

Linear response and correlation of a self-propelled particle in the presence of external fields.

Lorenzo Caprini¹, Umberto Marini Bettolo Marconi² and Angelo Vulpiani^{3,4}

¹ Gran Sasso Science Institute (GSSI), Via. F. Crispi 7, 67100 L'Aquila, Italy

² Scuola di Scienze e Tecnologie, Università di Camerino - via Madonna delle Carceri, 62032, Camerino, Italy

³ Dipartimento di Fisica, Università Sapienza - p.le A. Moro 2, 00185, Roma, Italy

⁴ Centro Interdisciplinare "B.Segre", Accademia dei Lincei, Roma, Italy

E-mail: lorenzo.caprini@gssi.it, angelo.vulpiani@roma1.infn.it

PACS numbers: 05.40.-a, 05.60.-k, 05.70.Ln

Abstract.

We study the non-equilibrium properties of non interacting active Ornstein-Uhlenbeck particles (AOUP) subject to an external nonuniform field using a Fokker-Planck approach with a focus on the linear response and time-correlation functions. In particular, we compare different methods to compute these functions including the unified colored noise approximation (UCNA). The AOUP model, described by the position of the particle and the active force acting on it, is usually mapped into a Markovian process, describing the motion of a fictitious passive particle in terms of its position and velocity, where the effect of the activity is transferred into a position-dependent friction. We show that the form of the response function of the AOUP depends on whether we put the perturbation on the position and keep unperturbed the active force in the original variables or perturb the position and maintain unperturbed the velocity in the transformed variables. Indeed, as a result of the change of variables the perturbation on the position becomes a perturbation both on the position and on the fictitious velocity. We test these predictions by considering the response for three types of convex potentials: quadratic, quartic and double-well potential. Moreover, by comparing the response of the AOUP model with the corresponding response of the UCNA model we conclude that although the stationary properties are fairly well approximated by the UCNA, the non equilibrium properties are not, an effect which is not negligible when the persistence time is large.

1. Introduction

Self-propelled particles represent a system inherently out of equilibrium as they take energy from the environment, convert it into directed motion and dissipate it to move in a viscous medium [1–3]. In recent years, a variety of models have been proposed in order to capture both the stationary and the time-dependent properties of these systems. Among these proposals, we mention the Run and Tumble [4–6], the active Brownian particle (ABP) model [7–9] and the Gaussian colored noise model also termed active Ornstein-Uhlenbeck particle (AOUP) model [10–12]. They all describe the overdamped motion of particles subjected to a drag force, due to the solvent, proportional to the particle’s velocity, to a deterministic force, F , due to an external driving or to interparticle interactions and to the so-called active force or self-propulsion. In the ABP the active force is modeled by a vector of constant norm and whose orientation performs a Brownian motion on the unit sphere. The orientation of the self-propulsion has a typical persistence time, τ i.e. it decorrelates with respect to its initial value exponentially as $\exp(-t/\tau)$. The existence of such correlation accounts for the persistence of the trajectories which is the distinguishing feature between the standard model of colloidal particles and the one describing self-propelled particles. Interestingly, in the presence of deterministic forces either due to external fields, such as confining walls or to particle-particle interactions self-propelled particles manifest novel phenomena such as a tendency to cluster [13–15] and correlations between the positions and the velocities reflecting their non-equilibrium nature.

The AOUP originates from the necessity of reducing the mathematical complexity of the ABP and is constructed by assuming the same deterministic forces as in the ABP but replacing the ABP active force by an active force whose components have a Gaussian distribution [13, 16]. The matching between ABP and AOUP is enforced by requiring that the active forces of each model have the same variance and the same exponential time-correlation, but the AOUP admittedly neglects the non-Gaussian nature of the ABP self-propulsion statistics. Apart from this non trivial aspect, the AOUP model has the advantage of lending itself to a simpler analysis and to the possibility of determining the steady state probability distribution function (pdf) of the active particle for small activity [28, 29]. Since the AOUP model is formulated as an overdamped particle subject to colored noise, it can be mapped into a new Markovian system, by adding a degree of freedom for each component of the noise. This new enlarged representation allows for the study the problem by using a standard approach based on the Kramers equation for which several approximate methods of solution are well-known [25, 26]. However, the choice of this enlarged space is not unique since the microstate of a single particle at a given instant can be identified by its position and velocity or by its position and by the value of the active force acting on it. The two descriptions are equivalent and for both one can write the corresponding Fokker-Planck equations and the associated approximate steady state distribution functions obtained by means of a perturbative analysis in terms of the parameter τ^{-1} . As far as only the steady state configurational properties are concerned it is possible to derive a closed, non-perturbative expression for the distribution function by means of the so-called unified colored noise approximation (UCNA) put forward by Hanggi and Jung [17, 18]. The static properties of the UCNA have been tested with success in the case of persistence times not too large, but very little is known about its dynamical properties. The present study aims to fill this gap by considering the response to a small external perturbation of a self-propelled particle driven by colored noise in the presence of a trapping potential. We shall compare both exact analytic and numerical results obtained by applying the fluctuation dissipation relation (FDR) [24] to the

AOUP model for the response to an initial displacement of the particle's position with the corresponding quantity computed within the UCNA. As a byproduct of this study, we obtain and explain a result which contradicts the naive expectation that the positional response function should not depend on the choice of the enlarged representation.

The paper is organized as follows. The description of the model and the theoretical results are presented in Section 2. In Sec. 3 we report the results of some numerical simulations obtained in the case of anharmonic potentials. Finally, we draw some conclusions in Sec. 4.

2. Models and theory

We model the effective dynamics for the space coordinates of an assembly of non-interacting active Brownian particles [12, 18], as:

$$\begin{aligned} \dot{x} &= \frac{f(x)}{\gamma} + a, & f(x) &= -\frac{d}{dx}\phi(x), \\ \dot{a} &= -\frac{a}{\tau} + \frac{\sqrt{2D}}{\tau}\eta, \end{aligned} \quad (1)$$

where $x(t)$ is the position of the particle, τ is the correlation time, γ the drag coefficient, $\phi(x)$ the potential acting on the system and the term $a(t)$, also called *active bath*, evolves as an Ornstein-Uhlenbeck process. The stochastic force $\eta(t)$ is a white noise, i.e. a Gaussian process with zero mean and $\langle \eta(t)\eta(t') \rangle = \delta(t-t')$. The parameter D is the diffusive coefficient due to the activity related and fixes the amplitude of the Ornstein-Uhlenbeck process, via:

$$\langle a(t)a(t') \rangle = \frac{D}{\tau} \exp\left[-\frac{t-t'}{\tau}\right]. \quad (2)$$

