, $v_{2,s}$. For $v_{2,s} \neq 0$, the energy exchange in the traps induces a deviation from thermal equilibrium conditions, and this process will result in sustained directed motion with an average net speed $v_{\text{net}}$, being the average distance travelled by the particle in a time interval $\tau_s$ between the stopping events, divided by $\tau_s$.  

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Fig. 5: (Colour on-line) Main figure: average (angular) net velocity $v_{\text{net}}$ of the rotating stop-and-go ratchet as a function of the time interval $\tau_0$ between stopping events. In the trapping mechanism, the second moment is set to $v_{2,s} = 1$ (upper curve), $v_{2,s} = -1$ (lower curve), with $v_2 = \langle \omega^2 \rangle - 1$. Insets: maximal average net velocity $v_{\text{net}}$ (for optimal $\tau_0$) as a function of the second moment of the velocity $v_{2,s}$ in the trap. Lines correspond to theory, dots represent results from molecular dynamics simulations, using the same setup as for fig. 4 (but without external torque). The net speed is obtained from simulating 1000 independent stopping intervals $\tau_0$ per realization and averaging over 10000 realizations for the three smallest stopping intervals and over 5000 realizations otherwise. Shown angular velocity is in units of thermal speed $v_\tau = \sqrt{k_B T / \ell}$ and time in units of relaxation time $\tau_\ell$. The asymmetry parameter is $\alpha = 0.0233$.

A simple analytical calculation, starting from eq. (3) with $f = 0$, gives an exact expression:

$$v_{\text{net}} = \frac{\alpha v_2}{2 \tau_0} \left( 1 - e^{-\tau_0} \right)^2. \quad (28)$$

The sense of motion is determined by the sign of $\alpha$ and of $v_{2,s}$, which is negative (positive) when the particle’s thermal motion is reduced (enhanced) by the trapping mechanism. A stopping interval $\tau_0^* \simeq 1.26$, given by the solution of $e^{\tau_0^*} = 2 \tau_0^* + 1$, yields a maximum net velocity ($v_{\text{net}}^{\text{max}} \simeq 0.204 \alpha v_{2,s}$) and an optimal distance between binding sites ($\simeq 0.256 \alpha v_{2,s}$, expressed in units $v_\tau \tau_\ell$).

These theoretical predictions are confirmed in a molecular dynamics simulation of the stop-and-go mechanism applied to a rotating (chiral) object, using the setup based on the prism in fig. 3(b), as in the previous section. In fig. 5, the resulting average net velocity $v_{\text{net}}$ as a function of different stop intervals $\tau_0$, for the values $v_{2,s} = -1$ and $1$ is shown. In the insets of fig. 5, we include the molecular dynamics results for $v_{\text{net}}$ at the optimal stopping interval as a function of $v_{2,s}$. The linear relation ($v_{\text{net}}^{\text{max}} = 0.204 \alpha v_{2,s}$) holds, even for large $v_{2,s}$.

**Conclusion.** – Intrinsic ratchets are characterized by an inherent asymmetry of the Brownian particle itself breaking the spatial symmetry. A generic formalism for the dynamical behaviour enables us to quantify the net particle velocity under unbiased periodic forcing. Molecular dynamics simulations of a rotational setup confirm the validity of this formalism. We predict drift speeds comparable to thermal speeds for nanosized asymmetric Brownian particles under ratchet operation. The relative simplicity of the setup (one heat bath, external symmetric forcing) could open avenues to experimentally test the nonlinear contribution of intrinsic asymmetry crucial in this and other work [11–19].

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