Theory for the dynamics of dense systems of athermal self-propelled particles
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A theory for the dynamics of dense systems of athermal self-propelled particles

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We present a derivation of a recently proposed theory for the time dependence of density fluctuations in stationary states of strongly interacting, athermal, self-propelled particles. The derivation consists of two steps. First, we start from the equation of motion for the joint distribution of particles' positions and self-propulsions and we integrate out the self-propulsions. In this way we derive an approximate, many-particle evolution equation for the probability distribution of the particles' positions. Second, we use this evolution equation to describe the time dependence of steady-state density correlations. We derive a memory function representation of the density correlation function and then we use a factorization approximation to obtain an approximate expression for the memory function. In the final equation of motion for the density correlation function the non-equilibrium character of the active system manifests itself through the presence of a new steady-state correlation function that quantifies spatial correlations of the velocities of the particles. This correlation function enters into the frequency term, and thus it describes the dependence of the short-time dynamics on the properties of the self-propulsions. More importantly, the correlation function of particles' velocities enters into the vertex of the memory function and through the vertex it modifies the long-time glassy dynamics.

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I. INTRODUCTION

There is a lot of interest in the static and dynamic properties of active matter systems [1–3]. These systems consist of particles that are self-propelled, and thus can move autonomously. The reason for this interest is twofold. First, there exists a great variety of biological and physical systems with self-propelled constituents. In this work we consider only a subset of these systems consisting of assemblies of particles without aligning interactions. Biological examples of such systems include some motile bacteria and physical systems are represented by synthetic Janus colloidal particles. The second reason for the interest in active matter systems is that they provide fascinating examples of intrinsically non-equilibrium driven systems with very rich and unusual phenomenology. From the point of view of a theoretical analysis active systems are a little easier to study than sheared systems, which used to be a workhorse of non-equilibrium statistical mechanics [4]. This follows from the fact that in active matter systems the driving is applied locally and, on average, isotropically. In contrast, sheared systems are intrinsically anisotropic.

Recently, it has been realized that dense active systems can exhibit glassy dynamics. The analogy between the dynamics in dense cell layers and the dynamics in a fluid approaching a glass transition was noted by Angelini et al. [5]. This study inspired a simulational investigation of a two-dimensional dense active system with aligning interactions in which a jammed phase was identified [6]. Glassy dynamics and the active glass transition was analyzed in a more general setting by Berthier and Kurchan [7]. They studied dynamic behavior of a simple model active system inspired by the spherical $p$-spin model. Their investigation showed that activity can shift the onset of glassy behavior but it does not always destroy the glass transition, unlike for similar models of sheared systems [8]. Berthier and Kurchan’s theoretical analysis was followed by several computational studies of strongly interacting systems of self-propelled particles without aligning interactions, which demonstrated glassy behavior of active matter. First, Ni et al. [9] simulated a system of active Brownian hard spheres and found that, with increasing magnitude of the self-propulsion, the long-time dynamics speeds up whereas the local structure, monitored through the steady-state structure factor, becomes less pronounced. Next, Berthier [10] simulated a slightly different, fully athermal (i.e. devoid of thermal Brownian motion) system of active hard disks and found that, with increasing departure from equilibrium, at intermediate volume fractions the dynamics could be non-monotonic but, again, the apparent glass transition is shifted towards higher volume fractions. Wysocki et al. [11] simulated a dense system of active Brownian particles with continuous interactions. More recently, Mandal et al. [12] simulated the classic model glassy system, the Kob-Andersen Lennard-Jones binary mixture [13], in which one of the components was endowed with self-propulsion. In qualitative agreement with Ni et al., they found that, upon increasing the magnitude of the self-propulsion, the long-time dynamics speeds up and that, beyond a critical strength of the self-propulsion, the glass phase disappears. Finally, Fily et al. [14] investigated the phase diagram of active Brownian harmonic spheres as a function of density, activity and noise, and identified a glassy phase in the high density, small self-propulsion speed regime.

The simulational investigations of active glassy dy-
namics stimulated interest in theoretical descriptions of the dynamics of dense systems of self-propelled particles. The main goal of these descriptions is to understand the effect of the non-equilibrium character of the active system on the glassy dynamics and the glass transition. We recall that, in spite of an extensive theoretical effort, a microscopic and quantitatively correct description of glassy dynamics of thermal “passive” systems remains a challenge [15]. Thus, we should not expect to obtain a microscopic and quantitatively accurate theory for much more complicated active systems. However, we might be able to get some insight into the role of activity. The precedent for this is the application of the well-known, albeit far from perfect, theory of the glassy dynamics, the mode-coupling theory [16], to the description of colloidal systems with short-range attractive interactions [17]. The theory, while in general not quantitatively correct, was able to account for the effect of attractions and to predict a re-entrant glass transition. Its qualitative predictions were subsequently confirmed by experiments [18]. We note that proposed theoretical descriptions of the dynamics of dense active systems use approaches similar the mode-coupling theory. This is hardly surprising since the mode-coupling theory provides one of very few microscopic descriptions of the glassy dynamics in thermal systems [19]. In addition, the virtues and flaws of this theory are quite well understood, which allows one to focus on phenomena that the theory describes reasonably well.

The first microscopic theory for the glassy dynamics of dense systems consisting of spherically symmetric self-propelled particles with non-aligning interactions was put forward by Farage and Brader [20]. This theory is a generalization of an earlier mode-coupling theory for sheared glassy colloidal fluids proposed by Fuchs and Cates [4]. Farage and Brader considered a system of self-propelled particles that were also subjected to thermal noise. They used the integration-through-transients approach introduced by Fuchs and Cates. In this approach one assumes that in the infinitely distant past the system was in an equilibrium state and then the drive, in this case the activity, was turned on. Using this procedure one can, in principle, calculate both equal time and dynamic properties of active systems. However, it is not clear how to use this approach to describe a fully athermal system which does not have an equilibrium state without the drive.

Recently, we proposed a different microscopic theory for dense athermal active systems [21]. Like the theory of Farage and Brader, our theory relies upon a factorization approximation, and thus it falls into a general category of mode-coupling-like approaches. There are, however, significant differences between our theory and that of Farage and Brader. First, our approach incorporates the influence of correlations between velocities of different particles on the dynamics of the active system. This effect is neglected in the theory of Farage and Brader. Second, we use a projection operator defined through a steady-state distribution function. This approach avoids using the integration-through-transients procedure and allows us to describe dynamics of fully athermal systems.

In Ref. [21] we presented an outline of the derivation of our theory. Here we present the details of the derivation and discuss all the approximations used. To make the present contribution self-contained we include some of the discussion from the appendices of Ref. [21]. In addition, we present a derivation of the theory for the time dependence of the tracer density fluctuations.

The main object of our theory is the (collective) intermediate scattering function, \( F(q; t) \), which describes the time dependence of the collective density fluctuations.

\[
F(q; t) = \frac{1}{N} \left\langle \sum_i e^{-i\mathbf{q} \cdot \mathbf{r}_i(t)} \sum_j e^{i\mathbf{q} \cdot \mathbf{r}_j(0)} \right\rangle .
\]

Here and in the following brackets \( \langle \ldots \rangle \) denote averaging over a steady-state distribution of positions and self-propulsions. We will also consider a closely related function, the self-intermediate scattering function, which describes the time dependence of the tagged particle (tracer) density fluctuations, \( F_s(q; t) \),

\[
F_s(q; t) = \frac{1}{N} \left\langle \sum_i e^{-i\mathbf{q} \cdot (\mathbf{r}_i(t) - \mathbf{r}_i(0))} \right\rangle .
\]

The latter function allows us to calculate quantities that are usually monitored in computer simulations, i.e. the relaxation time \( \tau_0 \) defined through the relation [22]

\[
F_s(q; \tau_0) = e^{-1},
\]

and the (long-time) self-diffusion coefficient \( D \) defined through the hydrodynamic limit of the self-intermediate scattering function,

\[
\lim_{t \to \infty, q \to 0, q^2 t = \text{const.}} F_s(q; t) \sim \exp \left(-Dq^2 t\right).
\]

The paper is organized as follows. In Section II we present and motivate the model active system that we analyze in the reminder of the paper. In Section III we discuss the main assumption on which our approach relies, the absence of steady-state currents. In Section IV we present the derivation of the approximate equation of motion for the many-body distribution of the positions of the active particles. This is followed by a brief discussion (Section V) of the short-time behavior of the scattering functions which illustrates the importance of the correlations between self-propulsions and positions. The derivations of the memory function representation and of the approximate expression for the memory function are presented in sections VI and VII, respectively. In Section VIII we discuss general conclusions that can be drawn from the final equation for the time dependence of the density correlations and in Section IX we summarize our findings and outline directions of future work. In the first appendix, Appendix A, we discuss an alternative equation of motion for the many-body distribution...
of the particles’ positions. In the second appendix, Appendix B, we present the derivation of the theory for the time dependence of the tagged particle (tracer) density fluctuations.

II. MODEL ACTIVE SYSTEM

We consider a system of $N$ interacting, self-propelled particles in a volume $V$. The average density is $\rho = N/V$. The particles interact via a spherically symmetric potential $V(r)$. They move in a viscous medium that is characterized by the friction coefficient of a single particle, which we denote by $\xi_0$. We assume that the friction felt by a particle is independent of the particle density and configuration, and thus we neglect hydrodynamic interactions [23]. Each particle moves under the combined influence of the interparticle force derived from the potential $V(r)$ and a self-propulsion force [24].

In the active Brownian particles model in Refs. [25, 26] it is assumed that the magnitude of the self-propulsion force is constant whereas its direction changes via rotational Brownian motion. If needed, to distinguish this model from other models of active particles we will refer to it as the rotational diffusion active Brownian particles model.

We use a slightly different model of active particles, introduced in Ref. [27] and then analyzed in Ref. [21]. An essentially identical model was independently introduced and studied by Maggi et al. [28].

Specifically, we assume that the self-propulsion force does not have a constant magnitude and it evolves in time according to the Ornstein-Uhlenbeck process. We note that the rotational diffusion active Brownian particles model and our model can be considered to be limiting cases of a more general model in which the direction of the self-propulsion force randomly rotates and its magnitude fluctuates. Most likely, neither limiting case perfectly describes active particles studied in experiments. The advantage of our model is that the equations of motion for the self-propulsion are linear, which makes some theoretical considerations somewhat easier. In particular, we showed that the complete steady-state distribution can be found for a single particle in a harmonic potential for our model [27]. We note that our model can be considered to be a continuous time version of the model used by Berthier [10]. Finally, we mention that a mapping was derived between the rotational diffusion active Brownian particles model and our model [26, 29]. This mapping preserves the self-propulsion autocorrelation function. However, higher moments of the self-propulsion are different.

We assume that the self-propelled particles are large enough so that any Brownian motion due to the thermal fluctuations of the viscous medium (solvent) can be neglected. Thus, the system is purely athermal and the particles move under the sole influence of the interparticle interactions and self-propulsion.

