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Mengkai Feng and Zhonghuai Hou

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Mode-coupling Theory for the Dynamics of Dense Underdamped Active Brownian Particle System

Mengkai Feng and Zhonghuai Hou*
Hefei National Research Center for Physical Sciences at the Microscale & Department of Chemical Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

We present a theory to study the inertial effect on glassy dynamics of the underdamped active Brownian particle (UABP) system. Using the assumption of the nonequilibrium steady-state, we obtain an effective Fokker-Planck equation for the probability distribution function (PDF) as a function of positions and momentums. With this equation, we achieve the evolution equation of the intermediate scattering function (ISF) through the Zwanzig-Mori projection operator method and the mode-coupling theory (MCT). Theoretical analysis shows that the inertia of the particle affects the memory function and corresponding glass transition by influencing the structure factor and a velocity correlation function. The theory provides theoretical support and guidance for subsequent simulation work.

I. INTRODUCTION

Active matter covers a broad range of different materials, including biological living tissues, self-propelled colloidal particles, etc. A number of different systems have been studied in depth, from experimental, theoretical and simulation aspects [1–8]. In recent years, a few novelties of glassy dynamics have been observed in dense active matter systems [9–22]. Results showed that activity changes the glassy behavior of dense passive colloidal fluids rather than simply erasing the glassy phase. Except for the features observed in equilibrium glass-forming liquids, such as dynamic slowing down, non-exponential relaxations and dynamical heterogeneity[23–27], glass transitions of the active matter systems have unique features like non-trivial velocity correlation [14, 20, 21] and different kinds of effective temperatures [20, 28–31]. Although a complete understanding of the glassy dynamics and mechanism of glass transition is still lacking until now [32–41], much less for the active matter glassy behavior with non-equilibrium property, the research of glassy dynamics in active system has received extensive attention[42–49].

In terms of theoretical research, the active glassy dynamics of a variety of models have been studied with different methods. For example, Farage and Brader [50] treated the active Brownian particle (ABP) as normal Brownian particles except the diffusion coefficient as single particle diffusion coefficient. Both this work and Liluashvili *et al.*'s [17] used the idea of integration-through-transient(ITT) to deal with the non-equilibrium characteristic. Meanwhile, Szamel derived an approximate theory for the glassy dynamics of athermal active Ornstein-Uhlenbeck particles (AOUP) at the non-equilibrium steady-state [15], and extended the theory to another system which includes the thermal noises [51]. Both his works depend on the assumption that the non-equilibrium steady-state currents are zeros. The result of the former one predicted a non-monotonic dependence of structural relaxation time on the persistent time of AOUPs, which is consistent with the computer simulations[14]. In this research field, we also proposed a theoretical work on the glassy behavior of ABPs [16], wherein we used the Fox's approximation to handle the active noise as a colored noise. By introducing an effective diffusion coefficient and a persudo-structure factor, our result showed that the activity of particles accelerates the structural relaxation and then pushes the glass transition point to a higher density, in accordance with prior simulation data [12].

Most recently, inertial effect on self-propelled particle system has been studied[30, 52–62]. Ordinarily, the typical Brownian particle moves in a solvent at a very low Reynolds number, which means these particles are highly overdamped, so that the mass of particle is neglectable. However, for some active Brownian particle systems such as self-propelled particles with large size or in solvent free environment, the low Reynolds number condition is on longer satisfied. Finite inertia is relevant for macroscopic objects covering at least three orders of magnitude in size($10^{-3} \sim 10^{0}$m) [63]. An important example is self-propelled granules generated by a vibrating plate, which has been commonly used as a model system in experiment recently [64–67]. In simulations, Löwen *et al.* observed a distinct inertial delay between orientation and velocity of particles [52]. Mandal *et al.* found that in the underdamped active particle system, a temperature difference exists when the motility induced phase separation (MIPS) appears [30]. They also found that a novel reentrant MIPS upon the particle inertia [30]. This result indicates a clear inertial effect on the system structure in nonequilibrium situation. It motivates us to further ask whether this effect exists in glass transition region. Other examples of inertial active particles include the swimmers at air-water interface [68], toy active particle model [69], etc. All these works lead us to contemplate whether the mass of active particles affects the glassy dynamics in dense colloidal systems. So far, the discussion about inertial effect of glass transition is little. Physi-

* E-mail: hzhlj@ustc.edu.cn

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cally, this question may not be a relevant issue in equilibrium statistical mechanics, since the structure factor of dense fluids is only dependent on the temperature and the interactions, instead of the mass of particle. However, this analysis is unsuitable for the non-equilibrium situation, based on the preceding discussions.

Here in this present paper, we developed a mode-coupling theory to study underdamped active Brownian particle in three dimensions. The model is mainly suitable for large particle or solvent-free systems, whose contribution of thermal noises can be neglected. We assume that a nonequilibrium steady-state (NESS) exists, and thereby a PDF can be identified along with the average over this distribution. To study the structure relaxation and glassy dynamics of such systems, we used the Zwanzig-Mori projection operator method and standard mode-coupling factorization approximations, which have been already successfully used in active systems [14–17, 36, 51, 70–72]. Results show that the inertial effect of ABPs is reflected as a correlation function of momentum and structure, which further influences the memory function. Our theory also gives a prediction that the inertia of particles accelerates the structure relaxation.

This paper is organized as follows. In Sec. II, we introduce and briefly discuss the underdamped active particle model with randomly rotational noise, and give some free particle properties for such model. In Sec.III, we discuss the steady-state assumption and corresponding distribution function. In Sec IV, we use the projection operator method and mode-coupling method to derive the evolution equation of a correlation function. We end with discussion in Sec. V.

II. UNDERDAMPED ACTIVE BROWNIAN PARTICLES

A. Modeling

We consider a three-dimensional system consisting of N-interacting self-propelled underdamped particles. Each particle i is propelled by an external force with randomly rotating direction $\mathbf{e}_i$ and constant magnitude f_0. The interaction between two particles is a spherically symmetric potential $V(|\mathbf{r}_i - \mathbf{r}_j|)$, and hydrodynamic interaction has been neglected. The equations of particle motion read

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m} \tag{1a}$$

$$\dot{\mathbf{p}}_i = -\frac{\gamma}{m}\mathbf{p}_i + \mathbf{F}_i\left(\mathbf{r}^N\right) + f_0\mathbf{e}_i \tag{1b}$$

$$\dot{\mathbf{e}}_i = \boldsymbol{\eta}_i \times \mathbf{e}_i \tag{1c}$$

where $\mathbf{r}_i$ and $\mathbf{p}_i$ are the position and momentum vectors of particle i, m and γ are the particle mass and the friction coefficient which are assumed to be the same for each particle, $\mathbf{F}_i = -\sum_{j\neq i}\nabla_i V(|\mathbf{r}_{ij}|)$ is the total interacting force acting on particle i. In Eq.(1c), $\boldsymbol{\eta}_i$ is a Gaussian white noise vector with zero mean $\langle\boldsymbol{\eta}_i(t)\rangle_{\text{noise}} = 0$ and variance $\left\langle\boldsymbol{\eta}_i(t)\boldsymbol{\eta}_j(t')\right\rangle_{\text{noise}} = 2D_r\mathbf{1}\delta_{ij}\delta(t-t')$, where D_r is the rotational diffusion coefficient and $\mathbf{1}$ the unit tensor. The correlation of the direction of propulsion force is $\langle\mathbf{e}_i(t)\mathbf{e}_j(t')\rangle_{\text{noise}} = \frac{1}{3}\exp\left(-2D_r|t-t'|\right)\mathbf{1}\delta_{ij}$ and $\tau_R = (2D_r)^{-1}$ gives the correlation time. Note that we have ingnored the thermal noises in Eq.(1b) and D_r and γ are set as independent parameters. In addition, when the characteristic time scale of inertia $\tau_I = \frac{m}{\gamma}$ tends to zero, Eq.(1b) reduces to $\dot{\mathbf{r}}_i = \gamma^{-1}\mathbf{F}_i\left(\mathbf{r}^N\right) + v_0\mathbf{e}_i$ with $v_0 = f_0/\gamma$, i.e. the overdamped athermal active Brownian particle model.

B. Free particle behavior

For a free UABP, i.e. $\mathbf{F}_i = 0$ in Eqn.(1b), the momentum satisfies $\langle\mathbf{p}_i\rangle = 0$ over the noise average (omitting subscript 'noise' for convenience), as well as variance

$$\left\langle\mathbf{p}_i^2\right\rangle = \frac{f_0^2}{(\gamma/m)(\gamma/m + 2D_r)}, \tag{2}$$

(see details in App.A). Although the system clearly violates the fluctuation-dissipation theorem and thereby the equilibrium state could never be reached, we can still assume that a formal equipartition theorem remains valid here, i.e. $\left\langle\mathbf{p}_i^2\right\rangle = 3mk_BT_{\text{eff}}$. Then, an effective temperature T_{eff} can be defined as

$$k_BT_{\text{eff}} = \frac{\left\langle\mathbf{p}_i^2\right\rangle}{3m} = \frac{f_0^2\tau_R\tau_I^2}{3m(\tau_I + \tau_R)}. \tag{3}$$

In the limit of $D_r \to \infty$, $\langle\mathbf{e}_i(t)\mathbf{e}_i(t')\rangle = (6D_r)^{-1}\delta(t-t')\mathbf{1}$ which corresponds to a white noise with infinitesimal variance. In this circumstance, if f_0 is a finite value, variance of momentum $\left\langle\mathbf{p}_i^2\right\rangle$ tends to zero too. Unless, if f_0^2/D_r is set as a nonzero finite value under $D_r \to \infty$ limit, one has $k_BT_{\text{eff}} = \frac{f_0^2}{6\gamma D_r}$. In this case, the particle actually undergoes an effective *passive* underdamped Brownian motion with effective diffusivity $D_{\text{eff}} = \frac{v_0^2}{6D_r}$.

Now we consider the mean square displacement (MSD) of free UABP. By integrating the momentum correlation function, we have

$$\begin{aligned}\left\langle\Delta\mathbf{r}^2(t)\right\rangle =& \frac{2t}{m^2}\int_0^t\left(1-\frac{s}{t}\right)\langle\mathbf{p}(s)\cdot\mathbf{p}(0)\rangle\,\mathrm{d}s\\ =& \frac{2v_0^2\tau_R}{\tau_R^2-\tau_I^2}\Big[\tau_R^2\left(t-\tau_R+\tau_Re^{-t/\tau_R}\right)\\ &-\tau_I^2\left(t-\tau_I+\tau_Ie^{-t/\tau_I}\right)\Big].\end{aligned} \tag{4}$$

For long-time limit $t\to\infty$, one has $\left\langle\Delta\mathbf{r}^2(t)\right\rangle = 2v_0^2\tau_Rt$, thereby an effective long-time diffusion coefficient can be defined as $D_{\text{eff}} = \lim_{t\to\infty}\frac{\left\langle\Delta\mathbf{r}^2(t)\right\rangle}{6t} = \frac{v_0^2\tau_R}{3} = \frac{v_0^2}{6D_r}$. Yet for

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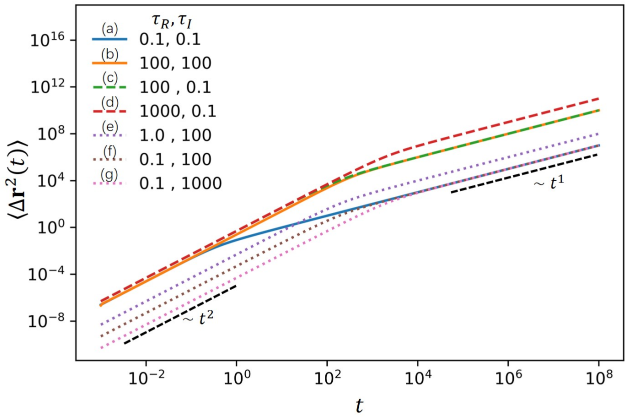

Figure 1. Mean square displacement of free UABP, with $v_0 = 1$, and different τ_R, τ_I. Lines(a,b): for $\tau_I = \tau_R$ case; lines(c,d): for $\tau_R \gg \tau_I$; lines(e,f,g): for $\tau_R \ll \tau_I$. All lines show ballistic movements at short-time region and turn to normal diffusions in long-time scale.

short-time limit $t \to 0$, one has $\left\langle \Delta \mathbf{r}^2(t) \right\rangle = \frac{v_0^2 \tau_R}{(\tau_R + \tau_I)} t^2$, which indicates a superdiffusion behavior at short-time region. Besides, the overdamped limit $\tau_I \to 0$ is also covered by $\left\langle \Delta \mathbf{r}^2(t) \right\rangle = 2 v_0^2 \tau_R \left(t - \tau_R + \tau_R e^{-t/\tau_R} \right)$. In Fig.1, the MSDs with constant v_0 and various τ_I and τ_R are plotted. Clearly, curves (b) and (c) share the same long-time behavior (also the same for (a), (f) and (g)), curves (a) and (d), (c) and (d) share the same short-time behaviors respectively. All MSD curves show crossovers between superdiffusion and normal diffusion. The time scale of transition point τ_c increases with both τ_I and τ_R, roughly $\tau_c \approx \max(\tau_I, \tau_R)$. In addition, it is worth noting that the interplay between τ_R and τ_I significantly influences the movements of the UABP, and consequently the MSDs. We discuss this issue with following cases: (i) $\tau_I \ll \tau_R$, the MSD reduces to $\left\langle \Delta \mathbf{r}^2(t) \right\rangle = v_0^2 t^2$ at short-time scale, thereby all MSDs collapse at this region, see curves (c) and (d); (ii) $\tau_I \gg \tau_R$, the short-time MSD reduces to $\left\langle \Delta \mathbf{r}^2(t) \right\rangle = \frac{v_0^2 \tau_R}{\tau_I} t^2$, therefore the spatial range of superdiffusion is very small in this case (curves (e-g)); (iii) specially $\tau_R = \tau_I$, the MSD reduces to $\left\langle \Delta \mathbf{r}^2(t) \right\rangle = 2 v_0^2 \tau_R \left(t - \tau_R + \tau_R e^{-t/\tau_R} \right)$, which is equivalent to the overdamped athermal ABP case.

