Effective equilibrium states in mixtures of active particles driven by colored noise

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We consider the steady-state behavior of pairs of active particles having different persistence times and diffusivities. To this purpose we employ the active Ornstein-Uhlenbeck model, where the particles are driven by colored noises with exponential correlation functions whose intensities and correlation times vary from species to species. By extending Fox’s theory to many components, we derive by functional calculus an approximate Fokker-Planck equation for the configurational distribution function of the system. After illustrating the predicted distribution in the solvable case of two particles interacting via a harmonic potential, we consider systems of particles repelling through inverse power laws potentials. We compare the analytic predictions to computer simulations for such soft-repulsive interactions in one dimension, and show that at linear order in the persistence times the theory is satisfactory.

I. INTRODUCTION

The study of active particles has recently attracted rapidly increasing attention of scientists belonging to different disciplines due to the current interest in the physical principles governing the behavior of fish schools, herds of animals, bacteria, collections of cells and/or man-made active colloids [1–3]. All these systems in order to move convert energy via metabolic or chemical reactions and are thus out of equilibrium [4]. On the theory side, many fundamental aspects of active systems can be described with some minimalistic models based on spherical particles [5, 6]. Even in the absence of attractive interactions such particles can exhibit intriguing individual and collective behavior, induced solely by their persistent motion, such as the accumulation at the system boundary [7, 8], the separation into a dilute and a dense phase [9, 10] and wetting or capillary condensation condensation transitions [11].

While the majority of studies are concerned with systems whose constituents are all identical, in real situations it is common to observe assemblies of active particles of different nature. The obvious question is how does the heterogeneity affect the collective behavior of such mixtures [12]. For example, doping a passive fluid with a small number of active particles significantly alters its structural and dynamical properties by supporting the formation of clusters [12] and, at higher densities, crystallization [12, 13]. On the other hand, active dopants with a short persistence length were reported to aggregate in cages [14]. On immersing large colloids into a bath of smaller active colloids, the former effectively are rendered active, which becomes manifest through activity-enhanced diffusivities [15, 16] and depletion forces [8, 17]. Employing shape-anisotropic colloids [10, 21] or manufacturing activity gradients [22], these effects can be used to generate directed motion of the colloids. Moreover, the segregation between two passive species has been reported as the result of coupling only one species to the active bath [23].

The mixtures described so far consist of species which differ in their shape (interaction potential) and particle number. Seeking for the closest analogy to the motility-induced phenomena observed for a single active species, we are particularly interested in particles solely distinguished by a difference in their activity. The most intriguing feature of such multicomponent active systems is their capability to demix, which cannot be attributed to the physical mechanisms also present in equilibrium mixtures. Some recent investigations have focused on such a binary mixture of an active and a passive species [24–26] or particles with different finite activities [26–29]. Quite intuitively, active phase separation phenomena can be described using the concept of an effective temperature, enhanced by activity [30], which has also been applied to mixtures [27, 31, 32]. Relatedly, the demixing of particles with the same mobility but different diffusion coefficients has been recently reported [33].

The model of active particles propelled by so-called Ornstein-Uhlenbeck processes (OUPs) provides a convenient starting point of many theoretical studies, since their equations of motion do not resolve the orientational degrees of freedom. A minimalistic strategy is based on the multidimensional generalizations of the unified colored noise approximation (UCNA) [34, 35] or a similar
II. THEORY

In order to study a system of $N$ active particles in $d$ spatial dimensions having species dependent diffusivities $D^{(i)}_a$ and persistence times $\tau^{(i)}_a$ where the index $i \in \{1 \ldots N\}$, we generalize the microscopic one-component active OUPs model of Refs. 38, 39, and 43 to the case where different types of Gaussian stochastic driving terms are present. To do so, we introduce a component-wise notation (compare, e.g., Ref. 43) for $dN$-dimensional arrays $\chi_tool{a}(t)$ denoting the coordinates of the particles evolving according to

$$\dot{x}_\alpha(t) = D_{\beta}F_{\alpha}(x_1, x_2, \ldots, x_{\alpha N}) + \chi_\alpha(t), \quad \text{(1)}$$

where $\alpha \in \{1 \ldots dN\}$, $F_{\alpha}$ is a conservative force due to passive interactions, $D_{\beta}$ is the inverse friction coefficient (related to the translational diffusivity $D_t$ in a Brownian system).