In order to proceed further, we will adopt non-dimensional variables for position, velocity, and time

$$X = \frac{x}{l}, \quad V = \frac{v}{v_T}, \quad \bar{t} = t \frac{v_T}{l} \quad (3)$$

where l is a suitable length and $v_T = \sqrt{\frac{D}{\tau}}$ is a reference velocity. We rescale forces and potential as follows:

$$F(X) = f(x) \frac{l}{D\gamma}, \quad U(X) = \frac{\phi(x)}{D\gamma}, \quad A = \frac{a}{v_T}, \quad (4)$$

and $\zeta = \frac{l}{\tau v_T}$ can be seen as the ratio between the characteristic length of the problem, l , such as the typical length-scale of the external potential $U(x)$, and the mean square diffusive displacement due to the active bath in a time interval τ . Rewriting Eq.(1) in terms of these new variables we have:

$$\dot{X} = -\frac{U'(X)}{\zeta} + A, \quad (5)$$

$$\dot{A} = -\zeta A + \sqrt{2\zeta}\xi(\bar{t}), \quad (6)$$

where $\langle \xi(\bar{t})\xi(\bar{t}') \rangle = \delta(\bar{t} - \bar{t}')$. In the following, we will use the symbol t for the non-dimensional time. If the particle is confined to a region of space by a potential $U(X)$, ζ^{-1} represents the ratio between the persistence length and size of the potential well and the amplitude of the fluctuating force in reduced

units is $\lim_{t \rightarrow \infty} \langle A(t)A(t) \rangle = 1$. For the pdf $\tilde{P}(X, A, t)$ of the (X, A) variables we have the following Fokker-Planck equation:

$$\frac{\partial}{\partial t} \tilde{P} - \frac{\partial}{\partial X} \left(\frac{U'(X)}{\zeta} - A \right) \tilde{P} = \zeta \frac{\partial}{\partial A} \left[\frac{\partial}{\partial A} + A \right] \tilde{P} \quad (7)$$

whose stationary solution $\tilde{P}_s(X, A)$ is in general unknown a part from simple potentials [26].

In order to apply techniques developed for the Kramers equation it is sometimes convenient to use instead of the (X, A) variables the phase-space variables (X, V) (see for instance [12, 28, 29]), through the following change of variables:

$$V \equiv \dot{X} = -\frac{U'(X)}{\zeta} + A, \quad (8)$$

$$X' = X. \quad (9)$$

In this way we recast the stochastic differential equation (5) as:

$$\dot{X} = V \quad (10)$$

$$\dot{V} = -U'(X) - \zeta g(X)V + \sqrt{2T\zeta}\eta \quad (11)$$

and the associated Kramers equation for the phase-space distribution $P(X, V, t)$:

$$\frac{\partial}{\partial t} P + V \frac{\partial}{\partial X} P - U'(X) \frac{\partial}{\partial V} P = \zeta \frac{\partial}{\partial V} \left[\frac{\partial}{\partial V} + g(X)V \right] P, \quad (12)$$

which means that the activity can be mapped into a space dependent friction term $g(X) = 1 + \frac{1}{\zeta^2} \frac{d^2}{dX^2} U(X)$ which depends on ζ . The second and third term on the left-hand side represent the streaming terms in the evolution of the phase-space distribution, whereas the right-hand side describes the dissipative part. Again the stationary distribution $P_s(X, V)$ is unknown, in general. Because the Jacobian of the transformation $(X, A) \rightarrow (X', V)$ is unitary, we have:

$$P_s(X, V) = \tilde{P}_s(X, A(V, X)). \quad (13)$$

We would like to stress that the X, V representation is relevant because it allows us to obtain the distribution function in terms of these variables and to develop an efficient perturbative scheme in powers of the non equilibrium parameter $1/\zeta$.

2.1. Steady state probability distributions in the extended space

Among the few cases whose stationary solution of the Fokker-Plank equation is known, one has the harmonic potential, $U(X) = \lambda X^2/2$. The steady state distribution in the (X, V) variables is a Gaussian, $P_s(X, V) \propto e^{-\frac{\beta}{2}(\lambda X^2 + V^2)}$ with inverse "effective temperature" $\beta = (1 + \lambda/\zeta^2)$, while in the variables (X, A) is the following multivariate Gaussian $\tilde{P}_s(X, A) \propto e^{-\frac{\beta}{2}(\lambda X^2 + (A - \lambda X/\zeta)^2)}$. For a generic potential the stationary pdf in the limit $1/\zeta \ll 1$, has the following approximated form (see [28, 29]):

$$P_s(X, V) \propto e^{-U(X) - \frac{V^2}{2}} \left\{ 1 - \frac{1}{2\zeta^2} \left[U'(X)^2 + V^2 U''(X) - 3U'''(X) \right] + \frac{1}{6\zeta^3} U''''(X) V^3 - \frac{1}{2\zeta^3} U''''(X) V \right\} + O\left(\frac{1}{\zeta^4}\right), \quad (14)$$

showing that positions and velocities are correlated for any finite ζ . In the (X, A) variables the stationary pdf reads:

$$\begin{aligned} \tilde{P}_s(X, A) \propto e^{-U(X) - \frac{(A - U'(X))^2}{2}} & \left\{ 1 - \frac{1}{2\zeta^2} \left[U'(X)^2 + \left(A - \frac{U'(X)}{\zeta} \right)^2 U''(X) - 3U'''(X) \right] + \right. \\ & \left. + \frac{1}{6\zeta^3} U''''(X) \left(A - \frac{U'(X)}{\zeta} \right)^3 - \frac{1}{2\zeta^3} U''''(X) \left(A - \frac{U'(X)}{\zeta} \right) \right\} + O\left(\frac{1}{\zeta^4}\right) \end{aligned} \quad (15)$$

Actually, there are no results in the opposite limit $\zeta \ll 1$, where the persistence time is large.

2.2. Reduced descriptions: distribution in positional space

Since in general the analytic solutions of eqs. (7) or (12) are not known, it is common practice to resort to a reduced description involving only the coordinate X for which it is possible to develop an efficient approximation method. This is the idea behind the reduction of the Kramers equation onto the Smoluchowski equation and it can be realized by different procedures such as multiple time-scale methods, functional integral techniques or adiabatic procedures. The unified color noise approximation (UCNA) was developed the first time by Hanggi et Jung by using an adiabatic elimination procedure to study the behavior of particles driven by colored noise [17, 30] and then recently extended [12, 18, 31] for systems of active particles. In the following, we consider two types of approximations: UCNA and an overdamped limit performed directly on the equation (5), with the idea of making a comparison among them. We shall study different regimes: $\zeta \gg 1$ and $\zeta \ll 1$. The first regime corresponds to a small departure from the equilibrium situation determined by the presence of a small τ , while the second regime to the case in which the persistent time is large and is more interesting, because it shows the peculiar features of the active particles, for instance the accumulation of active particles close to confining walls [12]. In order to gain some insight, we consider the distribution of positions in two special limits corresponding to short persistence time $\zeta \gg 1$ and to long persistence time $\zeta \ll 1$.

- (i) $\zeta \gg 1$. Let's consider the system of Eq. (5); a first approximation consists in neglecting \dot{A} . This means that A is well approximated by a white noise and we have:

$$\dot{X} = -\frac{U'(X)}{\zeta} + \sqrt{\frac{2}{\zeta}}\xi, \quad A = \sqrt{\frac{2}{\zeta}}\xi \quad \implies \quad P_1(X) \propto e^{-U(X)}, \quad (16)$$

where $P_1(X)$ is the configurational stationary probability distribution of an equilibrium system.