Comparing with the typical time scale of glassy dynamics, say τ_α, both τ_I and τ_R are much smaller than τ_α. However, based on the discussion above, we realize that τ_I and τ_R have effects on long-time behavior such as MSD. This motivates us to investigate how these characteristic time scales influence glassy dynamics, through theoretical method in the present work.

III. EFFECTIVE FOKKER-PLANCE EQUATION

The time evolution of the N-particle PDF $P\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N, t\right)$ is governed by the Fokker-Planck equation(FPE), which can be written as

$$\partial_t P\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N, t\right) = \hat{\Omega} P\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N, t\right), \tag{5}$$

$$\hat{\Omega} \equiv \sum_{j=1}^{N} \left[\frac{\partial}{\partial \mathbf{p}_j} \cdot \left(\frac{\gamma}{m} \mathbf{p}_j - \mathbf{F}_j - f_0 \mathbf{e}_j \right) - \frac{\partial}{\partial \mathbf{r}_j} \cdot \frac{\mathbf{p}_j}{m} + D_r \hat{R}_j^2 \right] \tag{6}$$

where $\omega_i = (\theta_i, \phi_i)$ denotes the orientational angle of $\mathbf{e}_i$, $\hat{\Omega}$ denotes the Fokker-Planck operator, $\hat{R}_j = \hat{\theta}_j \partial_{\theta_j} + \frac{1}{\sin\theta_j} \hat{\phi}_j \partial_{\phi_j}$ and $\hat{R}_j^2 = \frac{1}{\sin\theta_j} \partial_{\theta_j} \left(\sin\theta \partial_{\theta_j} \right) + \frac{1}{\sin^2\theta_j} \partial_{\phi_j}^2$ is the rotational diffusion operator in spherical coordinates (θ_i, ϕ_i). For convenience, we define $\hat{\Omega}_R = D_r \sum_{j=1}^{N} \hat{R}_j^2$ to describe the self-propulsion direction part.

A. NESS assumption and reduced PDF

The treatment of NESS is actually a fundamental difficulty in driven systems, due to the absence of detailed balance nature. In principle, it allows the existence of nonzero currents in such steady-state [73]. On the other hand, after the coarse-graining over a certain time scale, the currents vanish at a mesoscopic level, for some systems without any alignment interactions [74]. This indeed brings convenience to the theoretical study of dense active systems. However in the present underdamped system, it is unclear whether this conclusion is still reliable. To avoid this ambiguity, we just assume that the non-equilibrium steady-state exists, satisfying

$$\partial_t P^{ss}\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N\right) = 0, \tag{7}$$

where "ss" stands for steady-state, and do not place further restrictions on steady-state currents.

Our main target is to calculate the ISF $F_q(t)$, which is the time correlation function of density function in Fourier space (also knows as density fluctuations) $\rho_{\mathbf{q}}(t) = \sum_{j=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r}_j(t)}$,

$$\begin{aligned} F_q(t) &= \frac{1}{N} \left\langle \rho_{\mathbf{q}}^*(0) \rho_{\mathbf{q}}(t) \right\rangle \\ &= \frac{1}{N} \sum_{j=1}^{N} \sum_{l=1}^{N} \left\langle e^{-i\mathbf{q}\cdot\mathbf{r}_l(0)} e^{i\mathbf{q}\cdot\mathbf{r}_j(t)} \right\rangle \end{aligned} \tag{8}$$

Here the bracket $\langle \cdots \rangle$ is redefined as the average over the NESS distribution mentioned above, explicitly

$$\langle \cdots \rangle = \int (\cdots) P^{ss}\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N\right) \mathrm{d}\mathbf{r}^N \mathrm{d}\mathbf{p}^N \mathrm{d}\omega^N. \tag{9}$$

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Using the Fokker-Planck equation and operator, we can rewrite the ISF as

$$F_q(t) = \frac{1}{N}\left\langle \rho^*_{\mathbf{q}} e^{\hat{\Omega}t}\rho_{\mathbf{q}}\right\rangle \tag{10}$$

where we must emphasize that, in this bracket, any operator acts on all of the objects standing right of itself, including the steady-state distribution function P^{ss} [75].

According to Eqs.(1a)-(1c), the position and momentum variables do not influence the evolution of self-propulsion. This suggests that it should be available to derive an effective equation of motion for a reduced PDF without self-propulsion variables. Therefore, we introduce the reduced PDF as

$$P_e\left(\mathbf{r}^N, \mathbf{p}^N; t\right) \equiv \int P(\mathbf{r}^N, \mathbf{p}^N, \omega^N; t)\mathrm{d}\omega^N \tag{11}$$

where $\mathrm{d}\omega^N = d\omega_1 d\omega_2 \dots d\omega_N$ and $\mathrm{d}\omega_i = \sin\theta_i \mathrm{d}\theta_i \mathrm{d}\phi_i$. Considering the position, momentum and self-propulsion variables are coupled in the distribution function, one cannot write $P^{ss}\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N\right)$ as a product of steady-state distribution functions of each variable. Yet, we can integrate out the self-propulsion variable to obtain a reduced PDF at steady-state, *viz.*, $P_e^{ss}\left(\mathbf{r}^N, \mathbf{p}^N\right) = \int P^{ss}\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N\right)\mathrm{d}\omega^N$. Furthermore, since $\partial_t P_e^{ss} = \int \hat{\Omega} P^{ss}\mathrm{d}\omega^N = 0$, we get a continuity equation

$$\partial_t P_e^{ss} = -\sum_j \left(\frac{\partial}{\partial \mathbf{r}_j}\cdot \mathbf{j}_j^r + \frac{\partial}{\partial \mathbf{p}_j}\cdot \mathbf{j}_j^p\right) = 0 \tag{12}$$

with two current densities $\mathbf{j}_j^r = \frac{\mathbf{p}_j}{m}P_e^{ss}$ and $\mathbf{j}_j^p = -\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right)P_e^{ss}$, where

$$\langle\cdots\rangle_{lss} = \frac{1}{P_e^{ss}\left(\mathbf{r}^N, \mathbf{p}^N\right)}\int(\cdots)P^{ss}\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N\right)\mathrm{d}\omega^N. \tag{13}$$

is the so-called 'local steady-state' average[15]. Although these currents may not be zeros in such system without detailed balance, a main assumption of our theory is that for each j-particle $\frac{\partial}{\partial \mathbf{r}_j}\cdot \mathbf{j}_j^r + \frac{\partial}{\partial \mathbf{p}_j}\cdot \mathbf{j}_j^p = 0$ holds , i.e.,

$$\frac{\partial}{\partial \mathbf{p}_j}\cdot\left[\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right)P_e^{ss}\right] = \frac{\mathbf{p}_j}{m}\cdot\frac{\partial}{\partial \mathbf{r}_j}P_e^{ss}. \tag{14}$$

Comparing the Szamel's works Ref.[14, 15] where the overdamped athermal AOUP system were studied, the continuity equation leads to a vanishing currents assumption, $\mathbf{F}_j + \langle \mathbf{f}_j\rangle_{lss} = 0$, i.e. local system force $\mathbf{F}_j$ acting on particle j is balanced by the local steady-state averaged active force $\langle \mathbf{f}_j\rangle_{lss}$ in the NESS. Here in the underdamped case, however, such a force balance is violated because the particle has a momentum $\mathbf{p}_j$. Phenomenologically, during the time interval $\Delta t_j \sim \Delta \mathbf{r}_j/(\mathbf{p}_j/m)$, the momentum itself is balanced by the impulse net force $\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right)$ acting on the particle, which is $\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right)\Delta t_j \sim \Delta \mathbf{p}_j$, in accordance with Eq.(14). Such a qualitative discussion here highlights the difference between underdamped and overdamped systems. For shorthand notation, we may rewrite Eq.(14) as $\hat{\Omega}_I P_e^{ss} = 0$, where

$$\hat{\Omega}_I \equiv \sum_j\left[\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right) - \frac{\partial}{\partial \mathbf{r}_j}\cdot\frac{\mathbf{p}_j}{m}\right] \tag{15}$$

and the subscript I means "inertial" since $\hat{\Omega}_I$ would reduce to $\sum_j \gamma^{-1}\left[\mathbf{F}_j + f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right] = 0$ if inertial effect is not taken into account.

B. Projection operator and effective FPE

Here we follow the standard procedure of the Zwanzig-Mori's projector operator method [76]. Setting $\left(\mathbf{r}^N, \mathbf{p}^N\right)$ as the relevant subspace, we can define a projection operator

$$\mathcal{P}_{lss}(\cdots) = \frac{P^{ss}\left(\mathbf{r}^N, \mathbf{p}^N, \omega^N\right)}{P_e^{ss}\left(\mathbf{r}^N, \mathbf{p}^N\right)}\int(\cdots)\mathrm{d}\omega^N, \tag{16}$$

Acting this projection operator $\mathcal{P}_{lss}$ onto the distribution function $P(\mathbf{r}^N, \mathbf{p}^N, \omega^N, t)$, one has

$$\begin{aligned}\mathcal{P}_{lss}P(\mathbf{r}^N, \mathbf{p}^N, \omega^N; t) &= \frac{P^{ss}}{P_e^{ss}}\int P(\mathbf{r}^N, \mathbf{p}^N, \omega^N; t)\mathrm{d}\omega^N \\ &\equiv \frac{P^{ss}}{P_e^{ss}}P_e(\mathbf{r}^N, \mathbf{p}^N; t)\end{aligned} \tag{17}$$

Applying the Laplace transform, $\mathcal{LT}$, to both sides, we have $\mathcal{P}_{lss}\tilde{P}(z) = \left(P^{ss}/P_e^{ss}\right)\tilde{P}_e(z)$, where $\tilde{P}(z) \equiv \mathcal{LT}\left[P(\mathbf{r}^N, \mathbf{p}^N, \mathbf{e}^N; t)\right](z)$ and $\tilde{P}_e(z) \equiv \mathcal{LT}\left[P_e(\mathbf{r}^N, \mathbf{p}^N; t)\right](z)$ are Laplace transforms of the original and reduced PDFs, respectively. After a so-call "Dyson decomposition" (see details in App.B), time evolution of Eq.(17) in Laplace domain is written as

$$\mathcal{LT}\left[\partial_t \mathcal{P}_{lss}P(t)\right](z) = \mathcal{P}_{lss}\hat{\Omega}\mathcal{P}_{lss}\tilde{P}(z) + \mathcal{P}_{lss}\hat{\Omega}\left(z - \mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1}\mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}\tilde{P}(z). \tag{18}$$

Using the definition of $\hat{\Omega}$ and $\mathcal{P}_{lss}$, the first term is solved as

$$\mathcal{P}_{lss}\hat{\Omega}\mathcal{P}_{lss}\tilde{P}(z) = \frac{P^{ss}}{P_e^{ss}}\sum_j \left[\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right) - \frac{\partial}{\partial \mathbf{r}_j}\cdot\left(\frac{\mathbf{p}_j}{m}\right)\right]\tilde{P}_e(z) \equiv \frac{P^{ss}}{P_e^{ss}}\hat{\Omega}_I\tilde{P}_e(z) \tag{19}$$

where $\hat{\Omega}_I$ was introduced in Eq.(15). As already discussed in the last section, this term is nonzero, which is distinct from the case of overdamped systems. For the second term in the rhs of Eq.(18), we need to firstly deal with $\left(z - \mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1}$ term. Herein, an approximation has to be introduced

$$\mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss} \approx \hat{\Omega}_R = D_r\sum_j \hat{R}_j^2, \tag{20}$$

indicating that the rotation of the self-propulsion direction plays a major rule in the dynamical evolution in orthogonal phase space. Then the second term in Eq.(18) is calculated as

$$\begin{aligned}
&\mathcal{P}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\left(z - \mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1}\mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}\tilde{P}(z)\\
\approx&\frac{f_0^2}{z+2D_r}\frac{P^{ss}}{P_e^{ss}}\sum_{ij}\partial_{\mathbf{p}_i}\cdot\left\{\left(\left\langle \mathbf{e}_i\mathbf{e}_j\right\rangle_{lss} - \left\langle \mathbf{e}_i\right\rangle_{lss}\left\langle \mathbf{e}_j\right\rangle_{lss}\right)\cdot\left[\partial_{\mathbf{p}_j} - \left(\partial_{\mathbf{p}_j}\ln P_e^{ss}\right)\right]\right\}\tilde{P}_e(z)\\
\equiv&\frac{P^{ss}}{P_e^{ss}}\hat{\Omega}_A(z)\tilde{P}_e(z)
\end{aligned} \tag{21}$$

where the subscript A simply indicates "activity". Herein, $\left\langle \mathbf{e}_i\mathbf{e}_j\right\rangle_{lss} - \left\langle \mathbf{e}_i\right\rangle_{lss}\left\langle \mathbf{e}_j\right\rangle_{lss}$ is the steady-state correlations of the self-propulsion (directions), and $\hat{\Omega}_A(z)$ describes how such correlations would influence the evolution of particles motion in the subspace $\left(\mathbf{r}^N, \mathbf{p}^N\right)$.