The Gaussian stochastic noise $\chi_\alpha(t)$ evolves in time according to

$$\ddot{\chi}_\alpha(t) = -\frac{1}{\tau_\alpha^{(\alpha)}}\chi_\alpha(t) + \frac{\sqrt{D^{(\alpha)}_\alpha}}{\tau_\alpha^{(\alpha)}}\xi_\alpha(t), \quad \text{(2)}$$

with the white noise $\xi_\alpha(t)$, which has the time correlator $\langle \xi_\alpha(t)\xi_\beta(t') \rangle = 2D_t\delta_{\alpha\beta}\delta(t - t')$, and $D^{(\alpha)}_\alpha = D^{(\alpha)}_\alpha / D_t$. It has zero average and the tensorial time correlator

$$C_{\alpha\beta}(t - t') := \langle \chi_\alpha(t)\chi_\beta(t') \rangle = \frac{D^{(\alpha)}_\alpha}{\tau_\alpha^{(\alpha)}} \delta_{\alpha\beta} e^{-\frac{t - t'}{\tau_\alpha^{(\alpha)}}}. \quad \text{(3)}$$

The probability distribution functional of $\chi_\alpha(t)$ has the Gaussian representation:

$$P_N[\{\chi_\alpha\}] \propto \exp\left( -\frac{1}{2} \int ds\int ds' \sum_{\alpha\beta} \chi_\alpha(s)K_{\alpha\beta}(s - s')\chi_\beta(s') \right) \quad \text{(4)}$$

and is equipped with a tensorial kernel $K_{\alpha\beta}(t - t')$, the inverse of $C_{\alpha\beta}$.

In the appendix, by extending Fox’s approximation to an arbitrary number of (active) components, we show that the configurational distribution of positions of particles

$$f_N(\{y_\alpha\}, t) = \int D[\{\chi_\alpha\}] P_N[\{\chi_\alpha\}] \prod_\alpha \delta(y_\alpha - x_\alpha(t)) \quad \text{(5)}$$

evolves according to the following Fokker-Planck equation:

$$\frac{\partial f_N(\{y_\alpha\}, t)}{\partial t} = -\sum_\beta \frac{\partial}{\partial y_\beta} \left( D_{\beta}F_{\alpha}(\{y_\alpha\})f_N(\{y_\alpha\}, t) \right)$$

$$- D^{(\alpha)}_a \sum_\gamma \frac{\partial}{\partial y_\gamma} f_N(\{y_\alpha\}, t)\Gamma^{-1}_{\alpha\gamma}(\{y_\alpha\}) \quad \text{(6)}$$

with friction tensor

$$\Gamma_{\gamma\beta} = \delta_{\gamma\beta} - \tau^{(\beta)}_a D^{(\beta)}_a \frac{\partial F_{\alpha}}{\partial y_\beta}. \quad \text{(7)}$$

Switching to Cartesian coordinates we find the following Fokker-Planck equation:

$$\frac{\partial f_N(\{r_\alpha\}, t)}{\partial t} = -D_t \sum_i \nabla_i \cdot \left( \beta F_i(\{r_\alpha\})f_N(\{r_\alpha\}, t) \right)$$

$$- \sum_j \nabla_j \cdot \left( D_{ij}(\{r_\alpha\})f_N(\{r_\alpha\}, t) \right), \quad \text{(8)}$$

where the non dimensional diffusion tensor $D_{ij}$ is defined as $D_{ij}(\{r_\alpha\}) = D^{(i)}_a \Gamma^{-1}_{ji}(\{r_\alpha\})$. Assuming that the conservative force arises from an interaction potential $u_{ij}$ between each pair of particles and defining

$$\tilde{f}(\alpha) = D_{t}^{(\alpha)} \delta^{(\alpha)}_a,$$  \quad \text{(9)}$$

the friction tensor from Eq. (7) reads 38, 43

$$\Gamma_{ij}(\{r_\alpha\}) = 1\delta_{ij} + \tilde{f}(j) \nabla_i \nabla_j \sum_{k \neq i} u_{ik}(r_i, r_k). \quad \text{(10)}$$
In general, \( D_{ij}(r^N) \) is not symmetric, i.e., \( D_{ij} \neq D_{ji} \), if there are at least two different particle species. Regarding the structure of Eq. (3), transposing \( D_{ij} \) changes the components of the probability current but not the overall time evolution of the probability distribution. Further note that \( \Gamma_{ij} = \Gamma_{ji} \) only if \( i, j \) belong to the same species.