The above qualitative discussion translates into the following equations of motion for the positions and self-propulsions,

$$\begin{align*}
\dot{r}_i &= \frac{1}{\xi_0} \left[ f_i + F_i \right], \tag{5} \\
\dot{f}_i &= -r_p^{-1} f_i + \eta_i. \tag{6}
\end{align*}$$

In Eq. (5), $r_i$ is the position of particle $i$, $\xi_0$ the friction coefficient of an isolated particle, $f_i$ is the self-propulsion acting on particle $i$ and $F_i$ is the force acting on particle $i$ originating from the interactions,

$$F_i = -\sum_{j \neq i} \nabla J V(r_{ij}). \tag{7}$$

In Eq. (6), $\tau_p$ is the persistence time of the self-propulsion and $\eta_i$ is an internal Gaussian noise with zero mean and variance

$$\langle \eta_i(t) \eta_j(t') \rangle = 2 D_f I \delta_{ij} \delta(t - t'), \tag{8}$$

where $\langle \ldots \rangle_{\text{noise}}$ denotes averaging over the noise distribution, $D_f$ is the noise strength and $I$ is the unit tensor. Without interactions, particles evolving according to Eqs. (5-6) perform a persistent random walk with the mean-square displacement [30]

$$\langle (r_i(t) - r_i(0))^2 \rangle = 6 D_f f_p^2 \frac{t}{\xi_0} \left( t + \tau_p(e^{-t/\tau_p} - 1) \right). \tag{9}$$

According to Eq. (9), the short-time motion is ballistic,

$$\langle (r_i(t) - r_i(0))^2 \rangle \approx \frac{3 D_f f_p^2 t^2}{\xi_0^2} \quad t \ll \tau_p \tag{10}$$

and the long-time motion, $t \gg \tau_p$, is diffusive with diffusion coefficient $D_0$,

$$D_0 = D_f f_p^2 \frac{t}{\xi_0^2}. \tag{11}$$

Comparing expression (11) with the well-known formula for the diffusion coefficient of a Brownian particle moving in a viscous medium with friction constant $\xi_0$, $D_{\text{Brownian}} = k_B T / \xi_0$ (we use units such that the Boltzmann constant $k_B = 1$), we can define the single-particle effective temperature [27],

$$T_{\text{eff}} = D_0 \xi_0 = D_f f_p^2 / \xi_0. \tag{12}$$

The single particle effective temperature could be used as one of the independent control parameters, together with the number density $\rho$ and the persistence time $\tau_p$.

Eqs. (5-6) are a convenient starting point for computer simulations. In theoretical considerations it is more useful to describe the system using probability distributions and their associated evolution equations. The most fundamental description of our system, equivalent to equations of motion (5-6), uses the joint $N$-particle probability distribution of positions and self-propulsions,
$P_N(r_1, f_1, ..., r_N, f_N; t)$. This distribution evolves in time with evolution operator $\Omega$
\[ \partial_t P_N(r_1, f_1, ..., r_N, f_N; t) = \Omega P_N(r_1, f_1, ..., r_N, f_N; t), \quad (13) \]
which can be derived [30] from equations of motion (5-6),
\[ \Omega = -\xi_0^{-1} \sum_i \nabla_i \cdot (f_i + F_i) + \sum_i \frac{\partial}{\partial r_i} \left( \tau_p^{-1} f_i + D_f \frac{\partial}{\partial r_i} \right). \quad (14) \]

We recall that for non-interacting active particles Eqs. (13-14) are formally equivalent to the Fokker-Planck equation that describes the motion of non-interacting Brownian particles on a time scale on which their velocity relaxation can be observed [30]. Thus, a system of non-interacting active particles is formally equivalent to particles moving under the influence of thermal solvent fluctuations. This equivalence is absent for a system of interacting active particles. In particular, it should be emphasized that according to Eqs. (5-6) or, equivalently, Eqs. (13-14), self-propulsions evolve autonomously, independently of the configuration of the particles.

We will assume that our system can achieve a stationary state. In other words, there exists a steady-state probability distribution $P_{ss}^N(r_1, f_1, ..., r_N, f_N)$ such that
\[ \Omega P_{ss}^N(r_1, f_1, ..., r_N, f_N) = 0. \quad (15) \]

We emphasize that, in general, the joint steady-state distribution of positions and self-propulsions does not factorize into a product of steady-state distributions of particle positions and self-propulsions,
\[ P_{ss}^N(r_1, f_1, ..., r_N, f_N) \neq P_{ss}^N(r_1, ..., r_N) P_{ss}^N(f_1, ..., f_N), \quad (16) \]
where $P_{ss}^N(r_1, ..., r_N)$ and $P_{ss}^N(f_1, ..., f_N)$ are the steady-state distributions of positions and self-propulsions,
\[ P_{ss}^N(r_1, ..., r_N) = \int df_1 ... df_N P_{ss}^N(r_1, f_1, ..., r_N, f_N), (17) \]
\[ P_{ss}^N(f_1, ..., f_N) = \int dr_1 ... dr_N P_{ss}^N(r_1, f_1, ..., r_N, f_N). (18) \]

In general, neither the joint steady-state distribution $P_{ss}^N(r_1, f_1, ..., r_N, f_N)$ nor the steady-state distributions of positions $P_{ss}^N(r_1, ..., r_N)$ are known exactly (for approximate theories for the latter distribution see Refs. [28, 29]). However, the steady-state distribution of self-propulsions has a simple form,
\[ P_{ss}^N(f_1, ..., f_N) \propto \exp \left( -\frac{\sum_i f_i^2}{2 D_f} \tau_p \right). \quad (19) \]

Evolution operator (14) allows us to rewrite the definitions of the intermediate scattering functions (1-2),
\[ F(q; t) = \frac{1}{N} \langle n(q) \exp (\Omega t) n(-q) \rangle, \quad (20) \]
\[ F_s(q; t) = \langle n_s(q) \exp (\Omega t) n_s(-q) \rangle. \quad (21) \]

In Eq. (20) $n(q)$ is the Fourier transform of the microscopic density,
\[ n(q) = \sum_i e^{-iq \cdot r_i}, \quad (22) \]
and in Eq. (21) $n_s(q)$ is the Fourier transform of the microscopic tagged particle (tracer) density,
\[ n_s(q) = e^{-iq \cdot r_1}. \quad (23) \]

Note that we chose the tagged particle to be the particle number one; this choice is made arbitrarily and for convenience only. In Eqs. (20-21) $\Omega$ is the evolution operator (14), and brackets $\langle \ldots \rangle$ denote averaging over the joint steady-state distribution of positions and self-propulsions (15). We emphasize that in Eqs. (20-21) and in all similar formulas the steady-state distribution stands to the right of the quantity being averaged, and all operators act on it too.

### III. THE MAIN ASSUMPTION: ABSENCE OF CURRENTS

The fundamental difficulty posed by driven systems originates from the absence of detailed balance. The lack of detailed balance allows for the existence of non-trivial currents. It has been argued that at a mesoscopic level, in some systems without aligning interactions, i.e. after some coarse-graining (i.e. above a certain length and time scale), there are no currents and the active system becomes equivalent to a passive system [31].

Our main assumption is that in our model system, in the steady state the currents vanish after integrating out the self-propulsions. This assumption, together with additional coarse-graining over time, will allow us to approximate our system by a passive system with detailed balance.

A similar assumption was implicitly used by Farage and Brader. However, as discussed in the next section, their theory and ours use different passive systems to approximate an active system. In particular, we retain correlations between (overdamped) velocities of different particles.

To make our assumption explicit we first rewrite the equation of motion for the joint probability distribution of positions and self-propulsions, Eq. (13), in the form of a continuity equation,
\[ \partial_t P_N(r_1, f_1, ..., r_N, f_N; t) = \]
\[ - \sum_i \nabla_i \cdot j_i(r_1, f_1, ..., r_N, f_N; t) \]
\[ - \sum_i \frac{\partial}{\partial r_i} : j_f^i (r_1, f_1, ..., r_N, f_N; t), \quad (24) \]
where current densities are defined as
\[ j_i(r_1, f_1, ..., r_N, f_N; t) = \xi_0^{-1} (f_i + f_i) P_N(r_1, f_1, ..., r_N, f_N; t), \quad (25) \]
\[ j_i^{\text{f}}(r_1, f_1, \ldots, r_N, f_N; t) = \]
\[- \left( \tau_p^{-1} f_i + D_f \frac{\partial}{\partial f_i} \right) P_N(r_1, f_1, \ldots, r_N, f_N; t) \].

Current densities (25-26) are microscopic quantities, which may be non-zero in a system without detailed balance. Our main assumption is that in the steady state, the current density in the position space, integrated over self-propulsions, vanishes,
\[
\int \text{d}f_1 \ldots \text{d}f_N j_i^{\text{f}}(r_1, f_1, \ldots, r_N, f_N; t) = \int \text{d}f_1 \ldots \text{d}f_N \left[ f_i + \xi \right] P_N^{\text{ss}}(r_1, f_1, \ldots, r_N, f_N) = 0.
\]

Assumption (27) implies that the local steady-state average of the self-propulsion is equal to the negative of the force,
\[
\langle f_i \rangle_{\text{LSS}} = -F_i,
\]
where the local steady-state average is defined as
\[
\langle \ldots \rangle_{\text{LSS}} = \frac{1}{P_N^{\text{ss}}(r_1, \ldots, r_N)} \int \text{d}f_1 \ldots \text{d}f_N \ldots P_N^{\text{ss}}(r_1, f_1, \ldots, r_N, f_N).
\]

Eq. (28) could be interpreted as stating a balance of the self-propulsion of particle \( i \) and the total potential force acting on this particle, for a given configuration of the system.

We are not aware of any study that specifically focused on the existence of non-trivial steady-state currents in high density active systems without aligning interactions [33]. We note that the assumption (27) is made at the level of \( N \)-particle quantities. Thus, its direct simulational verification seems rather difficult. However, it might be possible to define and measure reduced (few-particle) current densities. Alternatively, it might be possible to analyze theoretically and then verify computationally the consequences of the presence/absence of currents. For example, one could try to derive a theory for an effective temperature of the active system and then to compare it with a recent simulational investigation [32]. Finally, one could try to develop an approximate expression for the \( N \)-particle joint steady-state distribution of positions and self-propulsions and investigate the validity of Eq. (27) directly. Preliminary results from such a project [34] suggest that, in general, steady-state currents exist and thus Eq. (27) constitutes an approximation. We will return to the consequence of the assumption made in Eq. (27) in future work.

IV. EFFECTIVE EQUATION OF MOTION FOR THE DISTRIBUTION OF PARTICLE POSITIONS

As emphasized in Sec. II, in our model active system the evolution of the self-propulsions does not depend on the configuration and density of the particles. On the other hand, for any interparticle interactions with a strongly repulsive short-range part of the interaction potential, in a dense system the positions of the particles change slowly. Intuitively, upon increasing the strength of the interactions in a dense active system, one expects qualitatively similar slowing down as in a passive system. By and large, this expectation has been borne out by computer simulations [9, 10, 12, 21] albeit with some caveats.

Thus, it seems reasonable to assume that in strongly interacting systems of active particles without aligning interactions the self-propulsions relax faster than the positions of the particles. This separation of times scales suggests that it should be possible to derive an approximate equation of motion for the probability of particles’ positions only. We expect that such an equation should become progressively more accurate in the strong interaction limit.

We should recall that our goal is to describe the dynamics of density fluctuations in the steady state of our model active system. Thus, we only need an approximate equation of motion for the probability of particles’ positions in the vicinity of the steady state. For this reason, in our considerations we introduce the steady-state distribution and, effectively, we use the gradient of the logarithm of this distribution with respect to the position of a given particle as a (normalized) effective force acting on this particle (see Eq. (42)). This construction is different from the approach of Furage and Brader [20] who concentrate on transient density fluctuations.