Combining all these results together, we have $\mathcal{LT}\left[\partial_t\mathcal{P}_{lss}P(t)\right](z) = \frac{P^{ss}}{P_e^{ss}}\left[\hat{\Omega}_I + \hat{\Omega}_A(z)\right]\tilde{P}_e(z)$. On the other hand, considering $\mathcal{LT}\left[\partial_t\mathcal{P}_{lss}P(t)\right](z) = \frac{P^{ss}}{P_e^{ss}}\mathcal{LT}\left[\partial_t P_e(t)\right](z)$, we achieve the evolution equation for reduced PDF that does not contain self-propulsion variables

$$\mathcal{LT}\left[\partial_t P_e(t)\right](z) = \hat{\Omega}^{\text{eff}}(z)\,\tilde{P}_e(z) \tag{22}$$

where

$$\begin{aligned}
\hat{\Omega}^{\text{eff}}(z) =& \hat{\Omega}_I + \hat{\Omega}_A(z)\\
=&\sum_{j=1}^N\left[\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right) - \frac{\partial}{\partial \mathbf{r}_j}\cdot\left(\frac{\mathbf{p}_j}{m}\right)\right]\\
&+\sum_{i,j=1}^N\frac{f_0^2}{z+2D_r}\partial_{\mathbf{p}_i}\cdot\left\{\left(\left\langle \mathbf{e}_i\mathbf{e}_j\right\rangle_{lss} - \left\langle \mathbf{e}_i\right\rangle_{lss}\left\langle \mathbf{e}_j\right\rangle_{lss}\right)\cdot\left[\partial_{\mathbf{p}_j} - \left(\partial_{\mathbf{p}_j}\ln P_e^{ss}\right)\right]\right\}
\end{aligned} \tag{23}$$

is the effective Fokker-Planck operator, wherein the first term $\hat{\Omega}_I$ comes from the inertial effect and the second term $\hat{\Omega}_A(z)$ results from particle activity. This operator serves as one of the main results of present work.

In an overdamped ABP system, Szamel obtained a similar effective evolution operator for distribution function[51],

$$\begin{aligned}
\Omega_{sz}^{\text{eff}}(z) = \sum_{ij}\nabla_i\cdot\Bigg[D_t\delta_{ij} + \frac{v_0^2}{z+D_r}\Big(&\left\langle \mathbf{e}_i\mathbf{e}_j\right\rangle_{lss}\\
&- \left\langle \mathbf{e}_i\right\rangle_{lss}\left\langle \mathbf{e}_j\right\rangle_{lss}\Big)\Bigg]\cdot\left[\nabla_j - \left(\nabla_j\ln P_e^{ss}\right)\right]
\end{aligned} \tag{24}$$

wherein we use subscript 'sz' to denote the operator in Szamel's work to avoid confusion. Comparing our result with this operator, $\hat{\Omega}_I$ in $\hat{\Omega}^{\text{eff}}(z)$ has no counterpart here, since particle momentum was not considered. Then, the second term $\hat{\Omega}_A(z)$ in $\hat{\Omega}^{\text{eff}}(z)$ is quite similar in form to the whole effective operator $\Omega_{sz}^{\text{eff}}(z)$, except that $\partial_{\mathbf{p}_i}$ in $\hat{\Omega}_A(z)$ was replaced by ∇_j in $\Omega_{sz}^{\text{eff}}(z)$, since the relevant reduced subspace only involved particle positions there. In addition, the last term $\partial_{\mathbf{p}_j} - \left(\partial_{\mathbf{p}_j}\ln P_e^{ss}\right)$ in $\hat{\Omega}_A(z)$ indicates the diffusion and drift effects of distribution func-

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tion evolution in momentum space, which is governed by self-propulsion force correlation.

Applying inverse Laplace transform on Eq.(22), we also have

$$\frac{\partial}{\partial t}P_e\left(\mathbf{r}^N,\mathbf{p}^N,t\right)=\hat{\Omega}_I P_e(t)+\hat{\Omega}'_A\int_{-\infty}^{t}e^{-2D_r(t-t')}P_e(t')\mathrm{d}t' \quad (25)$$

in real-time domain, where $\hat{\Omega}'_A=(z+2D_r)\hat{\Omega}_A(z)$ is z-independent. This equation shows that operator $\hat{\Omega}'_A$ contributes a memory effect of self-propulsion correlations on the distribution function evolution. In addition, for reduced steady-state distribution function $P_e^{ss}\left(\mathbf{r}^N,\mathbf{p}^N\right)$, considering $\lim_{t\to\infty}P_e(t)=P_e^{ss}$, we have $\frac{\partial}{\partial t}P_e^{ss}=\left[\hat{\Omega}_I+\hat{\Omega}_A(0)\right]P_e^{ss}=\hat{\Omega}^{\mathrm{eff}}(0)\,P_e^{ss}=0$.

IV. MODE-COUPLING THEORY

A. Dynamical variables and correlations

Using the effective operator $\hat{\Omega}^{\mathrm{eff}}(z)$, the intermediate scattering function can be rewritten as in the Laplace domain

$$\mathcal{LT}\left[F_q(t)\right](z)\equiv\tilde{F}_q(z)=\frac{1}{N}\left\langle\rho_{\mathbf{q}}^*\left(z-\hat{\Omega}\right)^{-1}\rho_{\mathbf{q}}\right\rangle \approx\frac{1}{N}\left\langle\rho_{\mathbf{q}}^*\left(z-\hat{\Omega}^{\mathrm{eff}}(z)\right)^{-1}\rho_{\mathbf{q}}\right\rangle_e, \quad (26)$$

wherein the last approximation sign is due to the approximation in the derivation of $\hat{\Omega}^{\mathrm{eff}}(z)$. This equation is the starting point of this section. We derive a memory function representation of $\tilde{F}_q(z)$ by using a projection operator approach similar to those used in in Ref.[77], [78]and[79].

Note that now the subspace involves particle positions and momenta, which is reminiscent of the standard mode-coupling theory for glass transition of supercooled atomic fluids[27, 32]. To proceed, we introduce a dynamical variable vector $\underline{A}=(A_1,A_2)=\left(\rho_{\mathbf{q}},j_{\mathbf{q}}^L\right)$, where

$$j_{\mathbf{q}}^L=\sum_j\hat{\mathbf{q}}\cdot\frac{\mathbf{p}_j}{m}e^{i\mathbf{q}\cdot\mathbf{r}_j}=\frac{1}{i\left|\mathbf{q}\right|}\dot{\rho}_{\mathbf{q}} \quad (27)$$

is the longitudinal current. We introduce its correlation function as

$$\omega_{\parallel}(q)=\frac{1}{N}\left\langle j_{\mathbf{q}}^{L*}j_{\mathbf{q}}^L\right\rangle =\frac{1}{N}\sum_{ij}\hat{\mathbf{q}}\cdot\left\langle\frac{\mathbf{p}_i\mathbf{p}_j}{m^2}e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\right\rangle\cdot\hat{\mathbf{q}}, \quad (28)$$

which can be obtained from direct simulations. The expression explicitly considers the correlations between velocity and density fluctuation. We emphasize that this correlation is necessary, since it has been revealed that a hidden velocity ordering exists in dense suspensions of self-propelled disks [21, 80]. In addition, we point out that for any dynamical variable A which does not explicitly contain self-propulsion variables, $\langle A\rangle=\langle A\rangle_e$ exactly holds.

To better illustrate the physical nature of $\omega_{\parallel}(q)$, we naively ignore the correlations between momentums of different particles, leading to

$$N\omega_{\parallel}(q)\approx\sum_{ij}\hat{\mathbf{q}}\cdot\left\langle\delta_{ij}\frac{\mathbf{p}_i\mathbf{p}_j}{m^2}e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\right\rangle\cdot\hat{\mathbf{q}} =\sum_i\frac{1}{3m^2}\left\langle\mathbf{p}_i^2\right\rangle\equiv\frac{Nv_T^2}{3}, \quad (29)$$

where v_T denotes an averaged velocity which could be dependent on system parameters like D_r, v_0 or particle density $\rho=N/V$. As a rough approximation, one may assume that $v_T^2=3k_BT_{\mathrm{eff}}/m$, where T_{eff} is the effective temperature defined for the free active particle. In this case, using Eq.(2), one has

$$v_T=\frac{f_0}{\sqrt{\gamma\left(\gamma+2D_r m\right)}}=\frac{v_0}{\sqrt{1+\tau_I/\tau_R}} \quad (30)$$

and $\frac{k_BT_{\mathrm{eff}}}{m}=\frac{v_0^2}{1+\tau_I/\tau_R}$,which should be suitable for dilute active particle systems. However, such approximation is not justified for moderate and dense systems, since for underdamped active systems, the 'temperature' could be different for different phases as demonstrated in some previous works on MIPS [30, 31]. For dense active particles system as studied here (beyond MIPS region), a well-defined effective temperature T_{eff}, should be homogeneous in space [20]. A similar system, overdamped active Ornstein-Uhlenbeck particle system, has been found that an effective temperature can be well-defined[28]. Nevertheless, Eq.(29) is instructive to understand the physics of correlation function $\omega_{\parallel}(q)$.

B. Projection for density fluctuation mode

With the treatments of last subsection, we can introduce the correlation function matrix $\underline{C}(t)=\langle\underline{A}^*\underline{A}(t)\rangle$, the Laplace transform of which reads $\underline{\tilde{C}}(z)=\left\langle\underline{A}^*\left[z-\hat{\Omega}^{\mathrm{eff}}(z)\right]^{-1}\underline{A}\right\rangle_e$. To obtain the evolution function of $\underline{\tilde{C}}(z)$, we introduce another projection operator

$$\mathcal{P}(\cdots)=\sum_{m,n=1}^{2}A_m\left[\langle\underline{A}^*\underline{A}\rangle_e\right]_{mn}^{-1}\langle A_m^*(\cdots)\rangle_e \quad (31)$$

where $\left[\langle\underline{A}^*\underline{A}\rangle_e\right]^{-1}=\begin{bmatrix}\left[NS(q)\right]^{-1} & 0\\ 0 & \left[N\omega_{\parallel}(q)\right]^{-1}\end{bmatrix}$ and $S_q=\frac{1}{N}\left\langle\rho_{\mathbf{q}}^*\rho_{\mathbf{q}}\right\rangle_e$ is the steady-state structure factor. We also introduce an orthogonal projection operator

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$\mathcal{Q} = 1 - \mathcal{P}$. Using the standard Mori-Zwanzig projection procedures[76], one can obtain the evolution equation of the correlation matrix as

$$z\underline{\tilde{C}}(z) - \underline{C}(t=0) = i\underline{\Omega}(z) \cdot \underline{\tilde{C}}(z) - \underline{\tilde{K}}(z) \cdot \underline{\tilde{C}}(z), \quad (32)$$

wherein $i\underline{\Omega}(z)$ is the collective frequency matrix and $\underline{\tilde{K}}(z)$ is the memory kernel matrix. The collective frequency is written as

$$\begin{aligned} i\underline{\Omega}(z) &= \left\langle \underline{A}^* \hat{\Omega}^{\text{eff}}(z) \underline{A} \right\rangle_e \cdot \langle \underline{A}^* \underline{A} \rangle_e^{-1} \\ &= \begin{bmatrix} 0 & -iq \\ -iq \frac{\omega_\parallel(q)}{S(q)} & -\frac{f_0^2 \Theta(q)}{(z+2D_r)m^2\omega_\parallel(q)} \end{bmatrix} \end{aligned} \quad (33)$$

where

$$\begin{aligned} \Theta(q) &= -\frac{2D_r m^2}{N f_0^2} \left\langle j_{\mathbf{q}}^* \hat{\Omega}^{\text{eff}}(z) j_{\mathbf{q}} \right\rangle_e \\ &= \frac{1}{N} \hat{\mathbf{q}} \cdot \left\langle \sum_{ij} \left(\langle \mathbf{e}_i \mathbf{e}_j \rangle_{lss} - \langle \mathbf{e}_i \rangle_{lss} \langle \mathbf{e}_j \rangle_{lss} \right) \right. \\ &\qquad \left. \times e^{-i\mathbf{q}\cdot\mathbf{r}_i} e^{i\mathbf{q}\cdot\mathbf{r}_j} \right\rangle_e \cdot \hat{\mathbf{q}} \end{aligned} \quad (34)$$

denotes a correlation function for active force directions between particle pairs (see derivation details in App.C), which can be obtained by direct simulations in practice. The memory kernel matrix is written as

$$\begin{aligned} \underline{\tilde{K}}(z) &= -\left\langle \underline{A}^* \hat{\Omega}^{\text{eff}} \mathcal{Q} \left(z - \mathcal{Q} \hat{\Omega}^{\text{eff}} \mathcal{Q} \right)^{-1} \mathcal{Q} \hat{\Omega}^{\text{eff}} \underline{A} \right\rangle_e \cdot \langle \underline{A}^* \underline{A} \rangle_e^{-1} \\ &= \begin{bmatrix} 0 & 0 \\ 0 & \tilde{m}_q(z) \end{bmatrix} \end{aligned} \quad (35)$$

where $\tilde{m}_q(z)$ is the memory function, reads

$$\tilde{m}_q(z) = -\frac{1}{N\omega_\parallel(q)} \left\langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\text{eff}} \mathcal{Q} \left(z - \mathcal{Q} \hat{\Omega}^{\text{eff}} \mathcal{Q} \right)^{-1} \mathcal{Q} \hat{\Omega}^{\text{eff}} j_{\mathbf{q}}^L \right\rangle_e \quad (36)$$

Comparing the left lower corner of the matrix equation(32), we get

$$\tilde{F}_q(z) = \cfrac{S_q}{z + \cfrac{\Omega_q^2}{z + \tilde{\nu}_q(z) + \tilde{m}_q(z)}} \quad (37)$$

where $\Omega_q^2 = \frac{q^2 \omega_\parallel(q)}{S_q}$, $\tilde{\nu}_q(z) = \frac{f_0^2 \Theta(q)}{(z+2D_r)m^2\omega_\parallel(q)} \equiv \frac{2D_r \nu_q}{z+2D_r}$ so that $\nu_q = \lim_{z\to 0} \tilde{\nu}_q(z)$. Applying inverse Laplace transform to bring this equation back to real-time space, one gets the evolution equation for ISF $F_q(t)$

$$\begin{aligned} &\partial_t^2 F_q(t) + \Omega_q^2 F_q(t) \\ &+ \int_0^t \left[m_q(t-u) + 2D_r \nu_q e^{-2D_r(t-u)} \right] \partial_u F_q(u) \, \mathrm{d}u = 0 \end{aligned} \quad (38)$$

This equation is one the main results of the present work.

C. Mode-coupling-like approximation

To make Eq.(38) practicable, one needs to solve the memory function $m_q(t)$. We use a factorization approximation which was developed in the mode-coupling theory for the glass transition.

Firstly, we introduce another projection operator, to project quantities onto the density pair subspace $\rho_{\mathbf{p}}\rho_{\mathbf{k}}$,

$$\mathcal{P}_2(\cdots) = \sum_{\mathbf{k},\mathbf{p}} \rho_{\mathbf{p}}\rho_{\mathbf{k}}\rangle_e G_{\mathbf{pk}}^{-1} \langle \rho_{\mathbf{p}}^* \rho_{\mathbf{k}}^* (\cdots) \rangle_e \quad (39)$$

where $G_{\mathbf{pk}} = 2N^2 S_p S_k$ is the normalization factor, due to the factorization approximation

$$\begin{aligned} \left\langle \rho_{\mathbf{p}}^* \rho_{\mathbf{k}}^* \rho_{\mathbf{p}'} \rho_{\mathbf{k}'} \right\rangle_e \approx& \left\langle \rho_{\mathbf{p}}^* \rho_{\mathbf{k}'} \right\rangle_e \left\langle \rho_{\mathbf{k}}^* \rho_{\mathbf{p}'} \right\rangle_e \\ &+ \left\langle \rho_{\mathbf{p}}^* \rho_{\mathbf{p}'} \right\rangle_e \left\langle \rho_{\mathbf{k}}^* \rho_{\mathbf{k}'} \right\rangle_e \\ =& (\delta_{\mathbf{pp}'} \delta_{\mathbf{kk}'} + \delta_{\mathbf{pk}'} \delta_{\mathbf{kp}'}) N^2 S_p S_k \end{aligned} \quad (40)$$

Secondly, we insert the projection operator $\mathcal{P}_2$ into the memory function, substitute the $\mathcal{Q}\hat{\Omega}^{\text{eff}} j_{\mathbf{q}}^L$ with $\mathcal{P}_2 \mathcal{Q} \hat{\Omega}^{\text{eff}} j_{\mathbf{q}}^L$, and at the same time, replace the evolution operator $\left(z - \mathcal{Q}\hat{\Omega}^{\text{eff}} \mathcal{Q} \right)^{-1}$ in the orthogonal space by $\left(z - \hat{\Omega}^{\text{eff}} \right)^{-1}$, leading to

$$\begin{aligned}
\tilde{m}_q(z) =& -\frac{1}{N\omega_\parallel(q)} \left\langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\text{eff}} \mathcal{Q} \left(z - \mathcal{Q}\hat{\Omega}^{\text{eff}} \mathcal{Q} \right)^{-1} \mathcal{Q}\hat{\Omega}^{\text{eff}} j_{\mathbf{q}}^{L} \right\rangle_e \\
\approx& -\frac{1}{N\omega_\parallel(q)} \left\langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\text{eff}} \mathcal{Q}\mathcal{P}_2 \left(z - \hat{\Omega}^{\text{eff}} \right)^{-1} \mathcal{P}_2 \mathcal{Q}\hat{\Omega}^{\text{eff}} j_{\mathbf{q}}^{L} \right\rangle_e \\
=& -\frac{1}{N\omega_\parallel(q)} \sum_{\mathbf{pp'kk'}} \langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\text{eff}} \mathcal{Q} \rho_{\mathbf{p}}\rho_{\mathbf{k}} \rangle_e G_{\mathbf{pk}}^{-1} \\
& \times \left\langle \rho_{\mathbf{p}}^* \rho_{\mathbf{k}}^* \left(z - \hat{\Omega}^{\text{eff}} \right)^{-1} \rho_{\mathbf{p'}}\rho_{\mathbf{k'}} \right\rangle_e \\
& \times G_{\mathbf{p'k'}}^{-1} \left\langle \rho_{\mathbf{p'}}^* \rho_{\mathbf{k'}}^* \mathcal{Q}\hat{\Omega}^{\text{eff}} j_{\mathbf{q}}^{L} \right\rangle_e
\end{aligned} \tag{41}$$

Thirdly, using factorization technique to solve $\left\langle \rho_{\mathbf{p}}^* \rho_{\mathbf{k}}^* \left(z - \hat{\Omega}^{\text{eff}} \right)^{-1} \rho_{\mathbf{p'}}\rho_{\mathbf{k'}} \right\rangle_e$, note that it has to be done in the time domain

$$\begin{aligned}
& \mathcal{LT}^{-1} \left[\left\langle \rho_{\mathbf{p}}^* \rho_{\mathbf{k}}^* \left(z - \hat{\Omega}^{\text{eff}} \right)^{-1} \rho_{\mathbf{p'}}\rho_{\mathbf{k'}} \right\rangle_e \right] \\
\approx & \mathcal{LT}^{-1} \left[\left\langle \rho_{\mathbf{p}}^* \left(z - \hat{\Omega}^{\text{eff}} \right)^{-1} \rho_{\mathbf{p'}} \right\rangle_e \right] \mathcal{LT}^{-1} \left[\left\langle \rho_{\mathbf{k}}^* \left(z - \hat{\Omega}^{\text{eff}} \right)^{-1} \rho_{\mathbf{k'}} \right\rangle_e \right] \\
& + \mathcal{LT}^{-1} \left[\left\langle \rho_{\mathbf{p}}^* \left(z - \hat{\Omega}^{\text{eff}} \right)^{-1} \rho_{\mathbf{k'}} \right\rangle_e \right] \mathcal{LT}^{-1} \left[\left\langle \rho_{\mathbf{k}}^* \left(z - \hat{\Omega}^{\text{eff}} \right)^{-1} \rho_{\mathbf{p'}} \right\rangle_e \right] \\
= & N^2 \left(\delta_{\mathbf{pp'}}\delta_{\mathbf{kk'}} + \delta_{\mathbf{pk'}}\delta_{\mathbf{kp'}} \right) F_p(t) F_k(t)
\end{aligned} \tag{42}$$

where $\mathcal{LT}^{-1}$ means inverse Laplace transform. Then we just need to calculate

$$\langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\text{eff}} \mathcal{Q} \rho_{\mathbf{p}}\rho_{\mathbf{k}} \rangle_e = \langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\text{eff}} \rho_{\mathbf{p}}\rho_{\mathbf{k}} \rangle_e - \langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\text{eff}} \rho_{\mathbf{q}} \rangle_e (NS_q)^{-1} \langle \rho_{-\mathbf{q}}\rho_{\mathbf{p}}\rho_{\mathbf{q}} \rangle_e \tag{43}$$

The second term includes a three-point correlation, that can be calculated by a standard procedure called "convolution approximation"[27]

$$\langle \rho_{-\mathbf{q}}\rho_{\mathbf{p}}\rho_{\mathbf{k}} \rangle \approx \delta_{\mathbf{p+k,q}} N S_k S_p S_q. \tag{44}$$

Using an equality $\hat{\Omega}^{\text{eff}} \left(\rho_{\mathbf{k}}\rho_{\mathbf{p}} P_e^{ss} \right) = -i \left(k j_{\mathbf{k}}^L \rho_{\mathbf{p}} + p j_{\mathbf{p}}^L \rho_{\mathbf{k}} \right) P_e^{ss}$, the first term can be reduced as

$$\langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\text{eff}} \rho_{\mathbf{p}}\rho_{\mathbf{k}} \rangle_e = -ik \left\langle j_{\mathbf{q}}^{L*} j_{\mathbf{k}}^{L} \rho_{\mathbf{p}} \right\rangle_e - ip \left\langle j_{\mathbf{q}}^{L*} j_{\mathbf{p}}^{L} \rho_{\mathbf{k}} \right\rangle_e \tag{45}$$

To proceed, we introduce an approximation which is a generalized version of convolution approximation (44), by involving particle momentums,

$$\begin{aligned}
\left\langle j_{\mathbf{q}}^{L*} j_{\mathbf{p}}^{L} \rho_{\mathbf{k}} \right\rangle_e =& \left\langle \sum_{ij} \frac{\mathbf{p}_i}{m} \cdot \hat{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}_i} \frac{\mathbf{p}_j}{m} \cdot \hat{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}_j} \rho_{\mathbf{k}} \right\rangle \\
\approx & \delta_{\mathbf{q-p,k}} \hat{\mathbf{q}} \cdot N\boldsymbol{\omega}(q) \cdot \left\langle \frac{1}{N} \sum_j \frac{\mathbf{p}_j\mathbf{p}_j}{m^2} \right\rangle^{-1} \cdot \boldsymbol{\omega}(p) \cdot \hat{\mathbf{p}} S_k \\
= & N\delta_{\mathbf{q-p,k}} \hat{\mathbf{q}} \cdot \hat{\mathbf{p}} \frac{\omega_\parallel(q)\omega_\parallel(p)}{\omega_\parallel(\infty)} S_k
\end{aligned} \tag{46}$$

where $\boldsymbol{\omega}(q) = \frac{1}{N}\sum_{ij} \left\langle \frac{\mathbf{p}_i\mathbf{p}_j}{m^2} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right\rangle$, $\omega_\parallel(\infty) = \lim_{q\to\infty} \omega_\parallel(q)$ and notice that $\lim_{q\to\infty} \boldsymbol{\omega}(q) = \left\langle \frac{1}{N}\sum_j \frac{\mathbf{p}_j\mathbf{p}_j}{m^2} \right\rangle$. As a result, memory function can be rewritten as

$$m_q(t) = \frac{\rho\omega_\parallel(q)}{16\pi^3 q^2} \int d\mathbf{k} \left[\mathbf{q} \cdot \left(\mathbf{p}\mathcal{C}_p + \mathbf{k}\mathcal{C}_k \right) \right]^2 F_p(t) F_k(t) \tag{47}$$

wherein a new correlation function is defined as $\mathcal{C}_k = \frac{1}{\rho}\left(1 - \frac{\omega_\parallel(k)}{\omega_\parallel(\infty) S_k} \right)$. Notice that if omitting the correlations between velocity and structure, we have $\left\langle j_{\mathbf{q}}^{L*} j_{\mathbf{p}}^{L} \rho_{\mathbf{k}} \right\rangle_e \approx \frac{k_B T_{\mathrm{eff}}}{m} N \delta_{\mathbf{q}-\mathbf{p},\mathbf{k}} \hat{\mathbf{q}} \cdot \hat{\mathbf{p}} S_k$, so that in the memory function (47), $\mathcal{C}_k$ reduces to ordinary direct correlation function $c_k = \rho^{-1}(1 - 1/S_k)$. We also note that the vertex term $\hat{\mathbf{q}} \cdot (\mathbf{p}\mathcal{C}_p + \mathbf{k}\mathcal{C}_k)$ does not explicitly include the activity parameters, which is different from our previous MCT study for dense active colloidal system[16, 81] but same as Ref.[15]. The direct reason is, herein we do not use effective interaction and diffusion approximations, but rather explicitly consider the correlation between velocity and structure.

V. DISCUSSION

Motivated by a series of works on inertial effect in active systems and recent research for glassy dynamics of dense active particle systems, we presented a theoretical method for studying the dynamics of dense underdamped active particle system, and showed the details of the derivation.

Comparing with our previous MCT work for ABP[16], the present framework no longer subjects to the small self-propulsion persistent time region since the starting points of these two theories are different. In terms of other MCT works for overdamped active particle [14, 15, 51] that share the same assumption of NESS, our theory can reduce to them when taking the overdamped limit.

In the limit of vanishing persistent time, our formulas can be reduced to an equivalent equilibrium Brownian particle system. For better comparison, we write the mode-coupling equation for dense underdamped Brownian particle system in equilibrium,

$$\partial_t^2 F_q(t) + \frac{\gamma}{m}\partial_t F_q(t) + \Omega_{\mathrm{eq},q}^2 F_q(t) + \int_0^t m_q^{\mathrm{eq}}(t-u)\partial_u F_q(u)du = 0, \tag{48}$$

$$m_q^{\mathrm{eq}}(t) = \frac{\rho k_B T}{16\pi^3 m q^2} \int [\mathbf{q} \cdot (\mathbf{p}c_p + \mathbf{k}c_k)]^2 F_p(t) F_k(t) \mathrm{d}\mathbf{k} \tag{49}$$

where $\Omega_{\mathrm{eq},q}^2 = \frac{k_B T}{m q^2 S_q}$. The mode-coupling equation and the memory kernel are similar to that in Eq.(38) and Eq.(47). The differences are given in turn: (i) the second term in Eq.(48) is γ/m rather than an exponential decaying memory kernel $2D_r\nu_q e^{-2D_r t}$ in UABP case; (ii) the coefficient of mode-coupling kernel in Eq.(49) is $\frac{k_B T}{m}$ rather than $\Omega_q^2 S_q/q^2 = \omega_\parallel(q)$ in UABP system; and (iii) direct correlation function $c_{k,p}$ in the memory kernel (49) rather than $\mathcal{C}_{k,p}$. In fact, it can be proved that when $D_r \to \infty$ while keeping f_0^2/D_r as a nonzero finite value, both our model and derived MCT equation reduce to the corresponding equilibrium version. Firstly, we have $\lim_{D_r\to\infty}\Theta(q) = \frac{1}{3}$, $\lim'_{D_r\to\infty}\omega_\parallel(q) = \frac{f_0^2}{6m\gamma D_r}$ (prime labels that f_0^2/D_r is a nonzero finite value), so that $\lim'_{D_r\to\infty}\nu_q = \frac{\gamma}{m}$. Considering $\lim_{D_r\to\infty}\int_0^t 2D_r\nu_q e^{-2D_r(t-u)}\frac{\partial}{\partial u}F_q(u)\mathrm{d}u = v_q\frac{\partial}{\partial t}F_q(t)$, the difference (i) is restored. Secondly, by simply defining $\frac{f_0^2}{6\gamma D_r} = k_B T_{\mathrm{eff}}$, then they share the same form. Finally, as we discussed above in last section, $\mathcal{C}_k$ reduces to ordinary version direction correlation function c_k.

The solution of Eqs.(37) and (38) provides a prediction of the glass transition through the ergodic parameter $f_q = \lim_{t\to\infty} F_q(t)/S_q$. When $f_q = 0$ the system is liquid, otherwise $f_q \neq 0$, the system is in glass state. According to Eq.(37), by taking the limit $f_q = \lim_{z\to 0} z\tilde{F}_q(z)/S_q$, we find out that

$$\frac{f_q}{1-f_q} = \lim_{t\to\infty} m_q(t)/\Omega_q^2, \tag{50}$$

which means that the glass transition point only depends on the memory function, or essentially the nonequilibrium steady-state structure factor S_k and function $\mathcal{C}_k$, rather than the correlation of active force direction $\Theta(q)$ directly. As for how the inertia influences the glass transition, Eqs.(47) and (50) show that the particle mass m does not change the critical point directly, and the question boils down to how the inertia influences the structure S_q and correlation function $\omega_\parallel(q)$, which requires further simulation research.

To analyse the structure relaxation of dense UABP system, i.e. the long-time scale behavior of ISF (Eq.(38) is inconvenient for this analysis), we review Eq.(37) in small z region and apply inversed Laplace transform, leading to

$$\frac{\partial}{\partial t}F_q(t) + \omega_q F_q(t) + \omega_q \int_0^t M_q(t-t')\frac{\partial}{\partial t'}F_q(t')\mathrm{d}t' = 0, \tag{51}$$

where the frequency term $\omega_q = \frac{\Omega_q^2}{\nu_q} = \frac{2D_r}{S_q\Theta(q)}\left(\frac{qm\omega_\parallel(q)}{f_0}\right)^2$ and the memory kernel

$$M_q(t) = \frac{m_q(t)}{\Omega_q^2} = \frac{\rho S_q}{16\pi^3 q^4}\int \mathrm{d}\mathbf{k}\,[\mathbf{q}\cdot(\mathbf{p}\mathcal{C}_p + \mathbf{k}\mathcal{C}_k)]^2 F_p(t)F_k(t) \tag{52}$$

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To briefly analysis the relaxation behavior, we firstly consider the small τ_R case, since $\omega_\parallel(q)$ has little oscillations [14, 42] and can be estimated with Eq.(29) in this case. According to Eq.(30), and keeping the friction and v_0 as constants, we may expect that $m\omega_\parallel(q) \approx \frac{v_0^2 m}{1+\tau_I/\tau_R}$ increases with the particle inertia, since $k_B T_{\text{eff}}/m$ is an estimation of $\omega_\parallel(q)$. Therefore, if the structure and active force correlation are not sensitive to a small change of mass, the increasing of the mass will accelerate the structural relaxation, which means a shorter relaxation time for larger mass. Beyond to small τ_R region, there might be a nontrivial influence of $m\omega_\parallel(q)$ on the relaxation behavior. Herein we emphasize that, this effect only exists in active underdamped system, since for passive system, the frequency term reads $\frac{m}{\gamma}\Omega^2_{\text{eq},q} = \frac{k_B T}{\gamma q^2 S_q} = \frac{D_t}{q^2 S_q}$, meaning that the relaxation is invariant with the change of the particle mass.

In summary, our theory begins with a non-equilibrium steady-state assumption. Using the projection operator technique on the distribution function, the variables of self-propulsion direction are eliminated so that we can achieve the effective evolution equation for the distribution function of positions and momentums of particles. After that, we proceed with the Zwanzig projection operator method and standard mode-coupling theory procedure, to obtain the evolution equation for intermediate scattering function. The form of the equation is very similar to other glassy systems, which means a mode-coupling transition is also valid for UABP system, although the quantitative results still require computer simulations to gain the steady-state structure and related correlation functions, which will be expressed in our upcoming work. In addition, our theory is essentially independent on the type of active particle, for example, one can easily extend our theoretical framework to a similar active particle model such as active Ornstein-Uhlenbeck particles.

In future work, we will firstly simulate the UABP system to obtain the steady-state structure and velocity correlations, then solve the equations numerically and study the inertial effect on glassy dynamics and ergodicity transition. And as a comparison, direct simulations of UABP in long-time scales are also required. Moreover, the projection method we used in two places are not limited in MCT study. Based on the non-equilibrium steady-state assumption, one can study many other questions further, such as effective temperature, stochastic thermodynamics for active systems and active bath problems.

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Appendix A: Velocity correlation for free active particle

For free ABP in d- dimensional space, the EOM is written as

$$\dot{\mathbf{r}} = \mathbf{p}/m \tag{A1a}$$
$$\dot{\mathbf{p}} = -\mathbf{p}\gamma/m + v_0\gamma\mathbf{e} \tag{A1b}$$
$$\dot{\mathbf{e}} = \sqrt{2D_r}\,\mathbf{e}\times\boldsymbol{\eta} \tag{A1c}$$

wherein the white noise term satisfies $\langle \eta_\alpha(t)\eta_\beta(t')\rangle = \delta_{\alpha\beta}\delta(t-t')$. Subequations (a) and (b) give the formal solution for the particle momentum

$$\mathbf{p}(t) = \mathbf{p}(0)e^{-\gamma t/m} + \gamma v_0 \int_0^t e^{-(t-u)\gamma/m}\mathbf{e}(u)\mathrm{d}u, \tag{A2}$$

and the final one can be rewritten as

$$\dot{\mathbf{e}}(t) = \mathbf{H}(t)\mathbf{e}(t), \tag{A3}$$

where $\mathbf{H}(t) = \sqrt{2D_r}\begin{pmatrix} 0 & \eta_z(t) & -\eta_y(t) \\ -\eta_z(t) & 0 & \eta_x(t) \\ \eta_y(t) & -\eta_x(t) & 0 \end{pmatrix}$ for 3D systems and $\mathbf{H}(t) = \sqrt{2D_r}\begin{pmatrix} 0 & \eta_z(t) \\ -\eta_z(t) & 0 \end{pmatrix}$ for 2D systems. This matrix equation has a formal solution

$$\begin{aligned}\mathbf{e}(t) &= \lim_{dt\to 0} e^{\mathbf{H}(t)dt}e^{\mathbf{H}(t-dt)dt}\cdots e^{\mathbf{H}(t_0)dt}\mathbf{e}(t_0) \\ &\equiv e_+^{\int_{t_0}^t \mathbf{H}(s)\mathrm{d}s}\mathbf{e}(t_0),\end{aligned} \tag{A4}$$

where subscript '+' labels to the summation order and its transposition is

$$\begin{aligned}\mathbf{e}^T(t) = \mathbf{e}(t_0)e_-^{\int_{t_0}^t \mathbf{H}^T(s)\mathrm{d}s} &= \lim_{dt\to 0}\mathbf{e}(t_0)e^{\mathbf{H}^T(t_0)dt}\cdots e^{\mathbf{H}^T(t-dt)dt}e^{\mathbf{H}^T(t)dt}\\ &= \mathbf{e}(t_0)e_-^{\int_{t_0}^t -\mathbf{H}(s)\mathrm{d}s},\end{aligned} \tag{A5}$$

since for all case $\mathbf{H}^T = -\mathbf{H}$. For convenience, we set $t_0 = 0$ in the following. The time correlation function of self-propulsion direction is

$$\begin{aligned}\langle \mathbf{e}(t)\mathbf{e}(t')\rangle =& \left\langle e_+^{\int_0^t \mathbf{H}(s)\mathrm{d}s}\mathbf{e}(0)\mathbf{e}(0)e_-^{\int_0^{t'} -\mathbf{H}(s)\mathrm{d}s}\right\rangle\\ =&\frac{1}{d}\left\langle e_+^{\int_0^t \mathbf{H}(s)\mathrm{d}s}e_-^{\int_0^{t'} -\mathbf{H}(s)\mathrm{d}s}\right\rangle\\ =&\frac{1}{d}\left\langle e_+^{\int_{t'}^t \mathbf{H}(s)\mathrm{d}s}\right\rangle\\ =&\frac{1}{d}\lim_{dt\to 0}\left\langle e^{\mathbf{H}(t)dt}\right\rangle\left\langle e^{\mathbf{H}(t-dt)dt}\right\rangle\cdots\left\langle e^{\mathbf{H}(t')dt}\right\rangle\end{aligned}$$

if $t' \leqslant t$, without loss of generality. Then, using $e^{\mathbf{H}(t')dt} = \sum_{n=0}^{\infty}\frac{1}{n!}(\mathbf{H}dt)^n$, and expectations for Gaussian variables, $\mathbb{E}\left[(\mathbf{H}dt)^2\right] = -(d-1)2D_r dt\mathbf{I}$, $\mathbb{E}\left[(\mathbf{H}dt)^{2k+1}\right] = 0$ and $\mathbb{E}\left[(\mathbf{H}dt)^{2k}\right] = (2k-1)!!\mathbb{E}\left[(\mathbf{H}dt)^2\right]^k$ (for $k \in \mathbb{Z}^+$), one has

$$\begin{aligned}\mathbb{E}\left[e^{\mathbf{H}(t')dt}\right] &= \mathbf{I} + \sum_{k=1}^{\infty}\frac{1}{(2k)!}\mathbb{E}\left[(\mathbf{H}dt)^{2k}\right]\\ &= \mathbf{I} + \sum_{k=1}^{\infty}\frac{1}{2^k k!}\left[-2(d-1)D_r dt\right]^k\mathbf{I}\\ &= e^{-(d-1)D_r dt}\mathbf{I}\end{aligned}$$

and therefore

$$\langle \mathbf{e}(t)\mathbf{e}(t')\rangle = d^{-1}\mathbf{I}e^{-(d-1)D_r\left|t-t'\right|} \tag{A6}$$

or in an inner product form

$$\langle \mathbf{e}(t)\cdot\mathbf{e}(t')\rangle = e^{-(d-1)D_r\left|t-t'\right|} \tag{A7}$$

For convenience, we define $\tau_I = m/\gamma$, $\tau_R = \left[(d-1)D_r\right]^{-1}$, and calculate the time correlation function of momentum $\langle \mathbf{p}(t)\cdot\mathbf{p}(t')\rangle$, (assume $t > t'$ and $t, t' \gg 0$)

$$\begin{aligned}\langle \mathbf{p}(t)\cdot\mathbf{p}(t')\rangle =& e^{-\left(t+t'\right)/\tau_I}\int_0^t \mathrm{d}u\int_0^{t'}\mathrm{d}u' e^{\left(u+u'\right)/\tau_I}f_0^2\langle \mathbf{e}(u)\cdot\mathbf{e}(u')\rangle\\ =& f_0^2 e^{-\left(t+t'\right)/\tau_I}\int_0^t \mathrm{d}u\int_0^{t'}\mathrm{d}u' e^{\left(u+u'\right)/\tau_I}e^{-|u-u'|/\tau_R}\\ =& f_0^2 e^{-\left(t+t'\right)/\tau_I}\left[\int_0^{t'}\mathrm{d}u\int_0^{t'}\mathrm{d}u' + \int_{t'}^t \mathrm{d}u\int_0^{t'}\mathrm{d}u'\right]e^{\left(u+u'\right)/\tau_I}e^{-|u-u'|/\tau_R}\\ =& f_0^2\left[(1)+(2)\right]\end{aligned}$$

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Let $x = u + u'$, $y = u' - u$, these two integrals become

$$
\begin{aligned}
(1) =& \frac{1}{2} e^{-\left(t+t'\right)/\tau_I} \int_{-t'}^{t'} e^{-y/\tau_R} \mathrm{d}y \int_{|y|}^{2t'-|y|} e^{x/\tau_I} \mathrm{d}x \\
=& e^{-\left(t+t'\right)/\tau_I} \int_0^{t'} e^{-y/\tau_R} \mathrm{d}y \int_y^{2t'-y} e^{x/\tau_I} \mathrm{d}x \\
=& e^{-\left(t+t'\right)/\tau_I} \tau_I \int_0^{t'} e^{-y/\tau_R} \left[e^{(2t'-y)/\tau_I} - e^{y/\tau_I} \right] \mathrm{d}y \\
=& \tau_I \left[e^{-(t-t')/\tau_I} \frac{1 - e^{-(\tau_I^{-1}+\tau_R^{-1})t'}}{\tau_R^{-1} + \tau_I^{-1}} - e^{-\left(t+t'\right)/\tau_I} \frac{1 - e^{-(\tau_R^{-1}-\tau_I^{-1})t'}}{\tau_R^{-1} - \tau_I^{-1}} \right] \\
\overset{\lim_{t,t'\to\infty}}{=} & \tau_I \frac{e^{-(t-t')/\tau_I}}{\tau_R^{-1} + \tau_I^{-1}}
\end{aligned}
$$

and

$$
\begin{aligned}
(2) =& e^{-\left(t+t'\right)/\tau_I} \int_{t'}^{t} \mathrm{d}u \int_0^{t'} \mathrm{d}u' e^{\left(u+u'\right)/\tau_I} e^{-(u-u')/\tau_R} \\
=& e^{-\left(t+t'\right)/\tau_I} \frac{e^{(\tau_I^{-1}-\tau_R^{-1})t} - e^{(\tau_I^{-1}-\tau_R^{-1})t'}}{\tau_I^{-1} - \tau_R^{-1}} \frac{e^{(\tau_I^{-1}+\tau_R^{-1})t'} - 1}{\tau_I^{-1} + \tau_R^{-1}} \\
=& \frac{1}{\tau_I^{-2} - \tau_R^{-2}} \left[e^{-t'/\tau_I} e^{-t/\tau_R} - e^{-t/\tau_I} e^{-t'/\tau_R} \right] \left[e^{(\tau_I^{-1}+\tau_R^{-1})t'} - 1 \right] \\
\overset{\lim_{t,t'\to\infty}}{=} & \frac{1}{\tau_I^{-2} - \tau_R^{-2}} \left[e^{-(t-t')/\tau_R} - e^{-(t-t')/\tau_I} \right]
\end{aligned}
$$

The momentum correlation reads

$$
\begin{aligned}
\langle \mathbf{p}(t) \cdot \mathbf{p}(t') \rangle =& f_0^2 \frac{1}{\tau_I^{-2} - \tau_R^{-2}} \left[e^{-(t-t')/\tau_R} - e^{-(t-t')/\tau_I} + \tau_I \left(\tau_I^{-1} - \tau_R^{-1} \right) e^{-(t-t')/\tau_I} \right] \\
=& f_0^2 \frac{1}{\tau_I^{-2} - \tau_R^{-2}} \left[e^{-(t-t')/\tau_R} - \frac{\tau_I}{\tau_R} e^{-(t-t')/\tau_I} \right] \\
=& \frac{f_0^2 \tau_R \tau_I^2}{(\tau_R^2 - \tau_I^2)} \left[\tau_R e^{-(t-t')/\tau_R} - \tau_I e^{-(t-t')/\tau_I} \right]
\end{aligned} \tag{A8}
$$

Therefore

$$
\begin{aligned}
\left\langle \mathbf{p}^2 \right\rangle &= \lim_{t\to\infty} \langle \mathbf{p}(t) \cdot \mathbf{p}(t) \rangle \\
&= \frac{f_0^2 \tau_R \tau_I^2}{(\tau_R + \tau_I)} = \frac{f_0^2}{\frac{\gamma}{m} \left(\frac{\gamma}{m} + (d-1) D_r \right)}
\end{aligned} \tag{A9}
$$

This is Eq.(2) in the main text.