Intriguingly, the generalized Unified Colored Noise Approximation (UCNA) [34, 35] gives rise to a mobility matrix

\[
\Gamma_{\text{ucna}} = \delta_{ij} - \frac{\tau_i^{(\gamma)}}{\tau_i^{(\gamma)} + 1} \frac{\partial F_i}{\partial y_j} = \Gamma_{\beta \gamma}
\]

which is the transpose of the Fox result in Eq. (7). However, we find that the corresponding effective diffusion tensor \( D_{ji}^{\text{ucna}} := D_{ji}^{(i)} (\Gamma_{\text{ucna}})^{-1} = D_{ji}^{(i)} \Gamma_{ji}^{\beta} \neq D_{ij} \) is totally unrelated to \( D_{ij} \), contrasting the relation in Eq. (11). Therefore, UCNA and Fox do not share the same steady state as it is the case in a one-component system at sufficiently high activity. As we will see below, this is even the case at linear order in the persistence time.

While the steady-state condition requires the vanishing of the divergence of the probability current, the condition of detailed balance involves the vanishing of all components of the probability current so that from Eq. (8) we find:

\[
f_N \left( \beta F - D_{\alpha}^{(\beta)} \sum_{\gamma} \frac{\partial}{\partial y_{\gamma}} \Gamma_{\gamma \beta} \right) = D_{\alpha}^{(\beta)} \sum_{\gamma} \Gamma_{\gamma \beta} \frac{\partial}{\partial y_{\gamma}} f_N.
\]

In general, the solution of such an equation is not known, but it reduces to a Boltzmann-like distribution in the case of a single species [39].

For completeness, we consider the most general case where some particles are subject to an additional translational Brownian white noise, referred to as thermal noise in the following, which is relevant, e.g., for studying a mixture of an active and a passive Brownian species. Generalizing Fox’s approximation [45], it is straightforward to rewrite Eq. (8) with the generalized tensor

\[
\mathcal{D}_{ji}(r^N) = \delta_{ji} I_t^{(i)} + D_{ji}^{(i)} \Gamma_{ji}^{-1}(r^N),
\]

where \( I_t^{(i)} \) takes the values 1 in the presence and 0 in the absence of thermal noise acting on particle \( i \). Equation (8) with Eq. (13) represents the full extension of Fox’s approximation [39, 37] for one component active fluids [38, 45, 46] to the multicomponent case where the fluid contains different species and each species is subjected to active (colored) noise whose intensity depends on the persistence time and the species.

III. AN ELEMENTARY TEST

Before discussing the more realistic case of a mixture, we consider perhaps the simplest model of interacting particles which lends itself to an analytic solution and may serve as a benchmark for our theory. An elastic dimer in a \( d = 1 \) dimensional well and subject to two different colored Gaussian baths is represented by two particles mutually coupled by a harmonic potential \( u(x_1 - x_2) = \alpha^2 (x_1 - x_2)^2/2 \) and each confined by a harmonic external potential \( v(x_a) = \omega^2 x_a^2/2 \). Their dynamics is described by the evolution equations

\[
\dot{x}_1(t) = D_{1} \beta F_1(x_1, x_2) + \chi_1(t),
\]

\[
\dot{x}_2(t) = D_{2} \beta F_2(x_1, x_2) + \chi_2(t),
\]

where \( F_a = -\frac{d}{dx_a}(v(x_a) + u(x_a - x_a)) \). The friction \( 1/(D_{a} \beta) \) is the same for both species, but the parameters \( \tau_a^{(\alpha)} \) and \( D_{a}^{(\alpha)} \) characterizing the stochastic driving term \( \chi_a(t) \), defined in Eq. (2), are different. Explicitly we have

\[
\dot{x}_1 = -D_{1} \beta (\omega^2 x_1 + \alpha^2 (x_1 - x_2)) + \chi_1(t),
\]

\[
\dot{x}_2 = -D_{2} \beta (\omega^2 x_2 - \alpha^2 (x_1 - x_2)) + \chi_2(t).
\]

This model has been first used in statistical mechanics in the context of the virial theorem by Riddell and Uhlenbeck [48] and recently by one of us [42] in the framework of active systems.