- (ii) $\zeta \ll 1$. In this case, we can neglect \dot{X} , therefore the variable X is related to A , so that the evolution is given by:

$$\dot{A} = -\zeta A + \sqrt{2\zeta}\xi, \quad \implies \quad \tilde{P}_2(A) \propto e^{-A^2/2}, \quad (17)$$

being $\tilde{P}_2(A)$ the stationary pdf for A . We can obtain a new probability distribution, $P_2(X)$, for the variable X , since $dA = \frac{U''(X)}{\zeta}dX$ and we have:

$$P_2(X) \propto \frac{U''(X)}{\zeta^2} \exp\left(-\frac{U'(X)^2}{2\zeta^2}\right). \quad (18)$$

Let us notice that for small ζ , $P_2(X)$ is a very peaked probability distribution.

Let us, now, consider the description based on the variables (X, V) given by Eq. (8) and perform the adiabatic elimination of the V variable, i.e. neglecting the acceleration \dot{V} , both for $\zeta \gg 1$ and $\zeta \ll 1$. We have the following single first order stochastic equation, the well known UCNA equation:

$$\dot{X} = -g(X)^{-1} \frac{U'(X)}{\zeta} + g(X)^{-1} \sqrt{\frac{2}{\zeta}} \xi. \quad (19)$$

whose stationary pdf of positions reads:

$$P_U(X) \propto g(X) \exp\left(-U(X) - \frac{1}{2\zeta^2} U'(X)^2\right). \quad (20)$$

Let's remark that

- when $\zeta \gg 1$ and $g \sim 1$ we have $P_U \sim P_1$.
- when $\zeta \ll 1$: since $g \sim U''(X)/\zeta^2$ we have $P_U \sim P_2$.

We note that P_U and P_1 are the approximations of the marginal distribution of the system described by the probability distribution given by Eq. (14). Indeed, by calling $P_M(X)$ the marginal distribution, with respect to V , associated to Eq. (14), we have:

$$P_M(X) \equiv \int dV P_s(X, V) = P_U(X) + O\left(\frac{1}{\zeta^4}\right) = P_1(X) + O\left(\frac{1}{\zeta^2}\right). \quad (21)$$

Therefore, we can say that when $\zeta \gg 1$, the UCNA-model is a better approximation than the model (i) and there is no reason to use the model (i) instead of the UCNA-model. In particular in the harmonic case the marginal distribution is exactly reproduced by the UCNA.

2.3. Linear response function

In this subsection, we shall study the response of our system when we slightly perturb the initial position of the particle and show that such a procedure yields different results, depending on the variables chosen to describe the system. In order to solve this apparent paradox, we first apply the well-known general fluctuation-dissipation relations [23, 24], in both representations (X, V) and (X, A) . We show that notwithstanding the Jacobian of the transformation is unitary, a perturbation of the position, X , in the A representation corresponds to a perturbation involving both the variables $(X$ and $V)$ in the V representation.

The response function R of the AOUP model was studied by Szamel and Fodor et al. in [10, 28]. In particular Fodor et al. numerically measured the susceptibility, defined as the time integral of the response and studied the system using the (X, V) coordinates, in the regime of small persistence time. In the present study, instead we directly measure the response of the system, both in the small and in the large persistence time limit. Let's call $R_A(t)$ the mean response of the system that we will compute numerically by adding a small impulsive force $h(t) = h_0 \delta(t)$, in the first equation of the system (5):

$$\dot{X}_h = -\frac{U'(X_h)}{\zeta} + A_h + h(t), \quad (22)$$

$$\dot{A}_h = -\zeta A_h + \sqrt{2\zeta} \xi, \quad (23)$$

where X_h and A_h are the variables of the system in presence of the perturbation. In a similar way we call $R_V(t)$ the response obtained by adding the small force to equations (10) in the (X, V) representation.

The study of $R_A(t)$ and $R_V(t)$ can be numerically performed by computing the following normalized quantity:

$$R(t) = \frac{\langle \delta X(t) \rangle}{\delta X(0)} = \frac{\langle X_h(t) - X(t) \rangle}{X_h(0) - X(0)}. \quad (24)$$

Although there are different versions of the FDR for the prediction of $R(t)$ [19,20], we focus the attention on the first version of the FDR, independently developed in [21] (for a recent work see [22]) and [23]. According to this version of FDR [24], we have the response in terms of an average, which involves the stationary pdf:

$$R_{V(A)}(t) = - \left\langle X(t) \left(\frac{\partial}{\partial X} \log Prob \right) \Big|_{t=0} \right\rangle_{V(A)}, \quad (25)$$

where depending on the choice of the variables one sets $Prob$ equal to $P_s(X, V)$ or $\tilde{P}_s(X, A)$ and the average $\langle \cdot \rangle$ is performed by using the corresponding stationary pdf and the symbol $t = 0$ means that the function is computed for the variables at $t = 0$.

By inserting Eq. (14) in relation (25), we obtain the response, $R_V(t)$ in the (X, V) representation:

$$\begin{aligned} R_V(t) = & - \left\langle X(t) \left(\frac{\partial}{\partial X} \log P_s(X, V) \right) \Big|_{t=0} \right\rangle_V = \\ & \left\langle X(t) \left(U'(X) + \frac{1}{\zeta^2} \left[U''(X)U'(X) + \frac{V^2}{2}U'''(X) - \frac{3}{2}U''''(X) \right] \right. \right. \\ & \left. \left. - \frac{1}{\zeta^3} \left[\frac{V^3}{6}U''''(X) - \frac{1}{2}VU''''(X) \right] \right) \Big|_{t=0} \right\rangle_V, \end{aligned} \quad (26)$$

up to the order $O(1/\zeta^4)$, while using Eq. (15) we obtain the response, $R_A(t)$ in the (X, A) representation:

$$\begin{aligned} R_A(t) = & - \left\langle X(t) \left(\frac{\partial}{\partial X} \log \tilde{P}_s(X, A) \right) \Big|_{t=0} \right\rangle_A = \\ & \left\langle X(t) \left(U'(X) - \frac{1}{\zeta}AU''(X) + \frac{1}{\zeta^2} \left(2U'(X)U''(X) + \frac{A^2}{2}U'''(X) - \frac{3}{2}U''''(X) \right) \right. \right. \\ & \left. \left. + \frac{1}{\zeta^3} \left(-A[U''(X)^2 + U'(X)U'''(X)] - \frac{A^3}{6}U''''(X) + \frac{A}{2}U''''(X) \right) \right) \Big|_{t=0} \right\rangle_A, \end{aligned} \quad (27)$$

where $\langle \cdot \rangle_A$ denotes the average with respect to $\tilde{P}(X, A)$. By expressing the response R_A in the variables (X, V) we obtain:

$$R_A(t) = R_V(t) - \frac{1}{\zeta} \left\langle X(t)V(0)U''(X(0)) \right\rangle_V - \frac{1}{\zeta^3} \left\langle X(t)V(0)U''(X(0))^2 \right\rangle_V, \quad (28)$$

showing that R_A and R_V differ by terms of order $1/\zeta$, which vanish in the limit $1/\zeta \ll 1$. Such a result seems somehow counterintuitive: how is it possible that the response of the system to an initial perturbation in the X variable depends on the choice of the coordinates that we use? To explain that, let's introduce the pdf of the perturbed system $\tilde{P}'_s(X, A) = \tilde{P}_s(X - \delta X_0, A)$ and $P'_s(X, V) = P_s(X - \delta X_0, V)$, and let's call $\tilde{W}((X_0, A_0) \rightarrow (X, A))$ and $W((X_0, V_0) \rightarrow (X, V))$ the transition probabilities from the state at time zero to the one at time t in the coordinates (X, A) and (X, V) , respectively. Under the usual hypothesis for the probability distribution it is easy [24] to show that the response of the position at time t , $R_A(t)$, in the variables (X, A) , is:

$$\langle \delta X(t) \rangle_A = \int X \left(\tilde{P}'_s(X_0, A_0) - \tilde{P}_s(X_0, A_0) \right) \tilde{W}((X_0, A_0) \rightarrow (X, A)) dX_0 dA_0 dX dA. \quad (29)$$

Since the Jacobian of the transformation is unitary, we can switch from the variables (X, A) to (X, V) :

$$\begin{aligned} \langle \delta X(t) \rangle_A = \\ \int X \left[P'_s(X_0, V_0(X_0, A_0)) - P_s(X_0, V_0(X_0, A_0)) \right] W((X_0, V_0) \rightarrow (X, V)) dX_0 dV_0 dX dV. \end{aligned} \quad (30)$$

For a small increment δX_0 we have:

$$\begin{aligned} P'_s(X, V(X, A)) - P_s(X, V(X, A)) &= -\delta X_0 \left[\frac{\partial}{\partial X} P_s(X, V(X, A)) + \frac{\partial V(X, A)}{\partial X} \frac{\partial P_s}{\partial V} \right] \\ &= -\delta X_0 \frac{d}{dX} P_s(X, V(X, A)). \end{aligned} \quad (31)$$

This version of the FDR involves a total derivative, which acts also on the velocity. This means that the response $R_A(t) = \frac{\langle \delta X(t) \rangle_A}{\delta X_0}$ is given by:

$$\begin{aligned} R_A(t) &= - \left\langle X(t) \left(\frac{d}{dX} \log P_s(X, V(A, X)) \right) \Big|_{t=0} \right\rangle_V \\ &\neq - \left\langle X(t) \left(\frac{\partial}{\partial X} \log P_s(X, V(A, X)) \right) \Big|_{t=0} \right\rangle_V = R_V(t), \end{aligned} \quad (32)$$

where the averages are performed by using $P_s(X, V)$. In other words we can say that, since A depends on X and V , the perturbation $(X, V) \rightarrow (X + \delta X_0, V)$ is not equivalent to the perturbation $(X, A) \rightarrow (X + \delta X_0, A)$.

3. Results

In the following, we shall present some results illustrating the predictions of the theory in some simple cases. We have performed the simulations for three different potentials $U(X)$: (a) harmonic potential $U(X) = \lambda X^2/2$, (b) quartic potential $U(X) = \lambda X^4/4$, (c) double well potential $U(X) = \lambda(X^4/2 - X^2/2)$.

The numerical computations of $R(t)$, both from data and FDR Eq.(25), were performed using the Euler-Maruyama method [27], neglecting order $(\Delta t)^{5/2}$.

3.1. Response in the limit $\zeta \ll 1$

In the case (a) the probability distribution of the system can be computed exactly and therefore we have an exact expression for the response: $R_A(t) \sim e^{-t\lambda/\zeta}$. In the cases (b) and (c) we know the probability distribution as a series in powers of $1/\zeta \ll 1$ so that we can obtain the FDR only perturbatively. Therefore, the numerical approach is necessary when the limit $\zeta \gg 1$ doesn't hold. In Fig. 1 we show $R_A(t)$ for the three different potentials and different values of ζ . Let us first discuss the case (a) and (b): when ζ is large, we are near the delta correlated noise, closed to the equilibrium situation. Therefore the shape of the potential does not change the form of the response, which decays roughly as an exponential. When $\zeta \sim 1$ or $\zeta \ll 1$ the results relative to the two potentials display large differences increasing as ζ decreases. In particular, when the attractive force becomes stronger, the response becomes slower, as we can see in Fig. 1. This is a consequence of the departure of the system from thermodynamic equilibrium: indeed the detailed balance holds only in the harmonic case [29] when the drag coefficient in the (X, V) variables is constant. Otherwise, $g(X)$ is not constant, and decreasing ζ the system goes far from equilibrium. Indeed, where ζ is small, in the harmonic case the shape obtained is the one predicted

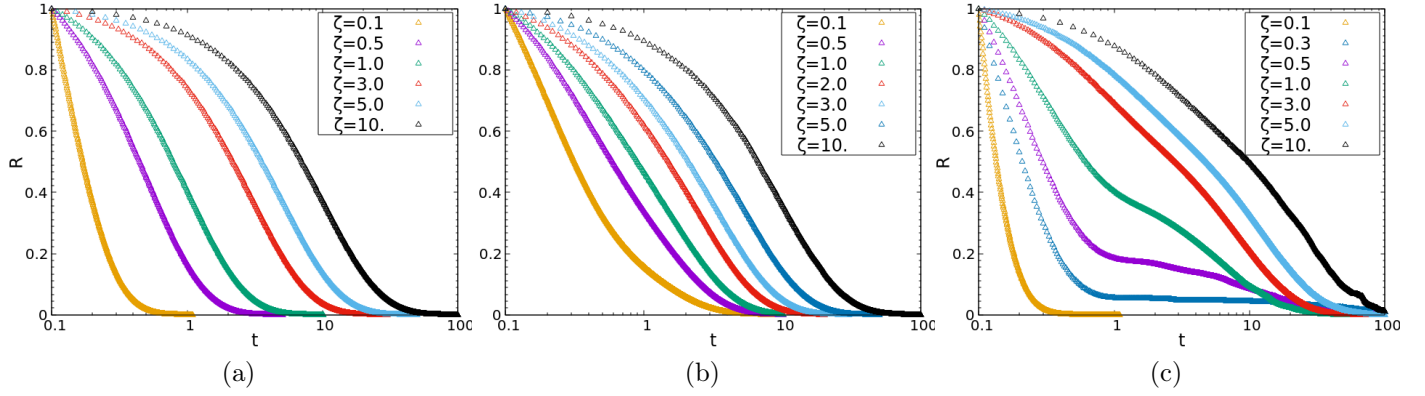


Figure 1: Responses $R_A(t)$ for the AOUP model computed, via numerical simulation, for different values of ζ by setting $\lambda = 1$. In figure (a) are plotted the responses for the harmonic potential $\lambda X^2/2$. The plots (b) and (c) correspond to a quartic potential $\lambda X^4/4$ and a double well potential $\lambda(X^4/4 - X^2/2)$, respectively.

by the theoretical computations $\sim e^{-\lambda t/\zeta}$. In the other cases we can distinguish between two regimes: up to $t \sim 1$ (in dimensional units this corresponds to $t \sim l/v_T$) there is *fast* relaxation, while for $t \gg 1$ there is a relaxation with an effective characteristic time $t_{slow} \gg \zeta$. The presence of these two regimes is a non-equilibrium effect and is more evident when the activity is large (ζ small). The presence of two times scales, when the system is far from equilibrium, is a clear consequence of the accumulation of particles near the confining walls [12]. This means that, even if the potential applied has a single well, the particle in the steady state experiences an effective double well potential. Such an observation is confirmed by the shape of the stationary pdf $P_U(X)$ in the UCNA-approximation. Phenomenologically, the drift term takes different values depending on the position of the particle: when X is near the minimum of the potential the effective drift force is proportional to $\sim \zeta V \ll V$, being $U''(X)/\zeta \sim 0$, and the particle moves just because of the deterministic force. For X far from the minimum, the drift force is proportional to $\sim V U''(X)/\zeta \gg V$, which means that the particle experiences a big Stokes force and moves very slowly. For X far from the minimum, the deterministic force is very big and steadily pushes the particle towards the minimum, preventing the particle from going too far. The balance between these two effects leads to a situation where the most probable value of the position does not coincide with the minima of the potential. This fact explains why the decay of the response function displays two different time-regimes, even in the presence of a single well potential $U(X) \propto X^{2n}$ with $n > 1$. Let us remark that this mechanism acts only when the detailed balance does not hold, as in the case where the curvature $U''(X)$ is not constant [29].

Finally, we consider the the double well potential (case (c)). In order to gain some insight, let us consider the situation where the noise is delta correlated: the response function displays two different decay behaviors (roughly exponential), in the first stage the typical decay time is associated with the relaxation in one of the two wells and is determined by the curvature of the potential, $U''(X_{min})$. For longer times the jumps of the particle between the two minima are relevant and the mean first passage time is determined by Kramers' formula [25]. If the persistence time, τ , is not very small is not easy to extend the above argument, however, in Fig. 1 (c) which displays the behavior of the response function

versus t , it is quite evident the presence of two different characteristic time scales. When the persistence time becomes larger the second relaxation becomes slower as clearly indicated by the plot of Fig. 1 (c), as if the effective barrier becomes higher.

3.2. The UCNA response function

It is known that the UCNA model well describes all the stationary properties of the system both for $1/\zeta \ll 1$ and $\zeta \ll 1$. This state of affairs is no longer true for the time-dependent dynamical properties such as the response to a small perturbation.

By using the FDR for a system under the action of a generic potential $U(X)$, we easily obtain the following expressions for the responses in the three cases, denoted by a subscript.

(i) if $\zeta \gg 1$ from eq. (26) we have:

$$R_1 = \langle X(t)U'(X(0)) \rangle_V. \quad (33)$$

(ii) while for $\zeta \ll 1$ the response is

$$R_2(t) = \frac{1}{\zeta^2} \langle X(t)U'(X(0))U''(X(0)) \rangle_V - \left\langle X(t) \frac{U'''(X(0))}{U''(X(0))} \right\rangle_V. \quad (34)$$

(iii) and within the UCNA we have:

$$R_U(t) = - \left\langle X(t) \left(\frac{\partial}{\partial X} \log P_U(X) \right) \Big|_{X=X(0)} \right\rangle_U, \quad (35)$$

and explicitly:

$$R_U(t) = \frac{1}{\zeta^2} \langle X(t)U'(X(0))U''(X(0)) \rangle_U + \langle X(t)U'(X(0)) \rangle_U - \left\langle X(t) \frac{U'''(X(0))}{\zeta^2 + U''(X(0))} \right\rangle_U. \quad (36)$$

where the subscript U means that the average is with respect to the UCNA steady state distribution, $P_U(X)$ given by (20).

3.3. Response function in the presence of a quadratic potential

In the harmonic case, $U(X) = \lambda X^2/2$, we can apply the FDR for all values of ζ without approximations and obtain from Eq. (26):

$$R_V(t) = \beta\lambda \langle X(t)X(0) \rangle_V \quad (37)$$

and from Eq. (28):

$$R_A(t) = \beta\lambda \left(\langle X(t)X(0) \rangle_V - \frac{1}{\zeta} \langle X(t)V(0) \rangle_V \right) = R_V(t) - \beta\frac{\lambda}{\zeta} \langle X(t)V(0) \rangle_V. \quad (38)$$

In general, the two responses are not the same, except in the limit $\zeta \rightarrow \infty$ which corresponds to the δ -correlated case. As shown in the Appendix the correlation functions appearing in r.h.s. of Eqs. (37) and (38) are given by:

$$\beta \langle X(t)X(0) \rangle_V = \frac{1}{\zeta - \lambda/\zeta} \left[\frac{\zeta}{\lambda} e^{-\lambda t/\zeta} - \frac{1}{\zeta} e^{-t\zeta} \right], \quad (39)$$

and

$$\beta \langle X(t)V(0) \rangle_V = \frac{1}{\zeta - \lambda/\zeta} [e^{-\lambda t/\zeta} - e^{-t\zeta}]. \quad (40)$$

Finally, the response functions read:

$$R_V(t) = \frac{\lambda}{\zeta - \frac{\lambda}{\zeta}} \left(\frac{\zeta}{\lambda} e^{-\lambda t/\zeta} - \frac{1}{\zeta} e^{-t\zeta} \right) \quad (41)$$

and

$$R_A(t) = e^{-\lambda t/\zeta}, \quad (42)$$

Perhaps contrary to intuition, the two responses are different for ζ not too large. For large ζ the two responses are very close. This is an effect of the memory: indeed, small ζ means big correlation time, being $\zeta \sim 1/\tau$.

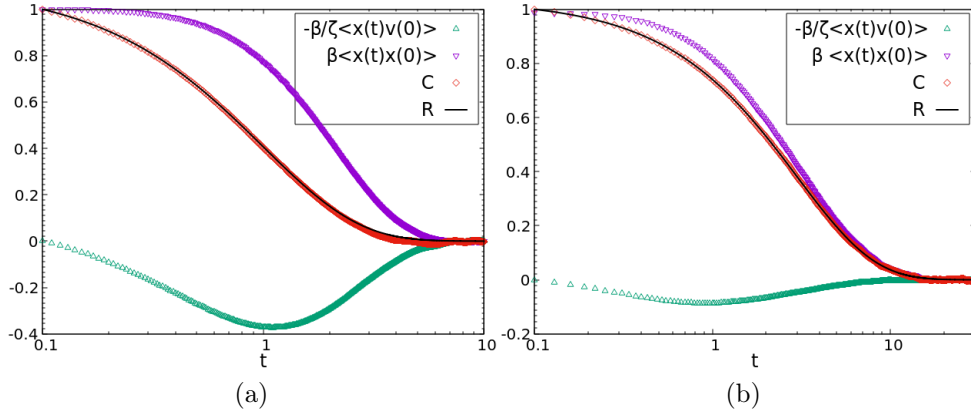


Figure 2: Response function $R_A(t)$ computed via numerical simulation for a harmonic potential $\lambda X^2/2$ with $\lambda = 1$ (black line). The red diamonds (C) represent the sum of the correlation functions given by the Eq. (38), i.e. $R_A(t) = \beta\lambda \left(\langle X(t)X(0) \rangle_V - \frac{1}{\zeta} \langle X(t)V(0) \rangle_V \right)$, a test employed in order to verify FDR. The green triangles represent the correlation $\beta \langle X(t)V(0) \rangle_V$ (Eq. (40)) and the violet inverse triangles represent the correlation $\beta \langle X(t)X(0) \rangle_V$ (Eq. (39)) and . Panel (a) corresponds to $\zeta = 1$ and panel (b) to $\zeta = 3$.

Consider now the response function as predicted by the UCNA theory in the harmonic case. By using the FDR given by Eq. (35) together with the UCNA stationary probability distribution (20) and the correlation function

$$\langle X(t)X(0) \rangle_U = \frac{1}{\beta\lambda} \exp\left(-\frac{\lambda t}{\zeta + \lambda/\zeta}\right),$$

the response function turns out to be:

$$R_U(t) = \exp\left(-\frac{\lambda t}{\zeta + \lambda/\zeta}\right). \quad (43)$$

Let's observe that this response is invariant for $\zeta \rightarrow \lambda/\zeta$. Then:

- $\zeta \gg 1 \implies R_U(t) \sim \exp\left(-\frac{\lambda t}{\zeta}\right)$, which is consistent with the response $R_A(t)$, given by Eq (42).
- $\zeta \ll 1 \implies R_U(t) \sim \exp(-t\zeta)$, which is not correct. Smaller ζ means a slower response, in disagreement with the result for $R_A(t)$, given by the Eq. (42).

3.4. Response function with varying ζ

Let us show the responses, numerically computed, for harmonic and quartic potentials, $U(X) = \lambda X^2/2$ and $U(X) = \lambda X^4/4$, respectively. In the harmonic case, the simulations are only intended as a check of the numerical codes. In the quartic case, we have only a perturbative result in power of $1/\zeta \ll 1$ for the probability distribution function (see eq. (14)). In general, it is difficult to predict the response in the small- ζ regime and we need a numerical study. In fig. 3 we show a comparison between the response of the AOUP-model and the UCNA. For $\zeta \gg 1$ the UCNA is a good approximation of the AOUP both in the case of a harmonic potential (Fig. 3a) and of a quartic potential (Fig. 3b). When ζ becomes smaller, the situation is completely different: in the harmonic case, as predicted by the theoretical computation, the response $R_A(t)$ becomes slower, according to the invariance $\zeta \rightarrow \lambda/\zeta$. Even in this simple case, the UCNA is not able to reproduce the response of the AOUP system for $\zeta \ll 1$. The scenario is similar in the case of the quartic potential $U(X) = \lambda X^4/4$. Moreover, we observe that the response $R_U(t)$

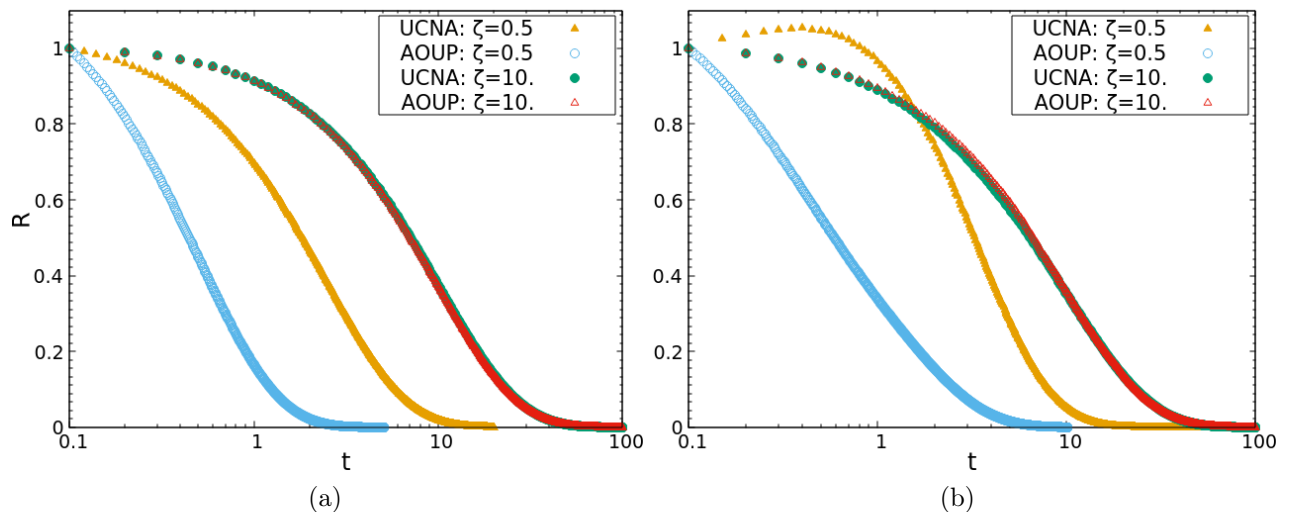


Figure 3: Responses functions computed via numerical simulations from the AOUP ($R_A(t)$) model and the UCNA-model ($R_U(t)$), for different values of ζ : $\zeta = 10, 0.5$ and $\lambda = 1$. The graphs are obtained for systems under the action of a harmonic potential $U = \lambda X^2/2$ (panel (a)) and a potential $U = \lambda X^4/4$ (panel (b)).

computed within the UCNA can be seen only as an approximation of the response $R_V(t)$ computed from Eq.(26).

In Fig. 4 we show a comparison between the response functions R_V , R_A and R_U . We have that the responses $R_V(t)$ and $R_A(t)$ display marked differences when $\zeta/\lambda \ll 1$ and $R_A(t)$ decays much faster. The explanation in the harmonic case comes from the FDR Eq.(38): Indeed the correlation between X and V plays an important role only for ζ small enough, giving a non-vanishing negative contribution. This means that the coupling between the X and V in the Eq.(38) is responsible for the faster decay of $R_A(t)$ with respect to $R_V(t)$, as is shown in Fig.2. On the other hand, $R_U(t)$ in the harmonic case is very close to $R_V(t)$, but in the initial stage the UCNA response is non-monotonic and only in a later stage behaves very closely to $R_V(t)$. In fact, $R_U(t)$ is only an approximation of $R_V(t)$ and fails in the limit $\zeta \ll 1$. This has been directly verified both for the harmonic potential (Fig. 4a) and the quartic potential (Fig. 4b).

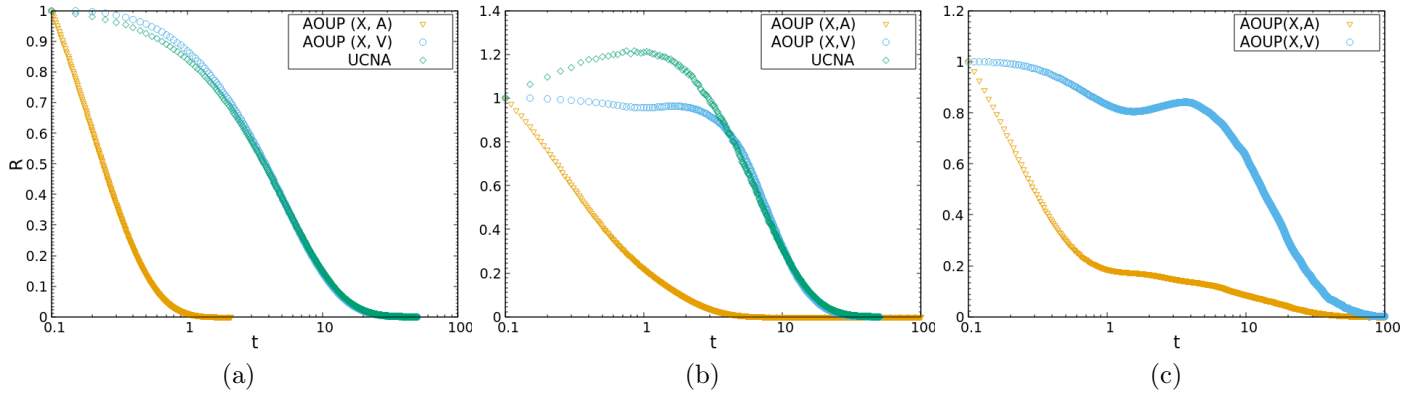


Figure 4: Response functions $R_A(t)$ and $R_V(t)$ computed via numerical simulations from the AOUP model and response $R_U(t)$ of the UCNA in the case of small ζ : $\zeta = 0.2$ and $\lambda = 1$. The graphs (a) and (b) are obtained for systems under the action of a harmonic potential $U = \lambda X^2/2$ and a quartic one $U = \lambda X^4/4$, respectively. The graph (c) is obtained for the double well potential $U = \lambda(X^4/4 - X^2/2)$, for $\zeta = 0.5$.

In Fig.4 we compare R_V and R_A in the case of a double well potential when ζ is small and so the system is far from equilibrium. As expected by the previous cases, $R_V(t)$ is slower than $R_A(t)$. Both responses show a first exponential relaxation for $t \sim 1$ and a relaxation slower than an exponential for a much longer time.

4. Summary and Conclusions

In this paper, we studied the response of a one-dimensional system of non-interacting AOUP under the action of an external potential. We have shown that, at variance with the equilibrium case which applies to passive particles, the standard formula connecting the response function after an initial perturbation in the particle position, X , to the partial derivative of the stationary phase-space distribution function, $P(X, V)$, with respect to X has to be modified in the case of active particles. Such a modification is necessary due to the dependence of the velocity of the particle, V , on the position X , a distinguishing feature of the active dynamics. The relevance of the derived formula is important when the persistence time τ is large. In order to validate our claims, we studied the analytically solvable case of a quadratic potential and by numerical methods the case of non quadratic potentials and compared the response of the AOUP system with the response in the overdamped regime corresponding to the UCNA both for small and large persistence time. This analysis shows that although the stationary properties are well approximated by the UCNA in both cases, this is not true regarding the dynamical properties. In particular, in the case of the response, the UCNA is a good approximation only when the persistence time is small. Finally, the present study has shown that when the persistence time is large enough, even in the case of a single well $U(X) \propto X^{2n}$ with $n > 1$, the response function relaxation is characterized by two time scales. This result is a clear manifestation of the non equilibrium nature of the system and appears only when the detailed balance does not hold.

Acknowledgments

We thank A. Puglisi for useful discussions and the anonymous referees for constructive criticisms.

5. Appendix: Exact computation of correlations and response functions for the harmonic potential

In the case of the harmonic potential the exact stationary probability distribution, $P_s(X, V)$, is well known, being a Gaussian with respect to both variables so that we can compute the time-dependent correlations and the responses $R_{A(V)}$ using the FDR. Indeed, by first multiplying by $X(0)$ the system of equations (5) and then taking their average with respect to the steady distribution $P_s(X, V)$, we obtain a system of ordinary differential equation for the correlation functions. Let's start from the evolution equations for the averages

$$\frac{d}{dt} \langle X(t)X(0) \rangle_V = \langle A(t)X(0) \rangle_V - \frac{\lambda}{\zeta} \langle X(t)X(0) \rangle_V, \quad (44)$$

$$\frac{d}{dt} \langle A(t)X(0) \rangle_V = -\zeta \langle A(t)X(0) \rangle_V. \quad (45)$$

We can solve

$$\langle A(t)X(0) \rangle_V = B e^{-\zeta t}, \quad (46)$$

where B is a constant to be fixed by the initial conditions. By substituting we get:

$$\frac{d}{dt} \langle X(t)X(0) \rangle_V = -\frac{\lambda}{\zeta} \langle X(t)X(0) \rangle_V + B e^{-\zeta t}, \quad (47)$$

whose solution is:

$$\langle X(t)X(0) \rangle_V = C e^{-\lambda t/\zeta} - \frac{B}{\zeta - \frac{\lambda}{\zeta}} e^{-\zeta t}, \quad (48)$$

where C is a second constant to be determined. Let us choose the following steady state initial conditions:

$$\lambda \langle X(0)X(0) \rangle_V = \frac{1}{\beta}, \quad (49)$$

$$\langle V(0)X(0) \rangle_V = \left(\langle A(0)X(0) \rangle_V - \frac{\lambda}{\zeta} \langle X(0)X(0) \rangle_V \right) = 0, \quad (50)$$

which mean that initially the "potential" energy $\lambda X^2/2$ obeys an equipartition principle and the velocity is not correlated with the position. In this way we can easily determine the constants: $B = 1/(\zeta\beta)$ and $\beta C = (\zeta/\lambda)/(\zeta - \lambda/\zeta)$. Finally, we have:

$$\beta \langle X(t)X(0) \rangle_V = \frac{1}{\zeta - \lambda/\zeta} \left[\frac{\zeta}{\lambda} e^{-\lambda t/\zeta} - \frac{1}{\zeta} e^{-\zeta t} \right] = \frac{1}{\lambda} R_V(t). \quad (51)$$

We can, now, easily compute $\langle V(t)X(0) \rangle_V$:

$$\beta \langle V(t)X(0) \rangle_V = \beta \frac{d}{dt} \langle X(t)X(0) \rangle_V = -\frac{1}{\zeta - \lambda/\zeta} [e^{-\lambda t/\zeta} - e^{-\zeta t}]. \quad (52)$$

By using the reversibility condition $\langle V(t)X(0) \rangle_V = -\langle X(t)V(0) \rangle_V$, the response of the AOUP system reads:

$$R_A(t) = \beta \lambda \langle X(t)X(0) \rangle_V - \beta \frac{\lambda}{\zeta} \langle X(t)V(0) \rangle_V = e^{-\lambda t/\zeta}, \quad (53)$$

which is our exact result.

By the same methods we can compute the correlation functions $\langle A(t)X(0) \rangle_V$ and $\langle X(t)A(0) \rangle_V$. Since the harmonic oscillator driven by colored noise obeys the detailed balance condition, if the variable $A(t)$ had a well defined parity under time-reversal one would obtain the relation

$$\langle A(t)X(0) \rangle_V = \pm \langle X(t)A(0) \rangle_V.$$

Indeed, this is not the case and as a matter of fact the result is:

$$\begin{aligned} \langle A(t)X(0) \rangle_V &= \langle V(t)X(0) \rangle_V + \frac{\lambda}{\zeta} \langle X(t)X(0) \rangle_V = \frac{1}{\beta} \frac{e^{-t\zeta}}{\zeta}, \\ \langle X(t)A(0) \rangle_V &= \langle X(t)V(0) \rangle_V + \frac{\lambda}{\zeta} \langle X(t)X(0) \rangle_V = \frac{1}{\beta} \frac{1}{\zeta - \lambda/\zeta} (2e^{-\lambda t/\zeta} - (1 + \lambda/\zeta^2)e^{-\zeta t}). \end{aligned}$$

References

- [1] Clemens Bechinger, Roberto Di Leonardo, Hartmut Löwen, Charles Reichhardt, Giorgio Volpe, and Giovanni Volpe. Active particles in complex and crowded environments. *Reviews of Modern Physics*, 88(4):045006, 2016.
- [2] Sriram Ramaswamy. The mechanics and statistics of active matter. *Annual Review of Condensed Matter Physics*, 1,323, 2010.
- [3] MC Marchetti, JF Joanny, S Ramaswamy, TB Liverpool, J Prost, Madan Rao, and R Aditi Simha. Hydrodynamics of soft active matter. *Reviews of Modern Physics*, 85(3):1143, 2013.
- [4] J. Tailleur and M. E. Cates. Sedimentation, trapping, and rectification of dilute bacteria. *EPL (Europhysics Letters)*, 86(6), 2009.
- [5] R. W. Nash, R. Adhikari, J. Tailleur, and M. E. Cates. Run-and-Tumble Particles with Hydrodynamics: Sedimentation, Trapping, and Upstream Swimming. *Physical Review Letters*, 104:258101, 2010.
- [6] M.E. Cates, and J. Tailleur. When are active Brownian particles and run-and-tumble particles equivalent? Consequences for motility-induced phase separation. *EPL (Europhysics Letters)*, 101(2): 20010, 2013.
- [7] A. P. Solon, and M. E. Cates, and J. Tailleur. Active brownian particles and run-and-tumble particles: A comparative study. *The European Physical Journal Special Topics*, 224(7): 1231-1262, 2015.
- [8] Pawel Romanczuk, Markus Bär, Werner Ebeling, Benjamin Lindner, Lutz Schimansky-Geier. Active brownian particles. *The European Physical Journal Special Topics*, 202(1):1-162, 2012.
- [9] B ten Hagen and S van Teeffelen and H Löwen. Brownian motion of a self-propelled particle. *Journal of Physics: Condensed Matter*, 23(19):194119, 2011.
- [10] Grzegorz Szamel. Self-propelled particle in an external potential: Existence of an effective temperature. *Physical Review E*, 90(1):012111, 2014.
- [11] Elijah Flenner, Grzegorz Szamel and Ludovic Berthier. The nonequilibrium glassy dynamics of self-propelled particles. *Soft matter*, 12(34):7136-7149, 2016.
- [12] Claudio Maggi, Umberto Marini Bettolo Marconi, Nicoletta Gnan, and Roberto Di Leonardo. Multidimensional stationary probability distribution for interacting active particles. *Scientific Reports*, 5, 2015.
- [13] Yaouen Fily and M Cristina Marchetti. Athermal phase separation of self-propelled particles with no alignment. *Physical review letters*, 108(23):235702, 2012.
- [14] Ivo Buttinoni, Julian Bialké, Felix Kümmel, Hartmut Löwen, Clemens Bechinger, and Thomas Speck. Dynamical clustering and phase separation in suspensions of self-propelled colloidal particles. *Physical review letters*, 110(23):238301, 2013.
- [15] Julian Bialké, Thomas Speck, and Hartmut Löwen. Active colloidal suspensions: Clustering and phase behavior. *Journal of Non-Crystalline Solids*, 407:367-375, 2015.
- [16] Thomas FF Farage, P Krinninger, and Joseph M Brader. Effective interactions in active brownian suspensions. *Physical Review E*, 91(4):042310, 2015.
- [17] Peter Hanggi and Peter Jung. Colored noise in dynamical systems. *Advances in Chemical Physics*, 89:239-326, 1995.
- [18] Umberto Marini Bettolo Marconi and Claudio Maggi. Towards a statistical mechanical theory of active fluids. *Soft matter*, 11(45):8768-8781, 2015.

- [19] Ryogo Kubo, Morikazu Toda and Natsuki Hashitsume. *Statistical physics II: nonequilibrium statistical mechanics*. Springer Science & Business Media, 2012.
- [20] Peter Hänggi and Harry Thomas. Stochastic processes: Time evolution, symmetries and linear response. *Physics Reports*, 88(4):207–319, 1982.
- [21] G. S. Agarwal, *Z. Phys*, **25**, 1972.
- [22] Debasish Chaudhuri, Abhishek Chaudhuri. Modified fluctuation-dissipation and Einstein relation at nonequilibrium steady states. *Physical Review E*, 85(2):021102, 2012.
- [23] Massimo Falcioni, Stefano Isola, and Angelo Vulpiani. Correlation functions and relaxation properties in chaotic dynamics and statistical mechanics. *Physics Letters A*, 144(6-7):341–346, 1990.
- [24] Umberto Marini Bettolo Marconi, Andrea Puglisi, Lamberto Rondoni, and Angelo Vulpiani. Fluctuation–dissipation: response theory in statistical physics. *Physics reports*, 461(4):111–195, 2008.
- [25] C. W. Gardiner. *Handbook of Stochastic Methods*. Springer, 1985.
- [26] Hannes Risken. *Fokker-Planck Equation*. Springer, 1984.
- [27] R. Toral and P. Colet. *Stochastic Numerical Methods: An Introduction for Scientists*. Wiley-VCH, 2014.
- [28] Étienne Fodor, Cesare Nardini, Michael E Cates, Julien Tailleur, Paolo Visco, and Frédéric van Wijland. How far from equilibrium is active matter? *Physical review letters*, 117(3):038103, 2016.
- [29] Umberto Marini Bettolo Marconi, Andrea Puglisi, and Claudio Maggi. Heat, temperature and clausius inequality in a model for active brownian particles. *Scientific Reports*, 7, 2017.
- [30] Lutz H'walisz, P Jung, P Hänggi, P Talkner, and Lutz Schimansky-Geier. Colored noise driven systems with inertia. *Zeitschrift für Physik B Condensed Matter*, 77(3):471–483, 1989.
- [31] Umberto Marini Bettolo Marconi, Nicoletta Gnan, Matteo Paoluzzi Claudio Maggi, and Roberto Di Leonardo. Velocity distribution in active particles systems. *Scientific Reports*, 6(33):23297 EP, 2016.
- [32] J Tailleur and ME Cates. Statistical mechanics of interacting run-and-tumble bacteria. *Physical review letters*, 100(21):218103, 2008.
- [33] Michael E Cates and Julien Tailleur. Motility-induced phase separation. *Annu. Rev. Condens. Matter Phys.*, 6(1):219–244, 2015.