To facilitate the derivation of the equation of motion for the probability of particles’ positions we introduce a projection operator that acts on an \( N \)-particle probability distribution of self-propulsions and positions and projects it on a local steady-state distribution, \( \text{i.e.} \) on a distribution in which self-propulsions have a steady-state distribution for a given sample of positions,

\[
P_{\text{LSS}} P_N(r_1, f_1, \ldots, r_N, f_N; t) =
\frac{P_N^{\text{ss}}(r_1, f_1, \ldots, r_N, f_N)}{P_N(r_1, \ldots, r_N)} \int \text{d}f_1 \ldots \text{d}f_N P_N(r_1, f_1, \ldots, r_N, f_N; t) =
\frac{P_N^{\text{ss}}(r_1, f_1, \ldots, r_N, f_N)}{P_N^{\text{ss}}(r_1, \ldots, r_N)} P_N(r_1, \ldots, r_N; t).
\]

We note that by integrating \( P_{\text{LSS}} P_N(r_1, f_1, \ldots, r_N, f_N; t) \) over self-propulsions we get the probability distribution of particles’ positions, \( P_N(r_1, \ldots, r_N; t) \).

Next, we define the orthogonal projection,
\[
Q_{\text{LSS}} = \mathcal{I} - P_{\text{LSS}},
\]
and write down equations of motion for \( P_{\text{LSS}} P_N(r_1, f_1, \ldots, r_N, f_N; t) \) and \( Q_{\text{LSS}} P_N(r_1, f_1, \ldots, r_N, f_N; t) \),
\[
\partial_t P_{\text{LSS}} P_N(r_1, f_1, \ldots, r_N, f_N; t) =
\mathcal{P}_{\text{LSS}} \mathcal{Q}_{\text{LSS}} P_N(r_1, f_1, \ldots, r_N, f_N; t) +
\mathcal{P}_{\text{LSS}} \mathcal{Q}_{\text{LSS}} P_N(r_1, f_1, \ldots, r_N, f_N; t),
\]
\[
(32)
\]
\( \partial_t \mathcal{Q}_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; t) = -Q_{\text{lss}} \Omega_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; t) + Q_{\text{lss}} \Omega \mathcal{Q}_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; t). \) \hspace{1cm} (33)

Since our goal is to calculate the intermediate scattering functions, Eqs. (20-21), which are functions of positions only, we can assume that

\[ Q_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; t = 0) = 0. \] \hspace{1cm} (34)

Then we can solve Eqs. (32-33) for the Laplace transform, \( \mathcal{L}T \), of \( \partial_t \mathcal{Q}_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; t) \) and we obtain

\[ \mathcal{L}T \left[ \partial_t \mathcal{Q}_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; t) \right] (z) = \left[ \mathcal{P}_{\text{lss}} \Omega \mathcal{Q}_{\text{lss}} \frac{1}{z - \mathcal{Q}_{\text{lss}} \Omega \mathcal{Q}_{\text{lss}}} \right] \mathcal{P}_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; z) \] \hspace{1cm} (35)

The first term inside the brackets on right-hand-side of Eq. (35) reads

\[ \mathcal{P}_{\text{loc}} \mathcal{Q}_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; z) = \frac{\mathcal{P}_{\text{loc}} \mathcal{Q}_{\text{lss}}}{\mathcal{P}_{\text{loc}}} P_N(r_1, f_1, ..., r_N, f_N) \cdot \left[ \nabla \frac{P_N(r_1, ..., r_N; z)}{P_N(r_1, ..., r_N)} \right] \] \hspace{1cm} (36)

We see that if current densities vanish in the steady state, Eq. (27), this term vanishes. Furthermore, one can show that

\[ \mathcal{Q}_{\text{lss}} \mathcal{Q}_{\text{lss}} P_N(z) = -\xi_0^{-1} \sum_i (f_i - \langle f_i \rangle_{\text{lss}}) \mathcal{P}_{\text{loc}} P_N(r_1, f_1, ..., r_N, f_N) \cdot \left[ \nabla \frac{P_N(r_1, ..., r_N; z)}{P_N(r_1, ..., r_N)} \right] \] \hspace{1cm} (37)

and

\[ \mathcal{P}_{\text{lss}} \mathcal{Q}_{\text{lss}} = -\frac{\mathcal{P}_{\text{loc}}}{\mathcal{P}_{\text{loc}}} P_N(r_1, f_1, ..., r_N, f_N) \xi_0^{-1} \sum_i \nabla_i \cdot \int df_1 ... df_N (f_i - \langle f_i \rangle_{\text{lss}}) \] \hspace{1cm} (38)

So far, we have not made any approximations. To proceed, we will need to deal with projected evolution operator \( \mathcal{Q}_{\text{lss}} \mathcal{Q}_{\text{lss}} \) in Eq. (35). This operator describes evolution in the space orthogonal to the local steady-state space. The simplest possible approximation is to assume that this evolution is entirely due to the free relaxation of the self-propulsions. In this case \( \mathcal{Q}_{\text{lss}} \mathcal{Q}_{\text{lss}} \) is approximated as follows

\[ \mathcal{Q}_{\text{lss}} \mathcal{Q}_{\text{lss}} \approx \sum_{i=1}^{N} \frac{\partial}{\partial f_i} \left( t_p^{-1} f_i + D_j \frac{\partial}{\partial f_j} \right). \] \hspace{1cm} (39)

We note that approximation (39) is equivalent to assuming that the time-scale of the self-propulsion’s relaxation is the same in non-interacting and interacting systems. This can be approximately valid for our model active system but, in particular, it would be an unreasonable approximation in the presence of aligning interactions. We recall that in our system the evolution of the self-propulsions is independent of the positions of the particles. Thus, the approximation (39) neglects the influence of the correlations between self-propulsions and positions on the evolution of the self-propulsions. Combining this approximation with Eqs. (37-38) we get the following approximate equality

\[ \mathcal{P}_{\text{lss}} \mathcal{Q}_{\text{lss}} (z - \mathcal{Q}_{\text{lss}} \mathcal{Q}_{\text{lss}})^{-1} \mathcal{Q}_{\text{lss}} \mathcal{Q}_{\text{lss}} P_N(r_1, f_1, ..., r_N, f_N; z) \approx \frac{\mathcal{P}_{\text{loc}} \mathcal{Q}_{\text{lss}}}{\mathcal{P}_{\text{loc}}} P_N(r_1, f_1, ..., r_N, f_N) \xi_0^{-2} \sum_i \nabla_i \cdot \int df_1 ... df_N (f_i - \langle f_i \rangle_{\text{lss}}) \] \hspace{1cm} (40)

Now, we expand \[ z - \sum_{j=1}^{N} \frac{\partial}{\partial f_j} \left( t_p^{-1} f_j + D_j \frac{\partial}{\partial f_j} \right) \] and integrate by parts. Finally, we integrate both sides of the resulting equation over self-propulsions and get the following expression for the Laplace transform of \( \partial_t P_N(r_1, ..., r_N; t) \)

\[ \mathcal{L}T \left[ \partial_t P_N(r_1, ..., r_N; t) \right] (z) = \xi_0^{-2} \sum_{i,j} \nabla_i \cdot (z + t_p^{-1})^{-1} (\langle f_i f_j \rangle_{\text{lss}} - \langle f_i \rangle_{\text{lss}} \langle f_j \rangle_{\text{lss}}) \cdot [-F_{ij} + \nabla_j] P_N(r_1, ..., r_N; z). \] \hspace{1cm} (41)
where $\mathbf{F}_{j}^{\text{eff}}$ is the (normalized) effective force acting on particle $j$ in the steady state,

$$
\mathbf{F}_{j}^{\text{eff}} = \nabla_j \log \mathcal{P}^\text{ss}_N(\mathbf{r}_1, \ldots, \mathbf{r}_N).
$$ (42)

The right-hand-side of Eq. (41) defines the effective evolution operator $\Omega^\text{eff}(z)$,

$$
\Omega^\text{eff}(z) = \xi_0^{-2} \sum_{i,j} \nabla_i \cdot \left( z + \tau_p^{-1} \right)^{-1} \left( \langle \mathbf{f}_i \mathbf{f}_j \rangle^\text{ss} - \langle \mathbf{f}_i \rangle^\text{ss} \langle \mathbf{f}_j \rangle^\text{ss} \right) \cdot \left[ -\mathbf{F}_{j}^{\text{eff}} + \nabla_j \right].
$$ (43)

We recall that in approximation (39) the influence of the correlations between self-propulsions and positions on the evolution of the self-propulsions was neglected. In the effective evolution operator (43) the influence of the same correlations on the evolution of the particles’ positions is included through the steady-state correlations of the self-propulsions, $\langle \mathbf{f}_i \mathbf{f}_j \rangle^\text{ss} - \langle \mathbf{f}_i \rangle^\text{ss} \langle \mathbf{f}_j \rangle^\text{ss}$.

Furthermore, we note that in the $z \to 0$ limit (which corresponds to coarse-graining in time) the evolution operator, Eq. (43), becomes formally similar to the evolution operator for a system of Brownian particles with hydrodynamic interactions [23]. This is the formal expression of the equivalence of a coarse-grained active system (i.e. in the space of positions only and on long time scales) and a passive system.

Farage and Brader [20] implicitly assumed the equivalence of a similarly coarse-grained active system (i.e. in the space of positions only and on long time scales) and a passive system without hydrodynamic interactions. Specifically, in order to obtain the effective evolution operator used in Ref. [20] from our operator (43), one needs to replace local steady-state correlations between the self-propulsions by the mean-square of the self-propulsions, $\langle \mathbf{f}_i \mathbf{f}_j \rangle^\text{ss} - \langle \mathbf{f}_i \rangle^\text{ss} \langle \mathbf{f}_j \rangle^\text{ss} \to D_{ij}^{\tau} \delta_{ij} \mathbf{I}$, where $\mathbf{I}$ is the unit tensor, and one needs to take the $z \to 0$ limit. Thus, our theory and the theory of Farage and Brader use different passive systems to approximate a coarse grained active system.

The most important assumption made in this section was approximating $\mathcal{Q}^\text{ss} \Omega^\text{ss}$ by the free relaxation of the self-propulsions. We shall see later that this assumption allows us to recover the correct short time dependence of the intermediate scattering function.

We recall once again that according to our model’s evolution equations, Eqs. (5-6), the self-propulsions evolve independently of the positions. However, in general, due to the coupled steady-state distribution of the self-propulsions and positions, the characteristic time for the transition from the short-time ballistic to diffusive motion (which is equal to $\tau_p$ for non-interacting particles, see Eq. (9)) depends on the strength of the interparticle interactions. We referred to this change in Ref. [21] as a renormalization of the relaxation rate of the self-propulsions by the interactions. As we will see later, approximating $\mathcal{Q}^\text{ss} \Omega^\text{ss}$ by the free relaxation of the self-propulsions is equivalent to neglecting of any such renormalization.

To improve upon this approximation one could try the alternative approach presented in Appendix A. This approach will likely lead to a more accurate description of the short-time dynamics. However, this advantage is outweighed by its computational complexity. In the remainder of this paper we will use the approximate effective evolution operator (43).

V. SHORT-TIME DYNAMICS: IMPORTANCE OF CORRELATIONS BETWEEN SELF-PROPELLSIONS AND POSITIONS

Here we briefly discuss the short-time dynamics of the scattering functions. First, we derive and discuss the explicit expressions for the second time derivatives of the scattering functions. We emphasize the importance of the correlations between the self-propulsions acting on the particles and their positions for the correct description of the short-time dynamics. Second, we point out that the effective evolution operator (43) leads to the correct results for the second time derivatives of the scattering functions.

To evaluate the short-time behavior of the intermediate scattering function we expand expression (20) in powers of $t$,

$$
F(q; t) = \frac{1}{N} \langle n(q)n(-q) \rangle + \frac{t}{N} \langle n(q)Qn(-q) \rangle + \frac{t^2}{2N} \langle n(q)Q^2n(-q) \rangle + \ldots
$$ (44)

The first term at the right-hand-side of Eq. (44) is the steady state static structure factor,

$$
S(q) = \frac{1}{N} \langle n(q)n(-q) \rangle,
$$ (45)

the second term vanishes due to symmetry, and the third term gives

$$
\frac{t^2}{2N} \langle n(q)Q^2n(-q) \rangle = -\frac{t^2q^2}{2N\xi_0} \langle \sum_i (\mathbf{f}_i + \mathbf{F}_i) e^{-i\mathbf{q}\cdot\mathbf{r}_i} \sum_j (\mathbf{f}_j + \mathbf{F}_j) e^{i\mathbf{q}\cdot\mathbf{r}_j} \rangle \cdot \hat{\mathbf{q}} = -\frac{t^2q^2}{2} \omega_{||}(q).
$$ (46)

In Eq. (46), $\omega_{||}(q)$ is a function that quantifies correlations of velocities of individual particles,

$$
\omega_{||}(q) = \frac{1}{N\xi_0^2} q \cdot \langle \sum_{i,j} (\mathbf{f}_i + \mathbf{F}_i)(\mathbf{f}_j + \mathbf{F}_j) e^{-i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \rangle \cdot \hat{\mathbf{q}}.
$$ (47)

The interpretation of function $\omega_{||}(q)$ comes from the fact that $\xi_0^{-1} \mathbf{f}_i + \mathbf{F}_i$ is the velocity of particle $i$ for our overdamped system, see Eq. (5). Computer simulation results [21] show that, at constant single particle effective
temperature $T_{\text{eff}}$, Eq. (12), with increasing the persistence time (i.e., with increasing departure from equilibrium), $\omega_\parallel(q)$ gradually develops significant oscillations while its overall magnitude decreases.

To summarize, the short-time expansion reads,

$$ F(q; t) = S(q) - \frac{q^2 t^2}{2} \omega_\parallel(\infty) + ... $$  \hspace{1cm} (48) 

This should be compared to the standard result for a colloidal suspension,

$$ F^{\text{BD}}(q; t) = S(q) - q^2 t D_0 H(q) + ... $$  \hspace{1cm} (49) 

where $D_0$ is the diffusion coefficient of a single isolated Brownian particle and $H(q)$ is the hydrodynamic factor [23] and the Newtonian dynamics result,

$$ F^{\text{ND}}(q; t) = S(q) - \frac{q^2 t^2 k_B T}{2m} + ... $$  \hspace{1cm} (50) 

where $k_B$ is the Boltzmann constant, $T$ is the temperature and $m$ is the particle mass.

The analogous calculation for the self-intermediate scattering function gives

$$ F_s(q; t) = 1 - \frac{q^2 t^2}{2} \omega_\parallel(\infty) + ... $$  \hspace{1cm} (51) 

whereas for a colloidal system one gets

$$ F^{\text{BD}}_s(q; t) = 1 - q^2 t D_0 H(\infty) + ... $$  \hspace{1cm} (52) 

where $D_0$ is the diffusion coefficient of a single isolated Brownian particle and $H(\infty) = \lim_{q \to \infty} H(q)$, and the result for a Newtonian system reads

$$ F^{\text{ND}}_s(q; t) = 1 - \frac{q^2 t^2 k_B T}{2m} + ... $$  \hspace{1cm} (53) 

The above results show that our active system has features of both colloidal and Newtonian systems. Its short-time dynamics involves a non-trivial steady-state correlation function $\omega_\parallel(q)$ quantifying spatial correlations of particles’ velocities which plays a role similar to that of the hydrodynamic factor $H(q)$. On the other hand, the short-time dynamics of the active system is ballistic, like in a Newtonian system. However, the origin of this ballistic behavior is self-propulsion rather than inertia.

It can be showed that the same results for the short-time dynamics are obtained if one starts from expressions for the scattering functions in terms of the effective evolution operator (43). The difference between the exact expressions and those involving the effective evolution operator appears at $t^4$ order.

VI. MEMORY FUNCTION REPRESENTATION

In this section we rewrite the formal expression (20) for the intermediate scattering function in terms of the so-called frequency matrix and irreducible memory matrix. The latter quantity contains all the (unknown) non-trivial dynamic information about the system. The resulting expression for the density correlation function in terms of the frequency matrix and the memory matrix is known as the memory function representation.

We start by re-writing of the Laplace transform of the intermediate scattering function in terms of the approximate evolution operator (43),

$$ \mathcal{L}T[F(q; t)](z) \equiv F(q; z) = N^{-1} \left\langle n(q) \left( z - \Omega \right)^{-1} n(-q) \right\rangle = N^{-1} \left\langle n(q) \left( z - \Omega^{\text{eff}}(z) \right)^{-1} n(-q) \right\rangle_r. $$  \hspace{1cm} (54) 

Here $\langle ... \rangle_r$ denotes averaging over the steady-state distribution of particles’ positions.

To derive the memory function representation of $F(q; z)$ we use the projection operator approach [16, 36, 39]. We define a projection operator on the microscopic density

$$ P_n = ... n(-q)_r \langle n(q) n(-q) \rangle^{-1}_r \langle n(q) \rangle ... . $$  \hspace{1cm} (55) 

We emphasize that projection operator $P_n$ is defined in terms of the steady-state distribution, unlike in the approach of Farage and Brader [20]. Next, we use the identity

$$ \frac{1}{z - \Omega^{\text{eff}}(z)} = \frac{1}{z - \Omega^{\text{eff}}(z) Q_n} + \frac{1}{Q_n} \frac{1}{z - \Omega^{\text{eff}}(z)} P_n \frac{1}{z - \Omega^{\text{eff}}(z)}, $$  \hspace{1cm} (56) 

where $Q_n$ is the projection on the space orthogonal to that spanned by the microscopic density,

$$ Q_n = \mathcal{I} - P_n, $$  \hspace{1cm} (57) 

to rewrite the Laplace transform of the time derivative of $NF(q; t)$ in the following way
The frequency matrix is given by the following expression

\[ \mathcal{L}[\partial_t N F(q; t)](z) = \left\langle n(q) \Omega_{\text{eff}}^{\text{eff}}(z) \frac{1}{z - \Omega_{\text{eff}}(z)} n(-q) \right\rangle_r = \left\langle n(q) \Omega_{\text{eff}}^{\text{eff}}(z) \mathcal{P}_n \frac{1}{z - \Omega_{\text{eff}}(z)} n(-q) \right\rangle_r \]

\[ + \left\langle n(q) \Omega_{\text{eff}}^{\text{eff}}(z) Q_n \frac{1}{z - \Omega_{\text{eff}}(z)} n(-q) \right\rangle_r = \left\langle n(q) \Omega_{\text{eff}}^{\text{eff}}(z) n(-q) \right\rangle_r \left\langle n(q) n(-q) \right\rangle_r^{-1} \left\langle n(q) \frac{1}{z - \Omega_{\text{eff}}(z)} n(-q) \right\rangle_r \]

\[ + \left\langle n(q) \Omega_{\text{eff}}^{\text{eff}}(z) Q_n \frac{1}{z - \Omega_{\text{eff}}(z)} Q_n \Omega_{\text{eff}}^{\text{eff}}(z) n(-q) \right\rangle_r \left\langle n(q) n(-q) \right\rangle_r^{-1} \left\langle n(q) \frac{1}{z - \Omega_{\text{eff}}(z)} n(-q) \right\rangle_r. \] (58)

The important part of the first term on the right-hand-side of the last equality sign in Eq. (58) is the matrix element of the effective evolution operator, \( \left\langle n(q) \Omega_{\text{eff}}^{\text{eff}}(z) n(-q) \right\rangle_r \), which can be expressed in terms of the frequency matrix \( \mathcal{H}(q; z) \),

\[ \left\langle n(q) \Omega_{\text{eff}}^{\text{eff}}(z) n(-q) \right\rangle_r = -q^2 N \mathcal{H}(q; z). \] (59)

The frequency matrix is given by the following expression

\[ \mathcal{H}(q; z) = \frac{\hat{q} \cdot \left\langle \sum_{i,j} \left( f_i f_j \right)_{\text{lss}} - \left( f_i \right)_{\text{lss}} \left( f_j \right)_{\text{lss}} \right\rangle_r e^{-i q \cdot (r_i - r_j)} \cdot \hat{q} \cdot N \xi_0^2 \left( z + \tau_p^{-1} \right) }{1} \] (60)

In Eq. (60) \( \hat{q} \) is a unit vector, \( \hat{q} = q / q \). In turn, the non-trivial part of the frequency matrix is represented by the function \( \omega_{\|}(q) \) introduced in Sec. V, which quantifies correlations of velocities of individual particles,

\[ \frac{1}{N \xi_0^2} \hat{q} \cdot \left\langle \sum_{i,j} \left( f_i f_j \right)_{\text{lss}} - \left( f_i \right)_{\text{lss}} \left( f_j \right)_{\text{lss}} \right\rangle_r e^{-i q \cdot (r_i - r_j)} \cdot \hat{q} = \frac{1}{N \xi_0^2} \hat{q} \cdot \left\langle \sum_{i,j} \left( f_i \right)_{\text{lss}} + F_i \right\rangle \left( f_j \right)_{\text{lss}} + F_j \left\rangle_r e^{-i q \cdot (r_i - r_j)} \cdot \hat{q} = \frac{1}{N \xi_0^2} \hat{q} \cdot \left\langle \sum_{i,j} \left( f_i + F_i \right) \left( f_j + F_j \right) \right\rangle_r e^{-i q \cdot (r_i - r_j)} \cdot \hat{q} = \omega_{\|}(q) \] (61)

To arrive at the penultimate line of Eq. (47) we utilized Eq. (28) and to arrive at the last line we used the fact that the local steady-state average followed by averaging over particles’ positions is equivalent to the full steady-state average,

\[ \langle \ldots \rangle_{\text{lss}} = \langle \ldots \rangle. \] (62)

We note that the penultimate line of Eq. (47) shows that \( \omega_{\|}(q) \) quantifies fluctuations around the force balance condition (28).