The model, being linear, can be solved analytically by direct integration of equations of motion. It is convenient to switch to collective variables \( q = x_1 - x_2 \) and \( Q = (x_1 + x_2)/2 \) and to the renormalized spring constant \( \Omega^2 = \omega^2 + 2\alpha^2 \). The steady-state equal-time pair correlations read

\[
\langle Q(t)Q(t') \rangle = \frac{1}{4\beta \omega^2} \left( \frac{D_{1}^{(1)}}{1 + \tau_t^{(1)} \Omega^2} + \frac{D_{2}^{(2)}}{1 + \tau_t^{(2)} \Omega^2} \right),
\]

\[
\langle q(t)q(t') \rangle = \frac{1}{\beta \Omega^2} \left( \frac{D_{1}^{(1)}}{1 + \tau_t^{(1)} \Omega^2} + \frac{D_{2}^{(2)}}{1 + \tau_t^{(2)} \Omega^2} \right).
\]

with \( \tau_t \) defined by [39]. Such an exact result will now be used to compare with the generalized Fox approximation.

A. Fox’s approximation for two oscillators

We now compute the averages featuring in Eqs. (17) and (18) using the approximate Fox theory for two components. The evolution of the probability distribution function of the state, \( \{y_a\} \), at time \( t \) described by the Fokker-Planck equation, Eq. (3), can be written in the compact form

\[
\frac{\partial}{\partial t} f_N(\{y_a\}, t) = \mathcal{L}_{FP} f_N(\{y_a\}, t)
\]

where \( \mathcal{L}_{FP} \) represents the Fokker-Planck operator. It follows that the average of an observable \( \mathcal{O}(\{y_a\}) \) evolves according to

\[
\frac{\partial}{\partial t} \langle \mathcal{O}(\{y_a\}, t) \rangle = \langle \mathcal{L}_{FP}^{\dagger} \mathcal{O}(\{y_a\}, t) \rangle
\]

where \( \mathcal{L}_{FP}^{\dagger} \) is the adjoint operator of the Fokker-Planck operator \( \mathcal{L}_{FP} \) and \( \langle \mathcal{O}(\{y_a\}, t) \rangle \equiv \int d\{y_a\} f_N(\{y_a\}, t) \mathcal{O}(\{y_a\}) \).
shall not digress to further discuss the multicomponent
our goal is to describe a system with
accurately described by the multicomponent Fox approach,
different diffusivities and (small) persistence times are ac-
tion, which is exact in the small $\tilde{\alpha}$
comparing Eq. (7) and Eq. (11) that UCNA results for
Planck equation (8) does, in general, not admit current-
and we obtain the following expression for the equal-time
theorem [49] the l.h.s of (21) vanishes as $t \to \infty$ as the system approaches the steady state. We obtain a simple
set of linear equations for the correlators $\langle x_\alpha x_\beta \rangle$, which can be easily solved.
Evaluating the inverse matrix $\Gamma^{-1}_{\alpha \beta}$ to first order in $\tilde{\alpha}(\alpha)
\Gamma_{11}^{1} = 1 - \tilde{\alpha}(1)(\omega^2 + \alpha^2)
\Gamma_{22}^{1} = 1 - \tilde{\alpha}(2)(\omega^2 + \alpha^2)
\Gamma_{12}^{1} = \tilde{\alpha}(2)\alpha^2
\Gamma_{21}^{1} = \tilde{\alpha}(1)\alpha^2
and we obtain the following expression for the equal-time correlations of the collective variables according to Fox's theory:
$\langle QQ \rangle = \frac{1}{4\beta\omega^2}(D^{(1)}_{0}(1 - \tilde{\alpha}(1)\omega^2) + D^{(2)}_{0}(1 - \tilde{\alpha}(2)\omega^2))$
$\langle q q \rangle = \frac{1}{\beta\Omega^2}(D^{(1)}_{0}(1 - \tilde{\alpha}(1)\Omega^2) + D^{(2)}_{0}(1 - \tilde{\alpha}(2)\Omega^2)).$
By comparing Eqs. (23) and (24) with the corresponding exact expressions [17] and [18] we see that Fox’s result agrees to linear order in $\tilde{\alpha}(\alpha)$. One can easily see from comparing Eq. (7) and Eq. (11) that UCNA results for
the off-diagonal friction matrix elements in Eq. (22) and the correlators in Eq. (21) are different from those found in the present treatment, based on the Fox approximation, which is exact in the small $\tilde{\alpha}(\alpha)$ limit. Therefore, we shall not digress to further discuss the multicomponent UCNA equations.