Appendix B: Derivation of effective Fokker-Planck equation

In this section, we show the details of the derivation for effective Fokker-Planck equation. Applying Laplace transform of Eq.(5), we get the equations for $\mathcal{P}_{lss} P(t)$ and $\mathcal{Q}_{lss} P(t)$,

$$
\begin{aligned}
\mathcal{LT} \left[\partial_t \mathcal{P}_{lss} P(t) \right](z) =& z \mathcal{P}_{lss} \tilde{P}(z) - \mathcal{P}_{lss} P(0) \\
=& \mathcal{P}_{lss} \hat{\Omega} \left(\mathcal{P}_{lss} + \mathcal{Q}_{lss} \right) \tilde{P}(z)
\end{aligned} \tag{B1}
$$

$$
\begin{aligned}
\mathcal{LT} \left[\partial_t \mathcal{Q}_{lss} P(t) \right](z) =& z \mathcal{Q}_{lss} \tilde{P}(z) - \mathcal{Q}_{lss} P(0) \\
=& \mathcal{Q}_{lss} \hat{\Omega} \left(\mathcal{P}_{lss} + \mathcal{Q}_{lss} \right) \tilde{P}(z)
\end{aligned} \tag{B2}
$$

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where $\mathcal{Q}_{lss}$ is defined as $\mathcal{Q}_{lss} = \mathcal{I} - \mathcal{P}_{lss}$ which is also a projection operator saytisfying $\mathcal{Q}_{lss}^2 = \mathcal{Q}_{lss}$ and $\mathcal{P}_{lss}\mathcal{Q}_{lss} = \mathcal{Q}_{lss}\mathcal{P}_{lss} = 0$. The second equation formally gives

$$\mathcal{Q}_{lss}\tilde{P}(z) = \left(z - \mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1} \mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}\tilde{P}(z) \tag{B3}$$

Herein, for arbitrary operator $\hat{O}$, the expression $\left(z - \hat{O}\right)^{-1}$ expresses the summation of infinite operator series $\left(z - \hat{O}\right)^{-1} = \sum_{i=0}^{\infty} z^{-(i+1)}\hat{O}^i$. And the fact that $\mathcal{Q}_{lss}P(0) = 0$ has been used in the second equality since the initial state is usually chosen to stay at the relevant subspace. Substituting Eq.(B3) into Eq.(B1), we get the closed equation for $\mathcal{P}_{lss}\tilde{P}\left(z\right)$

$$\mathcal{LT}\left[\partial_t \mathcal{P}_{lss}P(t)\right](z) = \mathcal{P}_{lss}\hat{\Omega}\mathcal{P}_{lss}\tilde{P}(z) + \mathcal{P}_{lss}\hat{\Omega}\left(z - \mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1} \mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}\tilde{P}(z). \tag{B4}$$

i.e. Eq.(18) in main text.

To solve this equation, we introduce two well-behaved function $g = g\left(\mathbf{r}^N, \mathbf{p}^N, \mathbf{e}^N, t\right)$ and $g_e = \int g\left(\mathbf{r}^N, \mathbf{p}^N, \mathbf{e}^N, t\right) \mathrm{d}\omega^N$, then we have

$$\mathcal{P}_{lss}\hat{\Omega}g = \sum_j \frac{P^{ss}}{P_e^{ss}}\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j\right) g_e - \frac{P^{ss}}{P_e^{ss}}\frac{\mathbf{p}_j}{m}\cdot\frac{\partial g_e}{\partial \mathbf{r}_j} - f_0\frac{P^{ss}}{P_e^{ss}}\frac{\partial}{\partial \mathbf{p}_j}\cdot\int \mathbf{e}_j g \mathrm{d}\omega^N, \tag{B5}$$

and

$$\begin{aligned}\mathcal{P}_{lss}\hat{\Omega}\mathcal{P}_{lss}g =& \sum_j \frac{P^{ss}}{P_e^{ss}}\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j\right) g_e - \frac{P^{ss}}{P_e^{ss}}\frac{\mathbf{p}_j}{m}\cdot\frac{\partial g_e}{\partial \mathbf{r}_j} - f_0\frac{P^{ss}}{P_e^{ss}}\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\left\langle \mathbf{e}_j\right\rangle_{lss} g_e\right)\\ =& \sum_j \frac{P^{ss}}{P_e^{ss}}\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right) g_e - \frac{P^{ss}}{P_e^{ss}}\frac{\mathbf{p}_j}{m}\cdot\frac{\partial g_e}{\partial \mathbf{r}_j},\end{aligned} \tag{B6}$$

This leads to the first term of rhs of Eq.(B4)

$$\mathcal{P}_{lss}\hat{\Omega}\mathcal{P}_{lss}\tilde{P}(z) = \frac{P^{ss}}{P_e^{ss}}\sum_j\left[\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\left\langle \mathbf{e}_j\right\rangle_{lss}\right) - \frac{\partial}{\partial \mathbf{r}_j}\cdot\left(\frac{\mathbf{p}_j}{m}\right)\right]\tilde{P}_e(z) \tag{B7}$$

Then, one has

$$\begin{aligned}\mathcal{P}_{lss}\hat{\Omega}\mathcal{Q}_{lss}g =& \mathcal{P}_{lss}\hat{\Omega}g - \mathcal{P}_{lss}\hat{\Omega}\mathcal{P}_l g\\ =& -f_0\frac{P^{ss}}{P_e^{ss}}\frac{\partial}{\partial \mathbf{p}_j}\cdot\int\left(\mathbf{e}_i - \left\langle \mathbf{e}_j\right\rangle_{lss}\right) g \mathrm{d}\omega^N,\end{aligned} \tag{B8}$$

as well as

$$\begin{aligned}\hat{\Omega}\mathcal{P}_{lss}g =& \sum_j \frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\mathbf{e}_j\right)\left(P^{ss}\frac{g_e}{P_e^{ss}}\right) - \frac{\mathbf{p}_j}{m}\cdot\frac{\partial}{\partial \mathbf{r}_j}\left(P^{ss}\frac{g_e}{P_e^{ss}}\right) + D_r\hat{R}_j^2\left(P^{ss}\frac{g_e}{P_e^{ss}}\right)\\ =& \sum_j \frac{g_e}{P_e^{ss}}\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\mathbf{e}_j\right)P^{ss} + \left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\mathbf{e}_j\right)P^{ss}\cdot\frac{\partial}{\partial \mathbf{p}_j}\frac{g_e}{P_e^{ss}}\\ &- \frac{g_e}{P_e^{ss}}\frac{\mathbf{p}_j}{m}\cdot\frac{\partial}{\partial \mathbf{r}_j}P^{ss} - P^{ss}\frac{\mathbf{p}_j}{m}\cdot\frac{\partial}{\partial \mathbf{r}_j}\frac{g_e}{P_e^{ss}} + D_r\frac{g_e}{P_e^{ss}}\hat{R}_j^2 P^{ss}\\ =& \sum_j\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\mathbf{e}_j\right)P^{ss}\cdot\frac{\partial}{\partial \mathbf{p}_j}\frac{g_e}{P_e^{ss}} - P^{ss}\frac{\mathbf{p}_j}{m}\cdot\frac{\partial}{\partial \mathbf{r}_j}\frac{g_e}{P_e^{ss}} + \frac{g_e}{P_e^{ss}}\hat{\Omega}P^{ss}.\end{aligned} \tag{B9}$$

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such that

$$\begin{aligned}\mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}g =&\hat{\Omega}\mathcal{P}_{lss}g - \mathcal{P}_{lss}\hat{\Omega}\mathcal{P}_{lss}g \\ =&\sum_j \frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\mathbf{e}_j\right)\left(P^{ss}\frac{g_e}{P^{ss}_e}\right) - \frac{P^{ss}}{P^{ss}_e}\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j\right)g_e + \frac{P^{ss}}{P^{ss}_e}\frac{\mathbf{p}_j}{m}\cdot\frac{\partial g_e}{\partial \mathbf{r}_j} \\ &-\frac{\mathbf{p}_j}{m}\cdot\frac{\partial}{\partial \mathbf{r}_j}\left(P^{ss}\frac{g_e}{P^{ss}_e}\right) + D_r\hat{R}^2_j\left(P^{ss}\frac{g_e}{P^{ss}_e}\right) + f_0\frac{P^{ss}}{P^{ss}_e}\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\langle\mathbf{e}_j\rangle_{lss}\,g_e\right) \\ =&\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j\right)g_e\cdot\partial_{\mathbf{p}_j}\frac{P^{ss}}{P^{ss}_e} - \frac{\mathbf{p}_j}{m}g_e\cdot\partial_{\mathbf{r}_j}\frac{P^{ss}}{P^{ss}_e} + D_r\hat{R}^2_j\left(P^{ss}\frac{g_e}{P^{ss}_e}\right) \\ &- f_0 g_e\langle\mathbf{e}_j\rangle_{lss}\cdot\partial_{\mathbf{p}_j}\frac{P^{ss}}{P^{ss}_e} - f_0\frac{\partial}{\partial \mathbf{p}_j}\cdot\left[\left(\mathbf{e}_j - \langle\mathbf{e}_j\rangle_{lss}\right)\frac{P^{ss}}{P^{ss}_e}g_e\right].\end{aligned} \tag{B10}$$

We emphasize that, so far, the projection method is exact, no matter the self-propulsion variables are fast variables or not. To deal with $\left(z-\mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1}$, nevertheless, an approximation has to be introduced. Now we rewrite the Fokker-Planck operator as $\hat{\Omega}=\hat{\Omega}_I+\delta\hat{\Omega}_I+\hat{\Omega}_R$, where

$$\delta\hat{\Omega}_I = \sum_{j=1}^{N}\left[f_0\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\langle\mathbf{e}_j\rangle_{lss} - \mathbf{e}_j\right)\right]. \tag{B11}$$

Since projector $\mathcal{Q}_{lss}$ evolves in a space that is orthogonal to the relevant subspace spanned by $\left(\mathbf{r}^N,\mathbf{p}^N\right)$, and operator $\hat{\Omega}_I$ does not contain ω variables, we have $\mathcal{Q}_{lss}\hat{\Omega}_I\mathcal{Q}_{lss}=0$. On the other hand, since $\mathcal{P}_{lss}\hat{\Omega}_R=0$, we have $\mathcal{Q}_{lss}\hat{\Omega}_R\mathcal{Q}_{lss}=\hat{\Omega}_R$. Considering the operator $\delta\hat{\Omega}_I$ (defined in Eq.(B11)) actually reflects a fluctuating effect $\left(\mathbf{e}_j-\langle\mathbf{e}_j\rangle_{lss}\right)$, it is reasonable to assume that the operator is entirely due to the free relaxation of the self-propulsion, i.e.

$$\mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss} \approx \hat{\Omega}_R = D_r\sum_j \hat{R}^2_j. \tag{B12}$$

Notice that this approximation is essentially same as the one used in Szamel's work [15, 51].Due to the structure of Eq.(18), to proceed, we need to calculate $\int \mathbf{e}_i\left(z-\mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1}g\mathrm{d}\omega^N$. Using the approximation $\mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\approx D_r\sum_j\hat{R}^2_j$, and the operator definition $\left(z-\mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1}\approx\sum_{k=0}^{\infty}\frac{\left(D_r\sum_j\hat{R}^2_j\right)^k}{z^{k+1}}$, with integration by parts technique, we have

$$\begin{aligned}&\int \mathbf{e}_i\left(D_r\sum_j\hat{R}^2_j\right)^k g\mathrm{d}\omega^N \\ =&-2D_r\int\mathbf{e}_i\left(D_r\sum_j\hat{R}^2_j\right)^{k-1}g\mathrm{d}\omega^N \\ =&\left(-2D_r\right)^k\int\mathbf{e}_i g\mathrm{d}\omega^N\end{aligned} \tag{B13}$$

($\hat{R}^2_j\mathbf{e}_j=-2\mathbf{e}_j$ in 3D) and therefore

$$\begin{aligned}&\int\mathbf{e}_i\sum_{k=0}^{\infty}\frac{\left(D_r\hat{R}\right)^k}{z^{k+1}}g\mathrm{d}\omega^N \\ =&\sum_{k=0}^{\infty}\frac{\left(-2D_r\right)^k}{z^{k+1}}\int\mathbf{e}_i g\mathrm{d}\omega^N \\ =&\frac{1}{z+2D_r}\int\mathbf{e}_i g\mathrm{d}\omega^N\end{aligned} \tag{B14}$$

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Hence we get

$$\int \mathbf{e}_i \left(z - \mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1} g\mathrm{d}\omega^N \approx \frac{1}{z + 2D_r}\int \mathbf{e}_i g\mathrm{d}\omega^N \tag{B15}$$

and similarly

$$\int \langle \mathbf{e}_i \rangle_{lss} \left(z - \mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1} g\mathrm{d}\omega^N = \frac{1}{z}\langle \mathbf{e}_i \rangle_{lss}\int g\mathrm{d}\omega^N \tag{B16}$$

Next we just need to calculate $\int \mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}g\mathrm{d}\omega^N$ and $\int \mathbf{e}_i\mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}g\mathrm{d}\omega^N$. The first one is

$$\begin{aligned}
&\int \mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}g\mathrm{d}\omega^N \\
=&\sum_j \frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j - f_0\langle \mathbf{e}_j\rangle_{lss}\right)g_e - \frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j\right)g_e \\
&+\frac{\mathbf{p}_j}{m}\cdot\frac{\partial g_e}{\partial \mathbf{r}_j} - \frac{\mathbf{p}_j}{m}\cdot\frac{\partial g_e}{\partial \mathbf{r}_j} + f_0\frac{\partial}{\partial \mathbf{p}_j}\cdot\left(\langle \mathbf{e}_j\rangle_{lss}g_e\right) = 0
\end{aligned} \tag{B17}$$

and the second one

$$\begin{aligned}
&\int \mathbf{e}_i\mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}g\mathrm{d}\omega^N \\
=&\sum_j -\langle \mathbf{e}_i\rangle_{lss}\frac{g_e}{P_e^{ss}}\partial_{\mathbf{p}_j}\left(\frac{\gamma}{m}\mathbf{p}_j - \mathbf{F}_j\right)P_e^{ss} - f_0\langle \mathbf{e}_i\mathbf{e}_j\rangle_{lss}\cdot P_e^{ss}\partial_{\mathbf{p}_j}\frac{g_e}{P_e^{ss}}P_e^{ss}\partial_{\mathbf{p}_j}\frac{g_e}{P_e^{ss}} \\
&+f_0\langle \mathbf{e}_i\rangle_{lss}\langle \mathbf{e}_j\rangle_{lss}P_e^{ss}\partial_{\mathbf{p}_j}\frac{g_e}{P_e^{ss}} + \langle \mathbf{e}_i\rangle_{lss}\frac{g_e}{P_e^{ss}}\partial_{\mathbf{p}_j}\cdot\left(f_0\langle \mathbf{e}_j\rangle_{lss}P_e^{ss}\right) \\
&+\langle \mathbf{e}_i\rangle_{lss}\frac{g_e}{P_e^{ss}}\frac{\mathbf{p}_j}{m}\cdot\partial_{\mathbf{r}_j}P_e^{ss} \\
=&-\sum_j f_0\left(\langle \mathbf{e}_i\mathbf{e}_j\rangle_{lss} - \langle \mathbf{e}_i\rangle_{lss}\langle \mathbf{e}_j\rangle_{lss}\right)\cdot P_e^{ss}\partial_{\mathbf{p}_j}\frac{g_e}{P_e^{ss}}
\end{aligned} \tag{B18}$$

The last step utilizes Eq.(14) in maintext. Then,

$$\begin{aligned}
&\sum_i \partial_{\mathbf{p}_i}\cdot\int \mathbf{e}_i\mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}g\mathrm{d}\omega^N \\
=&-\sum_{ij}\partial_{\mathbf{p}_i}\cdot f_0\left(\langle \mathbf{e}_i\mathbf{e}_j\rangle_{lss} - \langle \mathbf{e}_i\rangle_{lss}\langle \mathbf{e}_j\rangle_{lss}\right)\cdot P_e^{ss}\partial_{\mathbf{p}_j}\frac{g_e}{P_e^{ss}} \\
=&-\sum_{ij}\partial_{\mathbf{p}_i}\cdot\left\{f_0\left(\langle \mathbf{e}_i\mathbf{e}_j\rangle_{lss} - \langle \mathbf{e}_i\rangle_{lss}\langle \mathbf{e}_j\rangle_{lss}\right)\cdot\left[\partial_{\mathbf{p}_j} - \left(\partial_{\mathbf{p}_j}\ln P_e^{ss}\right)\right]g_e\right\}
\end{aligned} \tag{B19}$$

and finally

$$\begin{aligned}
&\mathcal{P}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\left(z - \mathcal{Q}_{lss}\hat{\Omega}\mathcal{Q}_{lss}\right)^{-1}\mathcal{Q}_{lss}\hat{\Omega}\mathcal{P}_{lss}g \\
\approx&\frac{P^{ss}}{P_e^{ss}}\frac{f_0^2}{z+2D_r}\sum_{ij}\partial_{\mathbf{p}_i}\cdot\left\{\left(\langle \mathbf{e}_i\mathbf{e}_j\rangle_{lss} - \langle \mathbf{e}_i\rangle_{lss}\langle \mathbf{e}_j\rangle_{lss}\right)\cdot\left[\partial_{\mathbf{p}_j} - \left(\partial_{\mathbf{p}_j}\ln P_e^{ss}\right)\right]g_e\right\} \\
\equiv&\frac{P^{ss}}{P_e^{ss}}\hat{\Omega}_A(z)\tilde{P}_e(z)
\end{aligned} \tag{B20}$$

Now we reconsider the approximation (B12) through this equation. Although the influence of the fluctuation $(\mathbf{e}_j - \langle \mathbf{e}_j\rangle_{lss})$ on the evolution of $\mathbf{e}^N$ was neglected (omitting of $\delta\hat{\Omega}_I$), its correlation function $\langle \mathbf{e}_i\mathbf{e}_j\rangle_{lss} - \langle \mathbf{e}_i\rangle_{lss}\langle \mathbf{e}_j\rangle_{lss}$ still contributes on $\hat{\Omega}_A$.

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Appendix C: Derivation details of MCT

In this part, we show the details of derivation for mode-coupling equation, including the frequency term, memory function, etc.

For convenience, we begin with some useful properties of density fluctuation, longitudinal current and steady-state distribution function. Firstly we introduce the adjoint operator $\mathcal{O}^\dagger$ for any operator $\mathcal{O}$, which is defined as $\int \left(\mathcal{O}^\dagger f\right) g \mathrm{d}\Gamma = \int f \mathcal{O} g \mathrm{d}\Gamma$. Using integration by parts, the adjoint of Ω^{eff} is

$$\begin{aligned}\hat{\Omega}^{\mathrm{eff}\dagger}(z) =& \sum_i -\left(\gamma \frac{\mathbf{p}_i}{m} - \mathbf{F}_i - f_0 \langle \mathbf{e}_i \rangle_{lss}\right) \cdot \partial_{\mathbf{p}_i} + \frac{\mathbf{p}_i}{m} \cdot \partial_{\mathbf{r}_i} \\ &+ \frac{f_0^2}{z + 2D_r} \sum_{ij} \left[\partial_{\mathbf{p}_j} + \left(\partial_{\mathbf{p}_j} \ln P_e^{ss}\right)\right] \cdot \left(\langle \mathbf{e}_i \mathbf{e}_j \rangle_{lss} - \langle \mathbf{e}_i \rangle_{lss} \langle \mathbf{e}_j \rangle_{lss}\right) \cdot \partial_{\mathbf{p}_i}\end{aligned} \tag{C1}$$

For convenience, we introduce the inversed gradient operator $\partial_{\mathbf{p}_i}^{-1}$, which is defined as $\partial_{\mathbf{p}_i}^{-1} \partial_{\mathbf{p}_j} = \delta_{ij} \mathbf{1}$, then the steady-state equation (14) formally becomes

$$\frac{\gamma}{m} \mathbf{p}_j - \mathbf{F}_j - f_0 \langle \mathbf{e}_j \rangle_{lss} = \frac{1}{P_e^{ss}} \partial_{\mathbf{p}_j}^{-1} \frac{\mathbf{p}_j}{m} \cdot \frac{\partial}{\partial \mathbf{r}_j} P_e^{ss} \tag{C2}$$

This equation associates the total force acting on each particle and the geometrical property of marginal steady-state distribution function. The non-equilibrium characteristic is also shown in this equation, because if we replace the distribution function with equilibrium distribution, right-hand side of the equation reduces to zero.

Now back to the derivation,

$$\begin{aligned}\left\langle j_{\mathbf{q}}^{L*} \hat{\Omega}^{\mathrm{eff}} j_{\mathbf{q}}^L \right\rangle_e =& \left\langle \left(\hat{\Omega}^{\mathrm{eff}\dagger} j_{\mathbf{q}}^L\right)^* j_{\mathbf{q}}^L \right\rangle_e \\ =& \sum_{ij} \left\langle -\frac{1}{m} \left(\gamma \frac{\mathbf{p}_j}{m} - \mathbf{F}_j - f_0 \langle \mathbf{e}_j \rangle_{lss}\right) \cdot \hat{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}_j} \hat{\mathbf{q}} \cdot \frac{\mathbf{p}_i}{m} e^{i\mathbf{q}\cdot\mathbf{r}_i} \right\rangle_e \\ &- iq \left\langle \left(\hat{\mathbf{q}} \cdot \frac{\mathbf{p}_j}{m}\right)^2 e^{-i\mathbf{q}\cdot\mathbf{r}_j} \hat{\mathbf{q}} \cdot \frac{\mathbf{p}_i}{m} e^{i\mathbf{q}\cdot\mathbf{r}_i} \right\rangle_e \\ &+ \frac{f_0^2}{z + 2D_r} \sum_{ijk} \left\langle \left(\partial_{\mathbf{p}_j} \ln P_e^{ss}\right) \cdot \left[\langle \mathbf{e}_i \mathbf{e}_j \rangle_{lss} - \langle \mathbf{e}_i \rangle_{lss} \langle \mathbf{e}_j \rangle_{lss}\right]^T \cdot \frac{\hat{\mathbf{q}}}{m} e^{-i\mathbf{q}\cdot\mathbf{r}_i} \hat{\mathbf{q}} \cdot \frac{\mathbf{p}_k}{m} e^{i\mathbf{q}\cdot\mathbf{r}_k} \right\rangle_e \\ =& \sum_{ij} -\frac{1}{m} \int \hat{\mathbf{q}} \cdot \left(\partial_{\mathbf{p}_j}^{-1} \frac{\mathbf{p}_j}{m} \cdot \frac{\partial}{\partial \mathbf{r}_j} P_e^{ss}\right) e^{-i\mathbf{q}\cdot\mathbf{r}_j} \hat{\mathbf{q}} \cdot \frac{\mathbf{p}_i}{m} e^{i\mathbf{q}\cdot\mathbf{r}_i} \mathrm{d}\mathbf{r}^N \mathrm{d}\mathbf{p}^N \\ &- \frac{f_0^2}{z + 2D_r} \sum_{ijk} \left\langle \partial_{\mathbf{p}_j} \cdot \left[\langle \mathbf{e}_i \mathbf{e}_j \rangle_{lss} - \langle \mathbf{e}_i \rangle_{lss} \langle \mathbf{e}_j \rangle_{lss}\right]^T \cdot \frac{\hat{\mathbf{q}}}{m} e^{-i\mathbf{q}\cdot\mathbf{r}_i} \hat{\mathbf{q}} \cdot \frac{\mathbf{p}_k}{m} e^{i\mathbf{q}\cdot\mathbf{r}_k} \right\rangle_e\end{aligned} \tag{C3}$$

the first term equals

$$\begin{aligned}&\sum_{ij} \frac{1}{m} \int \hat{\mathbf{q}} \cdot \left(\partial_{\mathbf{p}_j}^{-1} \frac{\mathbf{p}_j}{m} \cdot \frac{\partial}{\partial \mathbf{r}_j} P_e^{ss}\right) e^{-i\mathbf{q}\cdot\mathbf{r}_j} \hat{\mathbf{q}} \cdot \frac{\mathbf{p}_i}{m} e^{i\mathbf{q}\cdot\mathbf{r}_i} \mathrm{d}\mathbf{r}^N \mathrm{d}\mathbf{p}^N \\ =& \sum_{ij} \frac{1}{m} \int \hat{\mathbf{q}} \cdot \left(\partial_{\mathbf{p}_j}^{-1} \frac{\mathbf{p}_j}{m} \cdot \frac{\partial}{\partial \mathbf{r}_j} P_e^{ss}\right) e^{-i\mathbf{q}\cdot\mathbf{r}_j} \left(\partial_{\mathbf{p}_i} \partial_{\mathbf{p}_i}^{-1} \cdot \frac{\mathbf{p}_i}{m}\right) \cdot \hat{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}_i} \mathrm{d}\mathbf{r}^N \mathrm{d}\mathbf{p}^N \\ =& -\sum_{ij} \frac{1}{m} \int \hat{\mathbf{q}} \cdot \left(\delta_{ij} \mathbf{1} \frac{\mathbf{p}_j}{m} \cdot \frac{\partial}{\partial \mathbf{r}_j} P_e^{ss}\right) \cdot \hat{\mathbf{q}} \left(\partial_{\mathbf{p}_i}^{-1} \cdot \frac{\mathbf{p}_i}{m}\right) e^{-i\mathbf{q}\cdot\mathbf{r}_j} e^{i\mathbf{q}\cdot\mathbf{r}_i} \mathrm{d}\mathbf{r}^N \mathrm{d}\mathbf{p}^N \\ =& \sum_i \frac{1}{m} \int \left(\frac{\mathbf{p}_i}{m} \cdot \frac{\partial}{\partial \mathbf{r}_i} P_e^{ss}\right) \left(\frac{\mathbf{p}_i \cdot \mathbf{p}_i}{2m} + C\right) \mathrm{d}\mathbf{r}^N \mathrm{d}\mathbf{p}^N \\ =& \sum_i -\frac{1}{m} \int P_e^{ss} \frac{\partial}{\partial \mathbf{r}_i} \cdot \left[\frac{\mathbf{p}_i}{m} \left(\frac{\mathbf{p}_i \cdot \mathbf{p}_i}{2m} + C\right)\right] \mathrm{d}\mathbf{r}^N \mathrm{d}\mathbf{p}^N \\ =& -\frac{1}{m} \sum_i \left\langle \frac{\partial}{\partial \mathbf{r}_i} \cdot \left[\frac{\mathbf{p}_i}{m} \left(\frac{\mathbf{p}_i \cdot \mathbf{p}_i}{2m} + C\right)\right] \right\rangle_e = 0\end{aligned} \tag{C4}$$

since the terms containing $\mathbf{p}_i$ are all odd powers. Herein, we treat the operator $\partial_{\mathbf{p}_i}^{-1}$ as an integral essentially. The second part of Eq.(C3) is

$$\begin{aligned}
&\sum_{ijk}\left\langle \partial_{\mathbf{p}_j}\cdot\left[\langle\mathbf{e}_i\mathbf{e}_j\rangle_{lss}-\langle\mathbf{e}_i\rangle_{lss}\langle\mathbf{e}_j\rangle_{lss}\right]^T\cdot\frac{\hat{\mathbf{q}}}{m}e^{-i\mathbf{q}\cdot\mathbf{r}_i}\hat{\mathbf{q}}\cdot\frac{\mathbf{p}_k}{m}e^{i\mathbf{q}\cdot\mathbf{r}_k}\right\rangle_e \\
=&\sum_{ijk}\left\langle \hat{\mathbf{q}}\cdot\frac{\delta_{jk}}{m}\mathbf{1}\cdot\left[\langle\mathbf{e}_i\mathbf{e}_j\rangle_{lss}-\langle\mathbf{e}_i\rangle_{lss}\langle\mathbf{e}_j\rangle_{lss}\right]^T\cdot\frac{\hat{\mathbf{q}}}{m}e^{-i\mathbf{q}\cdot\mathbf{r}_i}e^{i\mathbf{q}\cdot\mathbf{r}_k}\right\rangle_e \\
=&\sum_{ij}\frac{1}{m^2}\hat{\mathbf{q}}\cdot\left\langle\left(\langle\mathbf{e}_i\mathbf{e}_j\rangle_{lss}-\langle\mathbf{e}_i\rangle_{lss}\langle\mathbf{e}_j\rangle_{lss}\right)e^{-i\mathbf{q}\cdot\mathbf{r}_i}e^{i\mathbf{q}\cdot\mathbf{r}_j}\right\rangle_e\cdot\hat{\mathbf{q}} \\
\equiv&\frac{1}{m^2}N\Theta(q)
\end{aligned}\tag{C5}$$

where $\Theta(q)$ is a function that quantifies correlations of active force direction for each particles. Finally, we get

$$\begin{aligned}
\left\langle j_{\mathbf{q}}^{L*}\hat{\Omega}^{\mathrm{eff}}(z)\,j_{\mathbf{q}}^{L}\right\rangle_e &= -\frac{f_0^2}{z+2D_r}\frac{1}{m^2}\hat{\mathbf{q}}\cdot\left\langle\sum_{ij}\left(\langle\mathbf{e}_i\mathbf{e}_j\rangle_{lss}-\langle\mathbf{e}_i\rangle_{lss}\langle\mathbf{e}_j\rangle_{lss}\right)e^{-i\mathbf{q}\cdot\mathbf{r}_i}e^{i\mathbf{q}\cdot\mathbf{r}_j}\right\rangle_e\cdot\hat{\mathbf{q}} \\
&\equiv -\frac{1}{z+2D_r}\frac{f_0^2}{m^2}N\Theta(q)
\end{aligned}\tag{C6}$$

and therefore the collective frequency term

$$\begin{aligned}
i\underline{\Omega}(z) &= \begin{pmatrix} 0 & \left\langle\rho_{\mathbf{q}}^*\hat{\Omega}^{\mathrm{eff}}(z)j_{\mathbf{q}}\right\rangle \\ \left\langle j_{\mathbf{q}}^*\hat{\Omega}^{\mathrm{eff}}(z)\rho_{\mathbf{q}}\right\rangle & \left\langle j_{\mathbf{q}}^*\hat{\Omega}^{\mathrm{eff}}(z)j_{\mathbf{q}}\right\rangle\end{pmatrix}\cdot\begin{pmatrix}[NS(q)]^{-1} & 0 \\ 0 & \left[N\omega_\parallel(q)\right]^{-1}\end{pmatrix} \\
&= \begin{pmatrix} 0 & -iqN\omega_\parallel(q) \\ -iqN\omega_\parallel(q) & -\frac{f_0^2}{(z+2D_r)m^2}N\Theta(q)\end{pmatrix}\cdot\begin{pmatrix}[NS(q)]^{-1} & 0 \\ 0 & \left[N\omega_\parallel(q)\right]^{-1}\end{pmatrix} \\
&= \begin{pmatrix} 0 & -iq \\ -iq\frac{\omega_\parallel(q)}{S(q)} & -\frac{f_0^2}{(z+2D_r)m^2}\frac{\Theta(q)}{\omega_\parallel(q)}\end{pmatrix}.
\end{aligned}\tag{C7}$$

This is Eq.(33) in the main text.

For equilibrium situation, i.e. the passive undredamped Brownian particle system,

$$\begin{aligned}
\left\langle j_{\mathbf{q}}^{L*}\hat{\Omega}^{\mathrm{eq}}j_{\mathbf{q}}^{L}\right\rangle_{eq} =& \left\langle\left(\hat{\Omega}^{\mathrm{eq}\dagger}j_{\mathbf{q}}^{L}\right)^* j_{\mathbf{q}}^{L}\right\rangle_{eq} \\
=&\sum_{ij}\left\langle-\frac{1}{m}\left(\gamma\frac{\mathbf{p}_j}{m}-\mathbf{F}_j\right)\cdot\hat{\mathbf{q}}e^{-i\mathbf{q}\cdot\mathbf{r}_j}\hat{\mathbf{q}}\cdot\frac{\mathbf{p}_i}{m}e^{i\mathbf{q}\cdot\mathbf{r}_i}\right\rangle - i\,|\mathbf{q}|\left\langle\left(\hat{\mathbf{q}}\cdot\frac{\mathbf{p}_j}{m}\right)^2e^{-i\mathbf{q}\cdot\mathbf{r}_j}\hat{\mathbf{q}}\cdot\frac{\mathbf{p}_i}{m}e^{i\mathbf{q}\cdot\mathbf{r}_i}\right\rangle \\
=&\sum_{ij}-\frac{1}{m}\int\hat{\mathbf{q}}\cdot\left(\partial_{\mathbf{p}_j}^{-1}\frac{\mathbf{p}_j}{m}\cdot\partial_{\mathbf{r}_j}P_{eq}-k_BT\gamma\frac{\partial}{\partial\mathbf{p}_j}P_{eq}\right)e^{-i\mathbf{q}\cdot\mathbf{r}_j}\hat{\mathbf{q}}\cdot\frac{\mathbf{p}_i}{m}e^{i\mathbf{q}\cdot\mathbf{r}_i}\mathrm{d}\mathbf{r}^N\mathrm{d}\mathbf{p}^N \\
=&\sum_{ij}-\frac{1}{m}\int\hat{\mathbf{q}}\cdot\left(\partial_{\mathbf{p}_j}^{-1}\frac{\mathbf{p}_j}{m}\cdot\partial_{\mathbf{r}_j}P_{eq}\right)e^{-i\mathbf{q}\cdot\mathbf{r}_j}\hat{\mathbf{q}}\cdot\left(\partial_{\mathbf{p}_i}\partial_{\mathbf{p}_i}^{-1}\cdot\frac{\mathbf{p}_i}{m}\right)e^{i\mathbf{q}\cdot\mathbf{r}_i}\mathrm{d}\mathbf{r}^N\mathrm{d}\mathbf{p}^N \\
&+\frac{1}{m}\int\hat{\mathbf{q}}\cdot k_BT\gamma\frac{\partial}{\partial\mathbf{p}_j}P_{eq}e^{-i\mathbf{q}\cdot\mathbf{r}_j}\hat{\mathbf{q}}\cdot\frac{\mathbf{p}_i}{m}e^{i\mathbf{q}\cdot\mathbf{r}_i}\mathrm{d}\mathbf{r}^N\mathrm{d}\mathbf{p}^N \\
=&\sum_{ij}\frac{1}{m}\int\hat{\mathbf{q}}\cdot\delta_{ij}\mathbf{1}\cdot\hat{\mathbf{q}}\frac{\mathbf{p}_j}{m}\cdot\left(\partial_{\mathbf{r}_j}P_{eq}\right)\left(\partial_{\mathbf{p}_i}^{-1}\cdot\frac{\mathbf{p}_i}{m}\right)e^{-i\mathbf{q}\cdot\mathbf{r}_j}e^{i\mathbf{q}\cdot\mathbf{r}_i}\mathrm{d}\mathbf{r}^N\mathrm{d}\mathbf{p}^N \\
&-\frac{1}{m}\int k_BT\gamma P_{eq}e^{-i\mathbf{q}\cdot\mathbf{r}_j}\hat{\mathbf{q}}\cdot\left(\partial_{\mathbf{p}_j}\frac{\mathbf{p}_i}{m}\right)\cdot\hat{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}_i}\mathrm{d}\mathbf{r}^N\mathrm{d}\mathbf{p}^N \\
=&\sum_{i}\frac{1}{m}\int\frac{\mathbf{p}_i}{m}\cdot\left(\partial_{\mathbf{r}_i}P_{eq}\right)\left(\frac{\mathbf{p}_i\cdot\mathbf{p}_i}{2m}\right)\mathrm{d}\mathbf{r}^N\mathrm{d}\mathbf{p}^N-\frac{Nk_BT\gamma}{m^2} \\
=&-\frac{Nk_BT\gamma}{m^2}
\end{aligned}\tag{C8}$$

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Thus the frequency term is

$$i\underline{\Omega} = \begin{pmatrix} 0 & -i\,|\mathbf{q}|\,\frac{Nk_BT}{m} \\ -i\,|\mathbf{q}|\,\frac{Nk_BT}{m} & -\frac{Nk_BT\gamma}{m^2} \end{pmatrix} \begin{pmatrix} \frac{1}{NS(q)} & 0 \\ 0 & \frac{m}{Nk_BT} \end{pmatrix}$$
$$= \begin{pmatrix} 0 & -i\,|\mathbf{q}| \\ -i\,|\mathbf{q}|\,\frac{k_BT}{mS(q)} & -\frac{\gamma}{m} \end{pmatrix} \tag{C9}$$

This eventually gives the MCT equation for underdamped passive Browian particle system, Eq.(48) in the main text.

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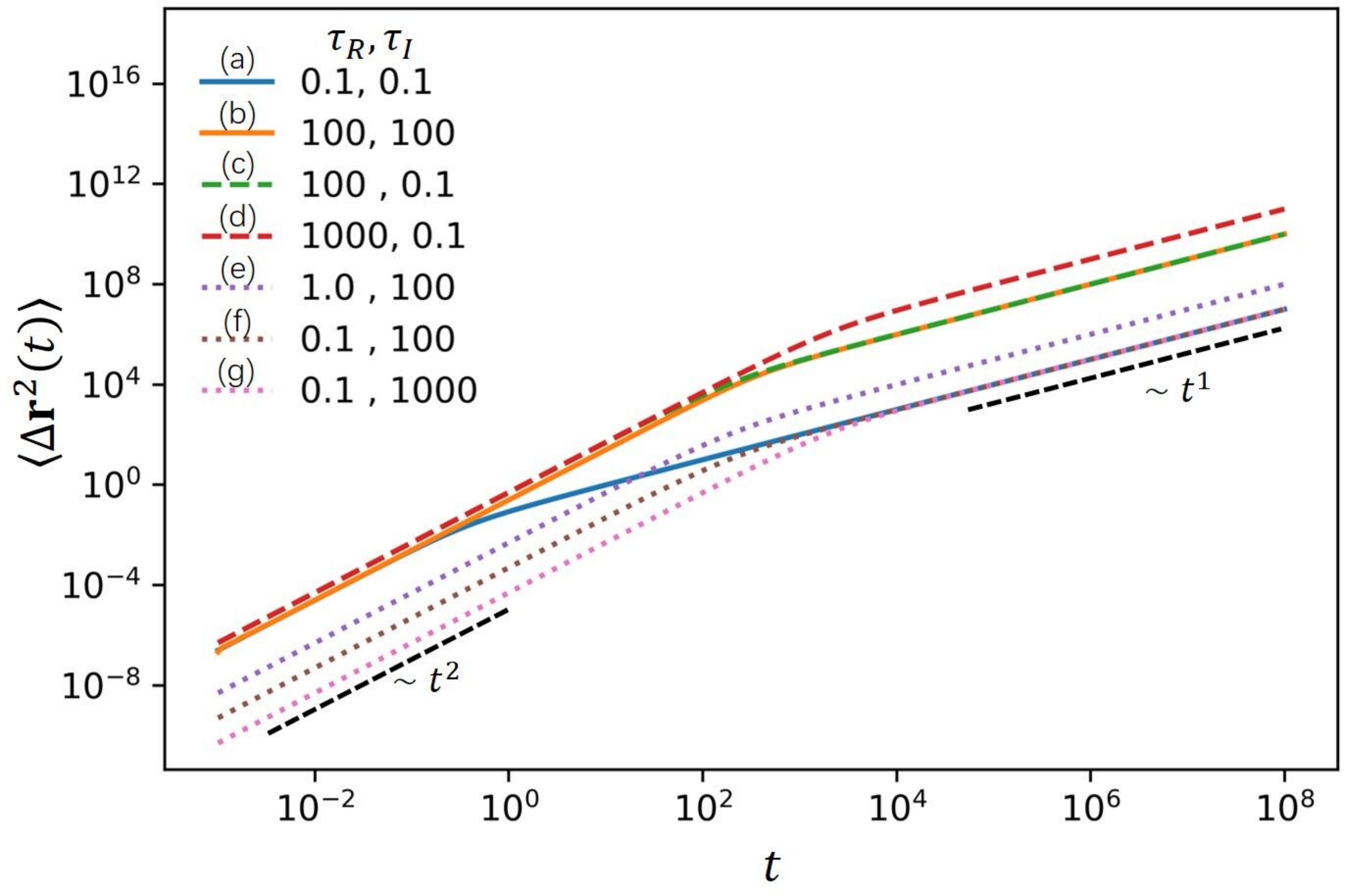

τ_R, τ_I
(a) 0.1, 0.1
(b) 100, 100
(c) 100 , 0.1
(d) 1000, 0.1
(e) 1.0 , 100
(f) 0.1 , 100
(g) 0.1 , 1000
$\langle \Delta \mathbf{r}^2(t) \rangle$
t
$\sim t^1$
$\sim t^2$
10^{16}
10^{12}
10^{8}
10^{4}
10^{0}
10^{-4}
10^{-8}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
10^{8}