The important part of the second term at the right-hand-side of the last equality sign in Eq. (58) can be expressed in terms of reducible [36, 37] memory matrix \( \mathcal{M}(q; z) \),

\[ \left\langle n(q) \Omega_{\text{eff}}^{\text{eff}}(z) Q_n \frac{1}{z - \Omega_{\text{eff}}^{\text{eff}}(z)} Q_n \Omega_{\text{eff}}^{\text{eff}}(z) n(-q) \right\rangle_r = q^2 N \mathcal{M}(q; z). \] (63)

The memory matrix is given by the following expression

\[ \mathcal{M}(q; z) = \left( N \xi_0^4 \left( z + \tau_p^{-1} \right)^2 \right)^{-1} \hat{q} \cdot \left\langle \sum_{i,j} e^{-i q \cdot r_i} \left( f_i f_j \right)_{\text{lss}} - \left( f_i \right)_{\text{lss}} \left( f_j \right)_{\text{lss}} \right\rangle_r \cdot \hat{q} \times \left[ -\nabla_j + F_j^{\text{eff}} \right] Q_n \frac{1}{z - \Omega_{\text{eff}}^{\text{eff}}(z)} Q_n \sum_{l,m} \nabla_l \cdot \left( f_l f_m \right)_{\text{lss}} - \left( f_l \right)_{\text{lss}} \left( f_m \right)_{\text{lss}} e^{i q \cdot r_m} \cdot \hat{q} \] (64)

We can now rewrite the Laplace transform of the intermediate scattering function in terms of the frequency

\[ F(q; z) = \frac{S(q)}{z + q^2 \left( \mathcal{H}(q; z) - \mathcal{M}(q; z) \right) / S(q)} \] (65)
where $S(q)$ is the steady-state structure factor,

$$S(q) = \langle n(q)n(-q) \rangle_r \equiv \langle n(q)n(-q) \rangle. \quad (66)$$

The second equality sign in Eq. (66) follows from the fact that for self-propulsion-independent quantities averaging over particles’ positions is equivalent to averaging over the full steady-state distribution of positions and self-propulsions.

Eq. (65) is the active matter equivalent of the memory function representation of the intermediate scattering function of a Brownian colloidal suspension derived by Ackerson [35]. As pointed out by Cichocki and Hess [36] and later elaborated by Kawasaki [37], the memory matrix that enters into Ackerson’s formula is not fully irreducible. Both Cichocki and Hess, and Kawasaki argued that approximations should be applied to the fully irreducible memory matrix. Therefore, we will follow the analysis presented in Refs. [36, 37] and derive an irreducible memory matrix.

We define the irreducible evolution operator $\Omega^{\text{irr}}(z)$,

$$\Omega^{\text{irr}}(z) = Q_n \Omega^{\text{eff}}(z) Q_n - \delta \Omega^{\text{irr}}(z) \quad (67)$$

where the subtraction term $\delta \Omega^{\text{irr}}(z)$ [38] reads

$$\delta \Omega^{\text{irr}}(z) = Q_n \left( -N \zeta_0^2 \left( z + t^{-1} \right)^2 \right) \sum_{i,j} \nabla_i \cdot \left( \langle f_i f_j \rangle_{bs} - \langle f_i \rangle_{bs} \langle f_j \rangle_{bs} \right) e^{iq \cdot r_j} \right) \cdot \hat{q} \left( \mathcal{H}(q; z) \right)^{-1}$$

$$= \hat{q} \left( \sum_k e^{-i q \cdot r_k} \left( \langle f_k f_i \rangle_{bs} - \langle f_k \rangle_{bs} \langle f_i \rangle_{bs} \right) \cdot \left( \nabla_i - \beta F_i^{\text{eff}} \right) Q_n \right)$$

Next, we define the irreducible memory matrix $M^{\text{irr}}(q; z)$, which is given by the expression analogous to Eq. (64) but with the projected evolution operator $Q_n \Omega^{\text{eff}}(z) Q_n$ replaced by irreducible evolution operator $\Omega^{\text{irr}}(z)$,

$$M^{\text{irr}}(q; z) = \left( N \zeta_0^2 \left( z + t^{-1} \right)^2 \right) \sum_{i,j} \nabla_i \cdot \left( \langle f_i f_j \rangle_{bs} - \langle f_i \rangle_{bs} \langle f_j \rangle_{bs} \right) \cdot \left( \nabla_i - \beta F_i^{\text{eff}} \right) Q_n$$

Finally, we use an identity similar to Eq. (56),

$$\frac{1}{z - Q_n \Omega^{\text{eff}}(z) Q_n} = \frac{1}{z - \Omega^{\text{irr}}(z)} + \frac{1}{z - \Omega^{\text{irr}}(z)} \delta \Omega^{\text{eff}}(z) \frac{1}{z - Q_n \Omega^{\text{eff}}(z) Q_n},$$

and we derive the following relation between $M(q; z)$ and $M^{\text{irr}}(q; z)$,

$$M(q; z) = M^{\text{irr}}(q; z) - M^{\text{irr}}(q; z) \mathcal{H}^{-1}(q; z) M(q; z). \quad (71)$$

Combining Eqs. (65) and (71) we arrive at the following representation of the intermediate scattering function in terms of the irreducible memory matrix,

$$F(q; z) = \frac{S(q)}{z + \frac{\mathcal{H}(q; z)/M(q; z)}{1 + M^{\text{irr}}(q; z)/M(q; z)}} \quad (72)$$

Eq. (72) is the active matter equivalent of the memory function representation of the intermediate scattering function of a Brownian colloidal suspension derived by Cichocki and Hess [36]. The latter equation was the starting point of the derivation of the mode-coupling theory for the glassy dynamics of colloidal systems [39].

In spite of the formal similarity between Eq. (72) and the irreducible memory function representation of the intermediate scattering function of a Brownian system, these equations are only equivalent if we take the limit $z \to 0$ in the frequency matrix term. In fact, as we have already stated a couple of times, active system performs interacting persistent Brownian motion and, therefore, its short time dynamics is ballistic rather than diffusive (we emphasize that, in this context, the term ballistic does not imply inertia, which is irrelevant for our overdamped system). The ballistic character of the short-time dynamics can be clearly seen if Eq. (72) is re-written in the following way. First, we rewrite Eq. (72) by introducing the irreducible memory function $M^{\text{irr}}(q; z)$,

$$\left(z + t^{-1} + M^{\text{irr}}(q; z) \right) \left(z F(q; z) - F(q; t = 0)\right) = - \left(\omega_q(q)^2/S(q)\right) F(q; z). \quad (73)$$

where the memory function reads

$$M^{\text{irr}}(q; z) = \left(z + t^{-1}\right)^2 M^{\text{irr}}(q; z)/\omega_q(q). \quad (74)$$
Next, we rewrite Eq. (73) in the time domain,

\[
\partial_t^2 F(q; t) + \tau_p \partial_t F(q; t) + \frac{\omega \parallel(q) q^2}{S(q)} F(q; t) = \int_0^t dt' M^{irr}(q; t - t') \partial_{t'} F(q; t'),
\]

(75)

where \(M^{irr}(q; t)\) is the inverse Laplace transform of \(M^{irr}(q; z)\). We note that the resulting equation, Eq. (75), has the same form as the memory function equation for the intermediate scattering function of a Newtonian system.

Let us discuss the meaning of the different terms in Eq. (75), starting with the three terms at its left-hand-side. The presence of the second time derivative implies ballistic dynamics at short times. For our system of self-propelled particles the origin of the ballistic behavior is the persistence of the self-propulsion. The first time derivative term describes the relaxation of the ballistic motion due to the evolution of the self-propulsion. Since we neglected the influence of the interactions on the evolution of the self-propulsion (recall Eq. (39)), the relaxation time of the self-propulsion is unchanged and equal to \(\tau_p\). The third term at the left-hand-side of Eq. (75) describes the collective random motion of the particles on time scale longer than the persistence time of the self-propulsion. On such a time scale, the second derivative term in Eq. (75) can be neglected. Then (recall that we are neglecting the right-hand side term for a moment), the intermediate scattering function \(F(q; t)\) evolves diffusively,

\[
F(q; t) \propto \exp \left( -\frac{\omega \parallel(q) \tau_p q^2}{S(q)} t \right).
\]

(76)

and \(\omega \parallel(q) \tau_p / S(q)\) plays the role of the short-time collective diffusion coefficient. This simple exponential time dependence of density correlations is modified by the presence of the memory function term at the right-hand-side of Eq. (75). The memory function term describes an internal time-delayed friction generated by the inter-particle interactions. This term leads to slow and glassy dynamics through a feedback mechanism implicit in the mode-coupling approximation (see discussion after Eq. (93)).

The non-equilibrium nature of the active system manifests itself in Eq. (75) through the presence of \(\omega \parallel(q)\), which quantifies spatial correlations between velocities of different particles. In particular, the second time derivative of the intermediate scattering function at \(t = 0\) is expressed in terms of \(\omega \parallel(q)\),

\[
\partial_t^2 F(q; t) \big|_{t=0} = -\frac{\omega \parallel(q) q^2}{S(q)} F(q; t = 0) \equiv -\omega \parallel(q) q^2,
\]

(77)

Eq. (77) agrees with the short-time expansion discussed in Sec. V. In the next section we will show that \(\omega \parallel(q)\) also enters an approximate expression for the so-called vertex function.

**VII. MODE-COUPLING-LIKE APPROXIMATION**

In order to make Eq. (75) useful we need an explicit expression for the memory function. Since the memory function contains all the non-trivial dynamic information about the system, there is little hope to derive an exact expression for it. Here we use the factorization approximation, which is also at the heart of the mode-coupling theory of glassy dynamics [16] and thus we call our approach a mode-coupling-like approximation.

Specifically, to derive an approximate expression for the memory function we follow the steps of the derivation of the mode-coupling theory for systems evolving with Brownian dynamics [39]. The derivation consists of three steps.

First, we project onto the subspace of density pairs,

\[
\hat{q} \cdot \left( \sum_{i,j} e^{-i \mathbf{q} \cdot \mathbf{r}_i} \left( \langle \mathbf{f}_i, \mathbf{f}_j \rangle_{\text{bs}} - \langle \mathbf{f}_i \rangle_{\text{bs}} \langle \mathbf{f}_j \rangle_{\text{bs}} \right) \cdot \left[ -\nabla_j + \mathbf{F}^{\text{eff}}_j \right] Q_n \right) \\
\approx \sum_{q_1, \ldots, q_4} \hat{q} \cdot \left( \sum_{i,j} e^{-i \mathbf{q} \cdot \mathbf{r}_i} \left( \langle \mathbf{f}_i, \mathbf{f}_j \rangle_{\text{bs}} - \langle \mathbf{f}_i \rangle_{\text{bs}} \langle \mathbf{f}_j \rangle_{\text{bs}} \right) \cdot \left[ -\nabla_j + \mathbf{F}^{\text{eff}}_j \right] Q_n \right)_{n_2}^{-1} \langle Q_n n_2(q_1, q_2) \rangle_{r}^{-1} \langle Q_n n_2(q_3, q_4) \rangle_{r}^{-1}.
\]

(78)

Here \(n_2(q_1, q_2)\) is the Fourier transform of the microscopic two-particle density,

\[
n_2(q_1, q_2) = \sum_{l,m} e^{-i q_1 \cdot r_l - i q_2 \cdot r_m},
\]

(79)

and \(\langle Q_n n_2(q_1, q_2) \rangle_{r}^{-1}\) is the inverse of the correlation matrix of microscopic pair densities. We should emphasize the importance of using in Eq. (78) only the parts of the microscopic pair density that are orthogonal to the microscopic density, i.e. using \(Q_n n_2(q_1, q_2)\) rather than \(n_2(q_1, q_2)\). The presence of the
operator $Q_n$ is necessary for the existence of the inverse of the correlation matrix $\langle Q_{n_2}(q_1, q_2) Q_{n_2}(-q_3, -q_4) \rangle_r$ \[40\].