IV. PROBABILITY DISTRIBUTION FUNCTION

Having seen that a system of two active particles with different diffusivities and (small) persistence times are accurately described by the multicomponent Fox approach, our goal is to describe a system with $\kappa$ components in $d$ dimensions. As shown in Sec. III the effective Fokker-Planck equation [23] does, in general, not admit current-free steady states. We thus write the condition for the existence of a steady-state solution in terms of the components
$J_{i\mu} = - \left( \beta F_{i\mu} \right) f_N - \sum_{\nu=1}^{\kappa} \sum_{J_{i\nu}=1}^{\kappa} \nabla_{j\mu} \cdot (D_{j\mu} f_N)$
of the probability current vector $J$, where the sum over particles $i$ has been transformed into a double sum over particle species $\mu$ and particles $i_{\nu}$ of each species, so that $N = \sum_{\mu} N_{\mu}$.
The steady-state condition then becomes
$\sum_{\mu=1}^{\kappa} \sum_{i_{\mu}=1}^{N_{\mu}} \nabla_{i_{\mu}} \cdot J_{i_{\mu}} = 0,$
generalizing the expression $J_1 = 0$ for one component [38]. Note that is not possible to write the above equation in a thermodynamical version [41] defining a conservative effective force [38, 46]. The prerequisite to derive an effective force of any kind is the existence of a Boltzmann-like configurational probability distribution $f_N(r^N)$, which is known analytically for a one-component system if no thermal noise is present [34].

A. Two-particle current

From now on, we restrict ourselves to $N = 2$ particles and silently omit the additional index denoting the species $\upsilon$ and $\mu$ of particle $1 \approx 1_{\upsilon}$, and of particle $2 \approx 2_{\upsilon}$ or $2 \approx 1_{\mu}$ if $\upsilon \neq \mu$. As both the interaction force and the effective diffusion tensor only depend on their distance $r = |r_1 - r_2|$ we can define a common derivative operator $\nabla \equiv \nabla_1 = -\nabla_2$. It then follows from Eq. (25) that
$\nabla \cdot J_1 - \nabla \cdot J_2 = 0.$
Explicitly, the two currents are given by:
$J_1(r) = f_2(r) \nabla (-\beta u(r) - D_{11} + D_{21})$
$+ (-D_{11} + D_{21}) \cdot \nabla f_2,$
$J_2(r) = f_2(r) \nabla (-\beta u(r) - D_{12} + D_{22})$
$+ (-D_{12} + D_{22}) \cdot \nabla f_2.$
Consider first a two-body system with a single component $\mu = \upsilon$, where $D_{11} = D_{22}$ and $D_{21} = D_{12}$ and thus Eq. (27) is trivially fulfilled. In general, the zero-divergence condition (27) is satisfied by $J_1 = J_2 + X$, where $X$ is a constant in $d = 1$ dimension or a divergence-free vector field for $d = 3$.
Let us now consider for the sake of simplicity and illustration purpose the one-dimensional case, where we define $x = x_1 - x_2$. The two particles belonging to different species interact with the same finite-range and symmetric pair potential $u(x)$ with $\lim_{x\to\pm\infty} u(x) = 0$. By subtracting the second current in Eq. (28) from the first one we obtain
$X = -2f_2(x) \frac{d}{dx} \left( \beta u(x) + D_m \right) - 2D_m \frac{d}{dx} f_2(x).$
where we defined
\[ D_m := \frac{1}{2}(D_{11} - D_{21} + D_{22} - D_{12}). \] (30)

Such an inhomogeneous first order linear differential equation can be solved by introducing the so-called integrating factor
\[ \psi_2(x) = \exp\left( -\frac{\int_0^x}{\int_{-\infty}^x D_m(s) \, ds} \right) \] (31)

Due to the symmetry of the pair potential the integrating factor has the property \( \lim_{x \to \pm \infty} \psi_2(x) = 1 \). The general solution of Eq. (29) must be of the form
\[ f_2(x) = \psi_2(x) \left( A - \frac{X}{2} \int_{-\infty}^x \frac{ds}{D_m(s) \psi_2(s)} \right) \] (32)

so that \( \lim_{x \to -\infty} f_2(x) = A \). Now, the value of the distribution function at infinity must be identical to the value at minus infinity ( \( \lim_{x \to -\infty} f_2(x) = A \) ) and we may conclude that:
\[ A = \lim_{x \to \infty} \psi_2(x) \left( A - \frac{X}{2} \int_{-\infty}^x \frac{ds}{D_m(s) \psi_2(s)} \right). \] (33)

The only solution is \( X = 0 \), thus the two currents \( J_1 = J_2 \) must be equal and \( f_2(x) = \psi_2(x) \) is given by Eq. (31), i.e., \( A = 1 \). Combining Eq. (29) for \( X = 0 \) with Eq. (28) we find
\[ J_1 = J_2 = \frac{f_2(x)}{2D_m} \left( (D_{11} - D_{21} - (D_{22} - D_{12})) \nabla \beta u(x) \right. \\
+ (D_{11} - D_{21}) \nabla (D_{22} - D_{12}) \\
- (D_{22} - D_{12}) \nabla (D_{11} - D_{21}) \right). \] (34)

One can see that \( J_1 = J_2 = 0 \) only if \( D_{11} - D_{21} = D_{22} - D_{12} = D_m \), a condition which is realized when the two particles are identical.

\[ f_2(x) \sim \exp\left( -\frac{x^2}{2(q_y)} \right) \sim \exp\left( -\frac{\beta u(x)}{2D_m} \right) \sim \exp\left( -\frac{\beta u(x)}{D_m} \right) \] (35)

explicitly as a Gaussian.

It is easily verified that a distribution of the form (35) gives \( X = 0 \) in Eq. (29), since \( D_m \) does not depend on \( x \) for the employed potential. We immediately get from Eq. (30) the position-dependent currents
\[ J_1 = J_2 = \frac{f_2(x)}{2D_m} \left( (D_{11} - D_{21} - (D_{22} - D_{12})) \nabla \beta u(x) \right. \\
= \alpha^2 x f_2(x) \left( \frac{(q_1^{(1)} q_2^{(2)}) (D_{11}^{(1)} + D_{21}^{(2)})}{(q_1^{(1)} q_2^{(2)}) (D_{11}^{(1)} - D_{12}^{(2)})} \right) \right). \] (36)

From these formulas it is easy to verify that the currents vanish for two identical particles with both \( \tau^{(1)} = \tau^{(2)} \) and \( D_1^{(1)} = D_2^{(2)} \). The full formula for the probability distribution \( f_2(x) \) follows from the consideration in the following section, which hold for an arbitrary bare interaction potential.

C. Effective potentials

With the knowledge of the two-particle probability distribution \( f_2 \), as given in one dimension by \( f_2(x) \equiv \psi_2(x) \) from Eq. (31), one can define an effective force \( \mathbf{F}_i^{\text{eff}} \) on particle \( i \in [1, 2] \) from the condition \( \beta \mathbf{F}_i^{\text{eff}} f_2 = -\nabla f_2 = 0 \). Note that defining an effective force \( \beta \mathbf{F}_i^{\text{eff}} \) equal to \( \beta \mathbf{F}_i \) of two particles of species \( \nu \) and \( \mu \) in \( d \) dimensions, obtained from equating the currents in Eq. (28) as
\[ \nabla \beta u_{\nu \mu}^{\text{eff}}(r) = -\nabla \ln f_2 = D_m^{-1} \cdot \nabla \left( \beta u(r) + D_m \right) \] (37)
with \( D_m \) defined as in Eq. (30).

The effective potentials \( u_{\nu \mu}^{\text{eff}} \) between members of the same species \( \nu \) can be obtained in various alternative ways, e.g., by setting either current in Eq. (28) to 0. The explicit form of the \( u_{\nu \nu}^{\text{eff}} \) has been discussed in detail in Ref. (58). Without thermal noise, i.e., setting in Eq. (15) \( T_i^{(0)} = 0 \) for all \( i \), the closed analytical expression
\[ \beta u_{\nu \nu}^{\text{eff}}(r) = \frac{u(r) + \dot{z}_0(r) \left( \frac{\partial u(r)}{\partial r} \right)}{D_h^{(v)}} - \ln \left\| E_1^{(v)} \right\|^{(0-1)} \left| E_2^{(v)} \right| \right), \] (38)
where the superscript \( (v) \) is short for \( (i) \). The above expression is valid in any spatial dimension \( d \), where
\[ E_n^{(v)}(r) = 1 + 2^{2(v + n - 2)} \frac{D_n^{(v)}}{\partial r} \] (39)
with \( n \in \{1, 2\} \) are the eigenvalues of \( \Gamma_{ij} \), defined in Eq. (10), for two particles of species \( \nu \). In this special case, \( E_n^{(v)} \) are equivalent (up to the factor \( D_h^{(v)} \) to the
FIG. 1. