Drift induced by dissipation

Reinaldo García-García,1,2,⋆ Pierre Collet,3, † and Lev Truskinovsky2, ‡

1Laboratoire de Physique Théorique-UMR CNRS Gulliver 7083,
PSL Research University, ESPCI, 10 rue Vauquelin, 75231 Paris cedex 05, France
2PMIH, CNRS UMR 7636, PSL Research University,
ESPCI, 10 rue de Vauquelin, 75231 Paris cedex 05, France
3Centre de Physique Théorique, CNRS UMR 7644 École Polytechnique, 91128 Palaiseau Cedex, France

Active particles have become a subject of intense interest across several disciplines from animal behavior to granular physics. Usually the models of such particles contain an explicit internal driving. Here we propose a model with implicit driving in the sense that the behavior of our particle is fully dissipative at zero temperature but becomes active in the presence of seemingly innocent equilibrium fluctuations. The mechanism of activity is related to the breaking of the gradient structure in the chemo-mechanical coupling. We show that the thermodynamics of such active particles depends crucially on inertia and cannot be correctly captured in the standard Smoluchowski limit. To deal with stall conditions, we generalize the definition of Stokes efficiency, assessing the quality of active force generation. We propose a simple realization of the model in terms of an electric circuit capable of turning fluctuations into a directed current without an explicit source of voltage.

Motile cells, living bacteria, synthetic swimmers and ‘walking’ grains are usually modeled as Active Brownian Particles (ABP) [1–4]. While it is clear that to achieve persistence, ABPs need to violate fluctuation dissipation theorem and extract energy from the environment, the underlying mechanisms of time reversal symmetry (TRS) breaking at the microscale are known only in few cases [5, 6]. Moreover, even in those cases, the stochastic thermodynamics of macroscopic directional drift is still replete with ‘hidden effects’ and ‘anomalies’ [7–10]. Directionality is usually imposed through the asymmetry of the background potential or the explicit external gradients [11–17], however, it can also arise from velocity-dependent forces [1, 18–23] allowing the effective friction coefficient to be negative [3, 24, 25]. Such forces are then capable of ‘pushing’ the particle and their activity can be interpreted as the presence of ‘anti-dissipation’ at the microscale.

In this Letter we study a more subtle mechanism of directional motility which relies on velocity dependent forces with strictly positive effective viscosity coefficient. Consider, for instance, an inertial dynamics of a particle \( m \dot{v} = F + f \), where \( m \) is the mass of the particle, \( f \) is an external fixed load, \( F = -\dot{\gamma}(v)v \) is a frictional force and \( \dot{\gamma} \geq 0 \) is an effective friction coefficient. At zero temperature this system is clearly dissipative with \( fv \geq 0 \). However, if one exposes the same particle to an equilibrium thermal reservoir writing dynamics in the form

\[ m \dot{v} = F + f + \xi, \]

where \( \langle \xi \rangle = 0 \) and \( \langle \xi(t)\xi(t') \rangle \sim \delta(t - t') \), it may, for particular choices of the function \( \dot{\gamma}(v) \), exhibit ‘anti-dissipative’ behavior with \( f \langle v \rangle \leq 0 \). In particular, such particle can behave as a Brownian motor with a nonzero drift \( \langle v \rangle \) at zero \( f \), apparently induced by dissipation. In this Letter we link this phenomenon with non-potential structure of dissipation and strong violation of detailed balance (DB). We address the nontrivial nature of the overdamped limit in such systems and show that the conventional Smoluchowski-type asymptotics fails to describe adequately the underlying energetics. To assess the efficiency of the new motor in the whole range of parameters, we had to go beyond the conventional definitions and view stall conditions as a regime with functional energy consumption.

To motivate the model we consider an underdamped Brownian particle moving in a fluid under the action of viscous friction and thermal noise. Suppose that the translational dynamics of the particle is additionally coupled to a chemical reaction:

\[
\begin{align*}
    m \dot{v} &= F(v, \Delta \mu) + f + \xi \\
    \dot{\mu} &= A(v, \Delta \mu)
\end{align*}
\]

where \( \langle \xi(t) \rangle = 0 \), and \( \langle \xi(t)\xi(t') \rangle = 2\gamma T\delta_{ij}\delta(t-t') \), \( \gamma \) is the corresponding ‘bare’ viscous coefficient, \( T \) is the temperature of the bath (we set Boltzmann constant equal to one) and \( A \) is the driving force acting on the reaction coordinate \( \zeta \). If chemistry and mechanics are decoupled and the particle is in equilibrium, we have \( F = -\gamma v \) and \( A = \Delta \mu \mu \) where \( \Delta \mu \) is the affinity of the chemical reaction. To break the TRS we assume that the fluxes are related to forces through pseudo-Onsagerian relations [26]

\[
\begin{align*}
    F &= -\gamma v + \lambda \Delta \mu(v/||v||) \\
    A &= -\lambda(v \cdot m) + \Delta \mu
\end{align*}
\]

where the coefficient \( \lambda \) characterizes chemo-mechanical coupling. The unit vector \( m \) indicates a preferred direction associated, for instance, with an external concentration gradient. Note that in (2, 3) the chemical subsystem
acts as a feedback controller for the mechanical degrees of freedom.

To ensure analytical transparency, we assume complete separation of time scales in the sense that the reaction is stationary $\dot{\zeta} = 0$. Then $F = -\gamma [1 - \epsilon (m \cdot v)/\|v\|]v$, where $\epsilon = \lambda^2/\gamma$ is a nondimensional parameter. This form of the friction force highlights the underlying anisotropy in dissipation. A helpful biological reference for this scenario is bacterial flagella whose efficiency for self-propulsion crucially depends on the fact that tangential and normal resistance coefficients are different [27].

Assume now that the vector field $m$ is constant and homogeneous and let us limit our analysis to one dimension. Then we recover our scalar model (1) with $\dot{\gamma}(v) = \gamma [1 + \epsilon \text{sgn}(v)]$, where $\text{sgn}(x)$ is the sign function, see also [28]. Note that $\dot{\gamma}(v) \neq \dot{\gamma}(-v)$ and therefore this model violates TRS even when the system is purely dissipative (for $|\epsilon| < 1$). If we write $F(v) = -\gamma v + g(v)$, where $g(v)$ is the non-linear contribution to friction, a broken TRS implies that $g(v) \neq -g(-v)$, which is, for instance, in stark contrast with the paradigmatic Rayleigh-Helmholtz model of ABP where always $g(v) = -g(-v)$ [19].

To clarify the difference between these two classes of models, assume that $F = -\gamma v + \epsilon g(v)$, where $g(v)$ is arbitrary and $\epsilon > 0$ is a small parameter. Assume for generality that the system is also perturbed spatially so that $m\dot{v} = -\gamma v + \epsilon g(v) + U'(x) + f + \xi$, where $v = \dot{x}$.

We begin by writing our Kramers equation for this system, $\partial_t P = -\nabla \cdot J$, where where $q = (x, v)$, $P(q, t)$ is the probability density and $J = (J_x, J_v)$ is the probability current which can be split in a reversible and a dissipative parts, $J = J_r + J_d$ [29], with $J_r = (v P, \epsilon m^{-1}[g_0(v) - U'(x)]P)$, and $J_d = (0, m^{-1}[\gamma g_0(v) - \gamma v]P - \gamma T m^{-2} \partial_v P)$ [30, 31]. Here we distinguished between the even and the odd contributions to the nonlinear force by defining $g_{r,o} = (g(v) \pm g(-v))/2$.

For the DB condition to be satisfied, we must have $J_d = 0$, which means that $\partial_v \ln P_s = (m/\gamma T)[\gamma g_0(v) - \gamma v]$, where $P_s(v, x)$ is the stationary distribution. This implies that $P_s$ must factorize into the product of a velocity-dependent and position-dependent functions. In the stationary state we must also have $\nabla \cdot J_r = 0$ or

$$\partial_v \ln P_s - \frac{\epsilon}{T} U' = \frac{\epsilon}{T} \left[ g_e - \frac{T \partial_v g_e}{m v} \right] + \frac{\epsilon^2}{\gamma v T} (g_e - U'). \quad (4)$$

Since the r.h.s. of (4) cannot depend on $v$ due to the factorization mentioned above, one must have $g_{r,0} = 0$. Moreover, we see from (4) that for systems with $g_0 = 0$ but $g_o \neq 0$ (Rayleigh-Helmholtz model), the DB condition holds to first order and breaks only at $O(\epsilon^2)$ (i.e., only in presence of a coupling with an external potential [20, 22]). Instead, when $g_o \neq 0$ but $g_0 = 0$, the DB breaks already at the first order in $\epsilon$ and without a need for external interactions. It is then clear that the degree of non-equilibrium in systems with $g_0 \neq 0$ is fundamentally stronger than in systems with $g_0 \neq 0$.

To illustrate the behavior of a system with $g_0 \neq 0$ we make the simplest assumption $g(v) = e \epsilon \text{sgn}(v) v$, which implies, in particular, that $g_0 = 0$. We can then drop the irrelevant potential $U(x)$ and, using dimensionless variables $\hat{v} = v/\sqrt{m/\gamma}$, $\hat{t} = t/\gamma$ and $\hat{f} = (f/\gamma)\sqrt{m/\gamma}$, write the dynamic equation in the form

$$\hat{\dot{\hat{v}}} = -[1 + e \text{sgn}(\hat{v})] \hat{v} + \hat{f} + \hat{\xi}, \quad (5)$$

where now $\langle \hat{\xi}(\hat{t})\hat{\xi}(\hat{t}') \rangle = 2\delta(\hat{t} - \hat{t}')$.

The $\hat{f}$ dependence of the steady-state drift velocity $\hat{v}_s = \langle \hat{v} \rangle$ can be written explicitly [32] and the typical $\hat{v}_s(\hat{f})$ curve, at $0 < \epsilon < 1$, is shown in Fig.1a. In addition to two purely dissipative regimes $\hat{v}_s(\hat{f}) = \hat{f}/(1 \pm \epsilon)$ reached at $\hat{f} \to \pm \infty$ the system also exhibits 'anti-dissipative' behavior at small forces when the particle can carry cargo (to the left, as long as $\epsilon > 0$). A simple expression can be obtained for $\hat{f} = 0$ where the velocity of active drift takes its maximum value

$$\hat{v}_s^m(\epsilon) = \sqrt{\frac{2}{\pi}} \sqrt{1 - \epsilon - \sqrt{1 + \epsilon}} / \sqrt{1 - \epsilon^2} < 0. \quad (6)$$

At $\epsilon \to 0$, we obtain $-\hat{v}_s^m \sim \epsilon$ or, in dimensional variables, $-v_s^m \sim \epsilon \sqrt{T/\gamma m}$. In the presence of cargo, the same scaling can be shown for the active part of the drift $v_s^a = v_s - f/\gamma$, so that again $-v_s^a \sim \epsilon \sqrt{T/\gamma m}$ for small $\epsilon$. This is a hint that in the overdamped regime the active behavior emerges only in the limit when $\epsilon \sim \sqrt{m}$.

The simplicity of the model allows one also to semi-analytically compute the force dependent effective diffusion coefficient $D = \lim_{\tau \to \infty} (\langle \hat{x}^2(\tau) \rangle - \langle (\hat{x}(\tau))^2 \rangle)/(2\tau)$, see...
Note that at $\epsilon \to 1$ the temperature of the ‘hot reservoir’ $T_+$ diverges and the velocity dynamics becomes Brownian for $\dot{v} < 0$. As a result both the average drift velocity and the recrossing time (from negative to positive velocity) diverge and the dynamics becomes critical exhibiting anomalous unidirectional persistence. At large times one can expect excursions into the preferred direction to dominate implying that $\langle \dot{x} \rangle \sim -t^{3/2}$, and $\dot{D} \sim t^2$; the associated transients are illustrated in Fig. 2.

Observe next that in the double limit $\epsilon \to 0, m \to 0$, with $\epsilon = -v_+^* \sqrt{\pi m/2T}$, when the active drift velocity has a finite limit, $v^*_a \to v_+^*$, the (dimensional) active diffusion coefficient $D^a = D - T/\gamma$ disappears with the scaling $D^a \sim \epsilon T/\gamma$. The limiting overdamped dynamics, rigorously justified in [32], takes the form

$$\dot{x} = f/\gamma + v_+^* + \sqrt{2T/\gamma} \xi,$$

which is often postulated in phenomenological models of ABP, e.g. [33]. Note, however, that the effective model (8), being only a weak limit of the original model (5), only reproduces trajectories faithfully while misrepresenting the structure of velocity fluctuations which are of order $\sim \sqrt{T/m}$ by equipartition. This leads to the appearance of the ‘hidden’ terms in the stochastic thermodynamics of such systems, e.g. [10, 34].

To elucidate this issue we now reintroduce dimensional variables and consider the energetics of a slightly more general model than (5):

$$m\dot{v} = -\gamma v + g_e + f + \xi,$$

where the even function $g_e(v)$ is arbitrary. The energy balance along a particular trajectory of duration $\tau$ can be derived by multiplying (9) by $v$ and integrating over time. It reads $E_\tau = U_\tau + W_\tau - Q_\tau$. Here $E_\tau = \langle m/2 \rangle \langle v^2(\tau) - v^2(0) \rangle$ is the change in kinetic energy of the particle, $U_\tau = \int_0^\tau dt g_\tau(v)$ is the active work performed on the particle, $W_\tau = -\int_0^\tau dt v$ is the work against the load, and $Q_\tau = \int_0^\tau dt v(\gamma - \xi)$ is the released heat [35]. The stochastic entropy production can be split into a part associated with the system (particle) and another part associated with the reservoir: $S_\tau = S^s_\tau + S^r_\tau$ [32, 36]. Here $S^s_\tau = \ln[\rho_0(v(0))/\rho_\tau(v(\tau))]$ is the change of the stochastic Shannon entropy of the particle, whose velocity at time $\tau$ is distributed with the probability density $\rho_\tau(v)$, and $S^r_\tau = Q_\tau/T - S^s_\tau$. The quantity $\hat{S}_\tau = m^{-1} \int_0^\tau dt \partial_v f(v) \rho_\tau(v)$ can be interpreted as a leftover of the information exchange between the system and the controller after eliminating the controller degrees of freedom [9, 25, 30, 31, 37–43]. To compute the total entropy production we used the standard representation $S_\tau = \ln(\mathcal{P}[v]/\mathcal{P}[\hat{v}])$ [36], where $\mathcal{P}[v]$ is the path probability of the trajectory $v$, while $\mathcal{P}[\hat{v}]$ is the probability for the time-reversed trajectory $\hat{v}$ [44].

The conventional forms of the first and second laws of thermodynamics can be obtained if we average the above expressions over the ensemble of possible trajectories and take time derivatives. Denote by italic capital letters such averages and assume that the system is in a stationary state with $\dot{E} = 0$ and $\dot{S}^s = 0$, where for instance $\dot{E} = (d/d\tau)\langle E_\tau \rangle$. Then we can write:

$$\dot{U}^a - \dot{W} - \dot{Q} = 0, \quad \dot{S} = \dot{Q}/T - \dot{S}^a = m^2/\gamma T \int J^2_d(v)/\rho_s(v) dv \geq 0,$$

where $J_d(v) = -m^{-1}[\gamma v + (\gamma T m^{-1}) \partial_v] \rho_s(v)$ denotes, as before, the dissipative part of the stationary current [32].
The main shortcoming of the limiting model (8) is that it underestimates entropy production. Indeed, for the overdamped dynamics (8), the stationary entropy production rate can be written as

$$\dot{S}_{od} = \frac{1}{\gamma T} (f + \gamma v_a^*)^2 \geq 0. \quad (11)$$

It is clearly associated with passive dissipation described in (10) by the term $\dot{Q}/T$. In stall conditions this expression vanishes because (8) does not see the fast dynamics at the microscale. If we now compute the entropy production for the full model (5) and go to the limit $m \to 0$ with $\epsilon \sim \sqrt{m}$ we obtain [32]

$$\dot{S} = \dot{S}_{od} + \left( \frac{\pi}{2} - 1 \right) \frac{\gamma (v_a^*)^2}{T} \geq 0, \quad (12)$$

where the second term constitutes the ‘hidden’ entropy production.

To assess the efficiency of our ABP it is natural to first introduce the injection rate of the Helmholtz free energy $\dot{F}^a = U^a - TS^a$. Then the inequality in (10) can be rewritten as $TS^a - \dot{W} \geq 0$, which suggests the following definition of the thermodynamic efficiency, $\eta_T = \dot{W}/\dot{F}^a \equiv \dot{W}/(TS^a + \dot{W}) \leq 1$ [45, 46]. This definition, however, neither accounts for the capacity of a motor to self-propel at zero force, nor for its ability to generate force in stall conditions: in both limits the machine works (either by achieving persistent unidirectional displacement or equally persistent localization) with apparently zero efficiency. A known way to resolve the first of these issues is to consider the Stokes efficiency [47], $\eta_S = (\dot{W} + \gamma v_a^*)/\dot{F}^a$, which still vanishes in stall conditions.

To fix this problem we observe that the (squared) total active force generated by the controller is $\langle g_a(v)^2 \rangle$, while only an amount $\langle g_a(v) \rangle^2$ is useful. The efficiency of active force generation can then be quantified as $\eta_a = \langle g_a(v)^2 \rangle / \langle g_a(v) \rangle^2$ or in thermodynamic terms [32]

$$\eta_a = \dot{W}^a / \dot{G}^a. \quad (13)$$

Here $\dot{W}^a = \gamma (v_a^*)^2$ is now interpreted as useful power, where $v_a^* = v_a - f/\gamma$ is the active velocity gain introduced previously; observe that it is finite in both zero force and zero velocity limits. The consumed power is naturally measured by the rate of injected Gibbs free energy $\dot{G}^a = \dot{F}^a - f v_a^* \geq \dot{F}^a$ which is also natural given that the system is performing work against the load. The typical behavior of thermodynamic, Stokes, and force generation (13) efficiencies is illustrated for our model in Fig. 3. Note that the definition (13) is different from the recently introduced notion of chemical efficiency [48] which may attain negative values and does not reduce to the Stokes efficiency $\eta_S$ in the absence of load.

We now briefly discuss a simple experimentally testable realization of the system (5) in the form of an electric circuit where an active current may appear in the absence of directed voltage, see Fig. 4. The ‘rectifier’ with the active component is made of two parallel branches, each containing a resistor $R_f$ and an ideal diode $D_i$ in series ($i = 1, 2$), and is in thermal contact with another bath with temperature $T_r << T_f$. This inequality is essential to ensure that electrical fluctuations are basically produced only in resistor $R_f$ while the ‘rectifier’ plays the role of the active mechanism alternating the effective resistance depending on the direction of the current in the ‘fluctuator’.

Standard circuit analysis leads to the following equation for the global current $I$ [32]:

$$L\dot{I} = -R_c(1 + \text{sgn}(I))I + \sqrt{2R_cT_c}\xi, \quad (14)$$

where the effective parameters are $R_c = R_f + (R_1 + R_2)/2$, $T_c = 2R_fT_f/(2R_f + R_1 + R_2)$ and $\epsilon = (R_2 - R_1)/(2R_f + R_1 + R_2)$. We assumed that the current is positive when flowing clockwise around the circuit. As the analogy between (5) in the absence of load, and (14) is complete, the circuit in Fig. 4 should be able to generate a directed current by rectifying thermal fluctuations: the ‘activity’ is then ensured by the device maintaining the temperature difference between the ‘fluctuator’ and the ‘rectifier’.

To conclude, we presented a model of an active particle exploiting ‘strong’ mechanism of TRS breaking. This model appears naturally if one makes the simplest pseudo-linear assumptions about the chemo-mechanical coupling of the vectorial (friction) and the scalar (reaction) processes which breaks the potentiality of the dissipative potential. While the realistic chemomechanical coupling is probably more complex, for instance quadratic, as in the case of KPZ equation [49] or the active model B [50], the main idea of the breaking the TRS symmetry through non-gradient dissipation can be already captured by our semi-analytical model. An important result of our analysis is that in systems with non-Maxwellian...
velocity distribution and persistence, the Smoluchowski limit aimed at capturing trajectories can grossly underestimate the associated dissipation, giving a misleading picture of the fluctuation rectification process.

Acknowledgments. The authors thank J.F. Joanny for helpful discussions. R.G.G. acknowledges financial support from the Grant ANR-10-LBX-0038 which is a part of the IDEX PSL (ANR-10-IDEX-0001-02 PSL). L. T. was supported by the Grants ANR-10-IDEX-0-0 01-02 PSL and ANR-17-CE08-0 047-02.

† Pierre.Collet@cpht.polytechnique.fr
‡ reinaldomeister@gmail.com

FIG. 4. Electric circuit imitating the behavior of the system (5) when $T_r \ll T_f$.  

\[ R_f \quad L \quad T_f \]

\[ D_1 \quad R_1 \quad T_r \quad D_2 \]
[45] F. J. Cao and M. Feito, Phys. Rev. E 79, 041118 (2009).
[46] P. Recho, J.-F. Joanny, and L. Truskinovsky, Phys. Rev. Lett. 112, 218101 (2014).
[47] H. Wang and G. Oster, Europhys. Lett. 57, 134 (2002).
[48] P. Baerts, C. Maes, J. Pešek, and H. Ramon, “Tension and chemical efficiency of myosin-ii motors,” (2017), arXiv preprint arXiv:1708.07454.
[49] M. Kardar, G. Parisi, and Y.-C. Zhang, Phys. Rev. Lett. 56, 889 (1986).
[50] R. Wittkowski, A. Tiribocchi, J. Stenhammar, R. J. Allen, D. Marenduzzo, and M. E. Cates, Nat. Commun. 5, 4351 (2014).