Second, we factorize averages resulting from substituting projection (78) into the expression for the memory function and at the same time replace the irreducible operator $\Omega^{irr}(z)$ by effective evolution operator $\Omega^{eff}(z)$. We should emphasize that this factorization has to be done in the time domain,

\[
\begin{align*}
\mathcal{L}^{-1} \left[ \left\langle Q_{n_2}(q_1, q_2) (z - \Omega^{irr}(z))^{-1} Q_{n_2}(-q_1, -q_4) \right\rangle_r \right] & \approx \\
\mathcal{L}^{-1} \left[ \left\langle n(q_1) (z - \Omega^{eff}(z))^{-1} n(-q_3) \right\rangle_r \right] & \mathcal{L}^{-1} \left[ \left\langle n(q_2) (z - \Omega^{eff}(z))^{-1} n(-q_4) \right\rangle_r \right] \{3 \leftrightarrow 4\}.
\end{align*}
\]

Here $\mathcal{L}^{-1}$ denotes the inverse Laplace transform and $\{3 \leftrightarrow 4\}$ means the preceding expression with labels 3 and 4 interchanged. Consistently with Eq. (80) we also factorize the steady-state correlation matrix of microscopic pair densities and for its inverse we get

\[
\begin{align*}
\langle Q_{n_2}(q_1, q_2) Q_{n_2}(-q_3, -q_4) \rangle_r^{-1} & \approx \\
\langle n(q_1) n(-q_3) \rangle_r^{-1} & \langle n(q_2) n(-q_4) \rangle_r^{-1} + \{3 \leftrightarrow 4\}.
\end{align*}
\]

Third, we approximate the vertex functions. Due to the presence of the velocity correlations, this last step is somewhat more complex than the approximation used in the derivation of the standard mode-coupling theory \[39\]. We will explain it on the example of the left vertex, $\mathcal{V}_l$, which is given by the following formula

\[
\begin{align*}
\mathcal{V}_l(q; q_1, q_2) &= \\
\xi_0^{-2} q \cdot \sum_{i,j} e^{-i(q-r_1)} (\langle f_i f_j \rangle_{bs} - \langle f_i \rangle_{bs} \langle f_j \rangle_{bs}) \cdot \\
& \times [ - \nabla_j + F_j^{eff} ] Q_{n_2}(-q_1, -q_2) / r \\
& = \xi_0^{-2} q \cdot \sum_{i,j} e^{-i(q-r_1)} (f_i + F_i) (f_j + F_j) \cdot \\
& \times [ - \nabla_j + F_j^{eff} ] Q_{n_2}(-q_1, -q_2).
\end{align*}
\]

Due to the presence of the projection operator $Q_n$, the left vertex consists of two terms,

\[
\begin{align*}
\mathcal{V}_l(q; q_1, q_2) &= \\
- \xi_0^{-2} q \cdot \sum_{i,j} e^{-i(q-r_1)} (f_i + F_i) (f_j + F_j) \cdot \\
& \times [ \nabla_j n_2(-q_1, -q_2) ] \\
+ & \xi_0^{-2} q \cdot \sum_{i,j} e^{-i(q-r_1)} (f_i + F_i) (f_j + F_j) \cdot \\
& \times [ \nabla_j n(-q) ] \langle n(q) n(-q) \rangle_r^{-1} \langle n(q) n_2(-q_1, -q_2) \rangle_r.
\end{align*}
\]

We will start with the second term, which is a bit easier to analyze. With the help of convolution approximation function and $\langle n(q) n_2(-q_1, -q_2) \rangle_r$ by effective evolution operator $\Omega^{eff}(z)$, we can rewrite the second term in the following form,

\[
\xi_0^{-2} q \cdot \sum_{i,j} e^{-i(q-r_1)} (f_i + F_i) (f_j + F_j) \cdot \\
\times [ \nabla_j n(-q) ] \langle n(q) n(-q) \rangle_r^{-1} \langle n(q) n_2(-q_1, -q_2) \rangle_r \\
\approx i \xi_0^{-2} q \cdot \sum_{i,j} (f_i + F_i) (f_j + F_j) e^{-i q \cdot (r_1 - r_2)} \cdot q \\
\times S(q_1) S(q_2) \delta_{q,q_1+q_2}.
\]

where in the last step we used the fact that for an isotropic system the tensor $\langle \sum_{i,j} (f_i + F_i) (f_j + F_j) e^{-i q \cdot (r_1 - r_2)} \rangle$ has only components parallel and perpendicular to $q$, and that its parallel component is proportional to $\omega(q)$, see Eq. (47).

The first term at the right-hand-side of Eq. (83) can be rewritten as follows,

\[
\begin{align*}
- \xi_0^{-2} q \cdot \sum_{i,j} e^{-i(q-r_1)} (f_i + F_i) (f_j + F_j) \cdot \\
\times [ \nabla_j n_2(-q_1, -q_2) ] \\
\approx - \xi_0^{-2} q \cdot \sum_{i,j} e^{-i(q-r_1)} (f_i + F_i) (f_j + F_j) \cdot \\
\times [ \nabla_j n(-q) ] \langle n(q) n(-q) \rangle_r^{-1} \langle n(q) n_2(-q_1, -q_2) \rangle_r \\
\times \left[ i q \cdot \sum_{i,j} e^{i q \cdot r_1} \sum_{l} e^{i q \cdot r_2} \{ 1 \leftrightarrow 2 \} \right].
\end{align*}
\]

Now, we use an approximation which is a generalization of the convolution approximation to correlation functions.
involving active particles’ velocities,
\[ \zeta_0^{-2} \left( \sum_{i,j} e^{-i\mathbf{q}_i \cdot \mathbf{r}_i} (f_i + F_i) (f_j + F_j) e^{i\mathbf{q}_j \cdot \mathbf{r}_j} \right) \approx \]
\[ NC_0^2 \omega(\mathbf{q}) (\langle \delta f \delta f \rangle)^{-1} \cdot \omega(\mathbf{q}_1)S(q_2) \delta_{q_1,q_1+q_2}. \quad (87) \]

Here \( \omega(\mathbf{q}) \) is the tensorial version of \( \omega_\parallel(q) \).
\[ \omega(\mathbf{q}) = \frac{1}{N \zeta_0} \left( \sum_{i,j} (f_i + F_i) (f_j + F_j) e^{-i\mathbf{q} \cdot \mathbf{r}_i} \right), \quad (88) \]

and \( (\langle \delta f \delta f \rangle)^{-1} \) is the inverse of the correlation matrix of single-particle velocities,
\[ \langle \delta f \delta f \rangle = \frac{1}{N} \left( \sum_i (f_i + F_i) (f_i + F_i) \right). \quad (89) \]

Note that \( \lim_{q \to \infty} \omega(\mathbf{q}) = \langle \delta f \delta f \rangle / \zeta_0^2 \). Using convolution approximation (87) and symmetry properties of tensors \( \omega(\mathbf{q}) \) and \( \langle \delta f \delta f \rangle \) we can finally write the first term (86) in the following form
\[ -iN \mathbf{q} \cdot \left[ \mathbf{q}_1 \omega_\parallel(q) \omega_\parallel(q_1) S(k_2) / \omega_\parallel(\infty) \right. \]
\[ + q_2 \omega_\parallel(q) \omega_\parallel(q_2) S(q_1) / \omega_\parallel(\infty) \] \( \left. \right] \delta_{q_1,q_1+q_2}, \quad (90) \]

where \( \omega_\parallel(\infty) = \lim_{q \to \infty} \omega_\parallel(q) = (3N/\zeta_0^2)^{-1} \left( \sum_i (f_i + F_i)^2 \right) \).

Combining Eqs. (85) and (90) we get the following approximate expression for the left vertex,
\[ \mathcal{V}(\mathbf{q}; q_1, q_2) \approx -iN S(q_1) S(q_2) \omega_\parallel(q) \]
\[ \times \left[ \mathbf{q} \cdot \mathbf{q}_1 \left( \frac{\omega_\parallel(q_1)}{\omega_\parallel(\infty) S(q_1)} - 1 \right) + \{1 \leftrightarrow 2 \} \right] \]
\[ = iN\rho S(q_1) S(q_2) \omega_\parallel(q) \left[ \mathbf{q} \cdot \mathbf{q}_1 C(q_1) + \mathbf{q} \cdot \mathbf{q}_2 C(q_2) \right] \quad (91) \]

where a new function \( C(q) \) reads
\[ \rho C(q) = 1 - \frac{\omega_\parallel(q)}{\omega_\parallel(\infty) S(q)}. \quad (92) \]

We note that if correlations between particles’ velocities are neglected (i.e. if \( \omega_\parallel(q) \) is set equal to 1), \( C(q) \) becomes an analogue of the direct correlation function for our steady-state active system.

The right vertex can be analyzed in the same way. We note that in the standard mode-coupling theory there is a close correspondence between the vertices that enter the expression for the memory function for the collective intermediate scattering function and those that enter the expression for the memory function for the self-intermediate scattering function. We should emphasize that this correspondence is also present in our approach; compare Eqs. (91) and (B27). Since the derivation of the vertices that enter the expression for the memory function for the self-intermediate scattering function is more straightforward, the presence of this correspondence serves as an additional check for the derivation presented above.

Combining the three steps and taking the thermodynamic limit we arrive at the following expression for the irreducible memory function,
\[ M^{irr}(q; t) = \frac{\rho \omega_\parallel(q)}{2} \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^3} \delta(\mathbf{q} - \mathbf{q}_1 - \mathbf{q}_2) \]
\[ \times (\mathbf{q} \cdot [\mathbf{q}_1 C(q_1) + \mathbf{q}_2 C(q_2)])^2 F(q_1; t) F(q_2; t). \quad (93) \]

Expression (93) resembles the corresponding expression derived within the standard mode-coupling theory. It describes a dynamic feedback mechanism: the time-delayed internal friction arising due to interparticle interactions decays due to the relaxation of the two-particle density, which is included at the level of factorization approximation (80). Thus, slow decay of density fluctuations feeds back into slow decay of the irreducible memory function.

Eq. (93) incorporates the non-equilibrium nature of the active system through the presence of the velocity correlations described through function \( \omega_\parallel(q) \). This function sets the overall scale of the memory function. More importantly, it enters into the expression for new function \( C(q) \), Eq. (92), and thus contributes to the vertices, which weight relative contributions of density fluctuations to the memory function. As we will see in the next section, it is the presence of the velocity correlations in the vertices that influences the location of the ergodicity breaking transition.

**VIII. ERGODICITY BREAKING TRANSITION AND LONG-TIME DYNAMICS CLOSE TO THE TRANSITION**

In general, one needs to solve the combined set of Eqs. (75) and (93) numerically. However, as we show in this section, even without a numerical solution we can draw some general conclusions from these equations.

First, let us assume that the system, as described by Eqs. (75) and (93), undergoes an ergodicity breaking transition. At such a transition, the intermediate scattering function does not decay to zero. The long-time limit of this function, \( \lim_{t \to \infty} F(q; t) = F(q) \equiv f(q) \), is the order parameter of the non-ergodic state. Following the procedure used in the standard mode-coupling theory [16] we can derive a self-consistent equation for the normalized order parameter, \( f(q) \),
\[ \frac{f(q)}{1 - f(q)} = m(q) \quad (94) \]

where \( m(q) \) is given by the following equation
\[ m(q) = \frac{\rho}{2q^2} \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^3} \delta(q - q_1 - q_2) S(q_1) S(q_2) \]
\[ \times (\mathbf{q} \cdot [\mathbf{q}_1 C(q_1) + \mathbf{q}_2 C(q_2)])^2 f(q_1) f(q_2). \quad (95) \]
The self-consistent equation for the order parameter is very similar to the equation derived in the standard mode-coupling theory. The only difference is that the role of the function describing the effective interaction, which in the standard mode-coupling theory is played by the direct correlation function, is now played by the new function $C(q)$ which involves both the steady-state structure factor, $S(q)$, and the function describing spatial correlations of the particles’ velocities, $\omega_{||}(q)$. The presence of $\omega_{||}(q)$ in the vertex function means that the location of the ergodicity breaking transition is not exclusively determined by the local steady-state structure.

Finally, to look at the long-time dynamics in the ergodic phase but close to the ergodicity breaking transition, it is convenient to introduce a normalized correlator, $\phi(q; t) = F(q; t)/S(q)$. The equation of motion, Eq. (75), in the Laplace space and re-written in terms of the correlator $\phi(q; z)$, has the following form,

$$
\frac{\phi(q; z)}{1 - z\phi(q; z)} = \frac{z + \tau^{-1} + (\omega_{||}(q)q^2/S(q))m(q; z)}{\omega_{||}(q)q^2/S(q)}, \quad (96)
$$

where $m(q; z)$ is the Laplace transform of the reduced memory function $m(q; t)$,

$$
m(q; t) = \frac{\rho}{2q^2} \int \frac{dq_1 dq_2}{(2\pi)^3} \delta(q - q_1 - q_2)S(q)S(q_1)S(q_2) \times (q \cdot [q_1 C(q_1) + q_2 C(q_2)])^2 \phi(q_1; t)\phi(q_2; t). \quad (97)
$$

Near the ergodicity breaking transition, for small $z$ the memory function $m(q; z)$ becomes very large. Thus, for small $z$ (i.e. for long times), we can approximate Eq. (96) by the following one,

$$
\frac{\phi(q; z)}{1 - z\phi(q; z)} = m(q; z). \quad (98)
$$

Eq. (98) has the structure identical to that of the equation of motion for the long-time dynamics near the ergodicity breaking transition described by the standard mode-coupling theory. This means that all analytical results based on the standard mode-coupling theory carry over to the present theory for the dynamics of the active system. In particular, the only quantity that one needs to do in order to predict the so-called mode-coupling exponents is to calculate the exponent parameter $\lambda$ [16]. This parameter can be calculated from the solution of the self-consistent equation for the order parameter, Eqs. (94-95) at the ergodicity breaking transition.

The reduced memory function $m(q; z)$ differs from the corresponding quantity of the standard mode-coupling theory by the presence of the new function $C(q)$, which involves $S(q)$ and $\omega_{||}(q)$. Again, due to the fact that the correlation function of particles’ velocities enters into $m(q; t)$, the static structure factor does not completely determine the system’s dynamics.

IX. DISCUSSION

We presented here the details of the derivation of a recently proposed theory for the dynamics of dense athermal active systems. The theory, in a natural way, identifies a new function that influences both short- and long-time dynamics. This new function quantifies spatial correlations of the particles’ velocities in the stationary state. The presence of the new function implies that the dynamics is not determined by the local structure only.

The influence of the additional steady-state function on the dynamics allows us to describe an un-expected result obtained in computer simulations [21]. We found that for a range of single-particle effective temperatures upon increasing departure from equilibrium (by increasing the relaxation time of the self-propulsion), the local structure becomes monotonically more pronounced whereas the long-time dynamics first speeds up and then slows down. We showed in Ref. [21] that our theory, combined with steady-state correlation functions obtained from computer simulations of a model single-component, moderately supercooled system, is able to describe qualitatively correctly the non-monotonic dependence of the long-time dynamics on the persistence time of the self-propulsion.

Our theory shares the most important approximation, the factorization approximation, with the mode-coupling theory of glassy dynamics. We showed that if there is an ergodicity breaking transition, our theory predicts that the dynamics upon approaching this transition is qualitatively similar to that predicted by the standard mode-coupling theory close to the corresponding mode-coupling transition.

In future work we would like to extend the present approach to binary mixtures in order to test the theory quantitatively against computer simulations, along the lines of our earlier test of the standard mode-coupling theory [42]. Of particular interest would be to check whether the present theory can predict the location of the dynamic crossover in an active system more accurately than the standard mode-coupling theory can predict the location of the crossover in an equilibrium (thermal) system.

In addition, we would like to investigate the very fundamental approximation of the theory concerning the absence of the steady-state currents. In this context, we would like to develop and test a theory for effective temperatures in the active system.

Finally, in real experimental active systems both self-propulsion and thermal Brownian forces are very often present. For this reason, we would like to develop a more general theory that would be able to account for the presence of the Brownian noise.
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Appendix A: Alternative approximation for $Q_{\text{las}} \Omega Q_{\text{las}}$

We start by noting that due to Eqs. (37) and (38) the quantity we need to calculate is a specific matrix element of the inverse operator $(z - Q_{\text{las}} \Omega Q_{\text{las}})^{-1}$

\[
\sum_{i,j} \nabla_i \cdot \left( (f_j - \langle f_j \rangle_{\text{las}}) (z - Q_{\text{las}} \Omega Q_{\text{las}})^{-1} (f_j - \langle f_j \rangle_{\text{las}}) \right)_{\text{las}} P_N^\text{ss}(r_1, ..., r_N) \cdot \nabla_m
\]

\[
\approx \sum_{i,j,l,m} \nabla_i \cdot \left( (f_l f_j - \langle f_j \rangle_{\text{las}} (f_j)_{\text{las}}) \cdot \left[ (f_j - \langle f_j \rangle_{\text{las}}) (z - Q_{\text{las}} \Omega Q_{\text{las}}) (f_l - \langle f_l \rangle_{\text{las}}) \right]_{\text{las}}^{-1} \right.
\]

\[
\cdot (f_l f_m - \langle f_l \rangle_{\text{las}} (f_m)_{\text{las}}) P_N^\text{ss}(r_1, ..., r_N) \cdot \nabla_m
\]  

(A2)

Then we note that

\[
\langle (f_j - \langle f_j \rangle_{\text{las}}) Q_{\text{las}} \Omega Q_{\text{las}} (f_l - \langle f_l \rangle_{\text{las}}) \rangle_{\text{las}} = \langle (f_j - \langle f_j \rangle_{\text{las}}) \Omega f_i \rangle_{\text{las}}
\]

\[
= [P_N^\text{ss}(r_1, ..., r_N)]^{-1} \int df_1 ... df_N (f_j - \langle f_j \rangle_{\text{las}}) \Omega f_i P_N^\text{ss}(r_1, f_1, ..., r_N, f_N) = \tau_p^{-1} (f_j f_l - \langle f_j \rangle_{\text{las}} (f_l)_{\text{las}}) - 2D_J f_{ij} \delta_{j\alpha} \delta_{i\beta}.
\]

(Eqs. (A2-3)) lead to the following approximate effective evolution operator,

\[
\Omega^{\text{eff}}(z) = \xi_0^{-2} \sum_{i,j,l,m} \nabla_i \cdot \left( (f_l f_j - \langle f_j \rangle_{\text{las}} (f_j)_{\text{las}}) \cdot \left[ (z - \tau_p^{-1}) (f_j f_l - \langle f_j \rangle_{\text{las}} (f_l)_{\text{las}}) + 2D_J f_{ij} \delta_{j\alpha} \delta_{i\beta} \right]^{-1} \right.
\]

\[
\cdot (f_l f_m - \langle f_l \rangle_{\text{las}} (f_m)_{\text{las}}) \cdot [-\mathbf{F}^{\text{eff}} + \nabla_j].
\]  

(A4)

Following the spirit of the first Enskog approximation used in the kinetic theory we introduce the following approximation,

\[
\mathcal{L}T [F_r(q; t)](z) \equiv F_r(q; z) = \langle n_s(q) (z - \Omega)^{-1} n_s(-q) \rangle = \langle n_s(q) (z - \Omega^{\text{eff}}(z))^{-1} n_s(-q) \rangle_r.
\]  

(B1)

To derive the memory function representation of $F(q; z)$ we use the projection operator approach [16, 36, 39]. We define a projection operator on the microscopic tagged particle density

\[
\mathcal{P}_s = \ldots n_s(-q) \mathcal{P}_s n_s(q) \ldots.
\]  

(B2)
Note that \((n_s(q)n_s(-q))_r \equiv 1\) and thus we do not need to include a normalization constant in definition (B2).

Next, we use the identity

\[
\frac{1}{z - \Omega_{\text{eff}}(z)} = \frac{1}{z - \Omega_{\text{eff}}(z)Q_s} + \frac{1}{z - \Omega_{\text{eff}}(z)Q_s} \Omega_{\text{eff}}(z)P_s \frac{1}{z - \Omega_{\text{eff}}(z)},
\]

where \(Q_s\) is the projection on the space orthogonal to that spanned by the microscopic tagged particle density,

\[
Q_s = I - \mathcal{P}_s,
\]

to rewrite the Laplace transform of the time derivative of \(F_s(q;t)\) in the following way

\[
\mathcal{L}[\partial_t F_s(q; t)] = \left\langle n_s(q)\Omega_{\text{eff}}(z) \frac{1}{z - \Omega_{\text{eff}}(z)} n_s(-q) \right\rangle_r = \left\langle n_s(q)\Omega_{\text{eff}}(z)P_s \frac{1}{z - \Omega_{\text{eff}}(z)} n_s(-q) \right\rangle_r + \left\langle n_s(q)\Omega_{\text{eff}}(z)Q_s \frac{1}{z - \Omega_{\text{eff}}(z)} n_s(-q) \right\rangle_r.
\]

The tagged particle frequency matrix, \(\mathcal{H}_s(q; z)\), is defined in terms of the matrix element of the effective evolution operator,

\[
\left\langle n_s(q)\Omega_{\text{eff}}(z) n_s(-q) \right\rangle_r = -q^2 \mathcal{H}_s(q; z),
\]

where

\[
\mathcal{H}_s(q; z) = \hat{q} \cdot \left( \langle f_i f_i \rangle_{\text{bs}} - \langle f_i \rangle_{\text{bs}} \langle f_i \rangle_{\text{bs}} \right) \cdot \hat{q} = \frac{\omega_i(\infty)}{\xi_0^2(z + \tau_p^{-1})} \frac{z + \tau_p^{-1}}{z},
\]

Explicitly, the memory matrix is given by the following expression

\[
\mathcal{M}_s(q; z) = \left( \xi_0^4(z + \tau_p^{-1})^2 \right)^{-1} \hat{q} \cdot \left( \sum_j e^{-iq \cdot r_j} \left( \langle f_i f_j \rangle_{\text{bs}} - \langle f_i \rangle_{\text{bs}} \langle f_j \rangle_{\text{bs}} \right) \right) \\
\times \left[ -\nabla_j + \mathbf{F}_{\text{eff}} \right] Q_s \frac{1}{z - \Omega_{\text{eff}}(z)Q_s} Q_s \sum_i \nabla_i \cdot \left( \langle f_i f_i \rangle_{\text{bs}} - \langle f_i \rangle_{\text{bs}} \langle f_i \rangle_{\text{bs}} \right) e^{iq \cdot r_i} \cdot \hat{q}.
\]

To define the irreducible tagged particle memory matrix we start by introducing an irreducible evolution operator for the tagged particle motion,

\[
\Omega_{\text{irr}}^s(z) = Q_s \Omega_{\text{eff}}(z)Q_s - \delta\Omega_{\text{eff}}^s(z)
\]

where the subtraction term \(\delta\Omega_{\text{eff}}^s(z)\) reads

\[
\delta\Omega_{\text{eff}}^s(z) = Q_s \xi_0^4(z + \tau_p^{-1})^2 \left( \sum_i \nabla_i \cdot \left( \langle f_i f_i \rangle_{\text{bs}} - \langle f_i \rangle_{\text{bs}} \langle f_i \rangle_{\text{bs}} \right) e^{iq \cdot r_i} \right) \cdot \hat{q} \left( \mathcal{H}_s(q; z) \right)^{-1}
\]
Next, we define the tagged particle irreducible memory matrix $\mathcal{M}_s^{\text{irr}}(q; z)$, which is given by the expression analogous to Eq. (B9) but with the projected evolution operator $Q_s \Omega^\text{eff}(z) Q_s$ replaced by irreducible evolution operator $\Omega_s^{\text{irr}}(z)$,

$$\mathcal{M}_s^{\text{irr}}(q; z) = \left( \frac{c_0}{\sqrt{\tau_p}} \right)^2 Q_s \left( \sum_j e^{-iq \cdot r_j} \left( \langle f_j f_j \rangle_{\text{bs}} - \langle f_j \rangle_{\text{bs}} \langle f_j \rangle_{\text{bs}} \right) \right) \cdot [-\nabla_j + \mathbf{p}^\text{eff}_j] Q_s,$$

$$\mathcal{M}^{\text{irr}}(q; t) = \left( z + 1 - q^2 \omega^\text{eff}(q; z) / H_s^{\text{eff}}(q; z) \right)^{-1} \mathcal{M}_s^{\text{irr}}(q; z) / \omega^{\text{eff}}(q; z),$$

and we derive a relation between $\mathcal{M}_s(q; z)$ and $\mathcal{M}_s^{\text{irr}}(q; z)$,

$$\mathcal{M}_s(q; z) = \mathcal{M}_s^{\text{irr}}(q; z) - \mathcal{M}_s^{\text{irr}}(q; z) \mathcal{H}_{s}^{-1}(q; z) \mathcal{M}_s(q; z).$$

The memory function representation for the self-intermediate scattering functions reads,

$$F_s(q; z) = \mathcal{M}_s^{\text{irr}}(q; z) / \omega^{\text{eff}}(q; z).$$

Finally, we use an identity similar to Eq. (B3),

$$\frac{1}{z - Q_s \Omega^\text{eff}(z) Q_s} = \frac{1}{z - \Omega_s^{\text{irr}}(z)} + \frac{1}{z - \Omega_s^{\text{irr}}(z)} \delta \Omega^\text{eff}(z) / z - Q_s \Omega^\text{eff}(z) Q_s,$$

where $M_s^{\text{irr}}(q; t)$ is the inverse Laplace transform of $M_s^{\text{irr}}(q; z)$. We note that for evolution on the time scale longer than the persistence time the second time derivative term in Eq. (B17) can be neglected. The resulting equation becomes equivalent to that describing the self-intermediate scattering function of a thermal Brownian system with a short time self-diffusion coefficient $\omega^\text{eff}(q; \infty)$. The last observation suggests that, in order to quantify the effect of the time-delayed friction (represented by the memory function term) on the evolution of the active system, one should normalize the time scale by the term describing the short-time dynamics, $\omega^\text{eff}(q; \infty) / \tau_p$.

Finally, we note that Eq. (B17) leads to the following expression for the second time derivative of the self-intermediate scattering function at $t = 0$,

$$\partial_t^2 F_s(q; t)|_{t=0} = -\omega^\text{eff}(q; \infty) q^2 F_s(q; t = 0) \equiv -\omega^\text{eff}(q; \infty) q^2,$$

which agrees with the exact result (51).

To derive an approximate expression for tagged particle memory function, we again follow the three steps [39], with some modifications due to the difference between the tracer (particle number $1$) and all other particles.

First, we project onto the subspace of joint tagged and fluid particle density,

$$Q_s \cdot \left( \sum_j e^{-iq \cdot r_j} \left( \langle f_j f_j \rangle_{\text{bs}} - \langle f_j \rangle_{\text{bs}} \langle f_j \rangle_{\text{bs}} \right) \cdot [-\nabla_j + \mathbf{p}^\text{eff}_j] Q_s \right)$$

$$\approx \sum_{q_1, \ldots, q_4} \left( \sum_j e^{-iq \cdot r_j} \left( \langle f_j f_j \rangle_{\text{bs}} - \langle f_j \rangle_{\text{bs}} \langle f_j \rangle_{\text{bs}} \right) \cdot [-\nabla_j + \mathbf{p}^\text{eff}_j] Q_s n_{s2}(q_1, q_2) Q_s n_{s2}(q_3, q_4) \right)^{-1} \left( Q_s n_{s2}(q_1, q_2) Q_s n_{s2}(q_3, q_4) \right)$$

Here $n_{s2}(q_1, q_2)$ is the Fourier transform of the microscopic joint tagged and fluid particle density,

$$n_{s2}(q_1, q_2) = \sum_{m>2} e^{-iq_1 \cdot r_1 - iq_2 \cdot r_m}.$$
necessary for the existence of the inverse of the correlation matrix \(Q_n s_{2} (q_{1}, q_{2}) \). Second, projecting onto joint tagged-fluid particle densities leads to an expression involving a four-particle correlation function which is factorized. This factorization approximation is the main approximation involved in the present derivation.

\[
\mathcal{L} \mathcal{T}^{-1} \left[ \langle Q_{s} n s_{2} (q_{1}, q_{2}) \rangle \right] \approx \mathcal{L} \mathcal{T}^{-1} \left[ \langle n_{s} (q_{1}) \rangle \right] \mathcal{L} \mathcal{T}^{-1} \left[ \langle n_{s} (q_{2}) \rangle \right].
\]

Consistently with Eq. (B21) we also factorize the steady-state correlation matrix of microscopic joint densities and for its inverse we get

\[
[\langle Q_{s} n s_{2} (q_{1}, q_{2}) Q_{s} n s_{2} (-q_{3}, -q_{4}) \rangle]_{r}^{-1} \approx \delta_{q_{1} q_{3}} \langle n (q_{2}) n (-q_{4}) \rangle_{r}^{-1}.
\]

The final, third step, is concerned with the vertices. The left vertex reads,

\[
\mathcal{V}_{dl}(q; q_{1}, q_{2}) = \xi_{0}^{-2} q \cdot \left( \sum_{j} e^{-i \mathbf{q} \cdot \mathbf{r}_{1}} \left( (f_{j} f_{j})_{bs} - (f_{1})_{bs} (f_{1})_{bs} \right) \right) \cdot \left[ -\nabla_{j} + F_{j}^{\text{eff}} \right] Q_{s} n s_{2} (-q_{1}, -q_{2})_{r} \approx \xi_{0}^{-2} q \cdot \sum_{j} e^{-i \mathbf{q} \cdot \mathbf{r}_{1}} (f_{1} + F_{1}) (f_{j} + F_{j}) \cdot \left[ -\nabla_{j} + F_{j}^{\text{eff}} \right] Q_{s} n s_{2} (-q_{1}, -q_{2}).
\]

Due to the presence of the projection operator \(Q_{n}\), the left vertex consists of two terms,

\[
\mathcal{V}_{dl}(q; q_{1}, q_{2}) = \xi_{0}^{-2} q \cdot \left( \sum_{j} e^{-i \mathbf{q} \cdot \mathbf{r}_{1}} (f_{1} + F_{1}) (f_{j} + F_{j}) \right) \cdot \left[ -\nabla_{j} n s_{2} (-q_{1}, -q_{2}) \right] \approx \xi_{0}^{-2} q \cdot \sum_{j} e^{-i \mathbf{q} \cdot \mathbf{r}_{1}} (f_{1} + F_{1}) (f_{j} + F_{j}) \cdot \left[ -\nabla_{j} n s_{2} (-q_{1}) \right] \langle n_{s} (q) n s_{2} (-q_{1}, -q_{2}) \rangle.
\]

The second term can be expressed in terms of \(\omega_{\|}(\infty)\) and the steady-state structure factor,

\[
\xi_{0}^{-2} q \cdot \sum_{j} e^{-i \mathbf{q} \cdot \mathbf{r}_{1}} (f_{1} + F_{1}) (f_{j} + F_{j}) \cdot \left[ -\nabla_{j} n s_{2} (-q_{1}) \right] \langle n_{s} (q) n s_{2} (-q_{1}, -q_{2}) \rangle = i \omega_{\|}(\infty) \hat{q} \cdot (q_{1} + q_{2}) (S(q_{2}) - 1) \delta_{q_{1} q_{1} + q_{2}}.
\]

The first term at the right-hand-side of Eq. (B24) can be rewritten as follows,

\[
-\xi_{0}^{-2} \hat{q} \cdot \sum_{j} e^{-i \mathbf{q} \cdot \mathbf{r}_{1}} (f_{1} + F_{1}) (f_{j} + F_{j}) \cdot \left[ -\nabla_{j} n s_{2} (-q_{1}, -q_{2}) \right] \approx -\xi_{0}^{-2} \hat{q} \cdot \sum_{j} e^{-i \mathbf{q} \cdot \mathbf{r}_{1}} (f_{1} + F_{1}) (f_{j} + F_{j}) \cdot \left[ i q_{1} e^{i \mathbf{q} \cdot \mathbf{r}_{1}} + i q_{2} e^{i \mathbf{q} \cdot \mathbf{r}_{1}} \right] f_{j} f_{j} + F_{j} f_{j} + F_{j}.
\]

Combining Eqs. (B25) and (B25) we get the following approximate expression for the left vertex,

\[
\mathcal{V}_{dl}(q; q_{1}, q_{2}) \approx -i S(q_{2}) \omega_{\|}(\infty) \hat{q} \cdot (q_{1} + q_{2}) \left( C(q) - 1 \right) \delta_{q_{1} q_{1} + q_{2}},
\]

where function \(C(q) = (1 - 1/S(q))/\rho\), Eq. (92) of the main text. The right vertex can be analyzed in the same way.
Combining the three steps and taking the thermodynamic limit we arrive at the following expression for the irreducible memory function for the tagged particle motion

\[ M_{ii}^{irr}(q; t) = \rho \omega \int_{\mathbb{R}^d} dq_1 dq_2 \frac{1}{(2\pi)^d} \delta(q - q_1 - q_2) \times (q \cdot q_2 C(q_2))^2 F_1(q_1; t) F(q_2; t). \]  

(28)

As we mentioned in the main text of the article, the relation between the approximate expressions for the irreducible memory functions for the collective and tagged particle motion, Eqs. (93) and (B28), is the same as in the standard mode-coupling theory.

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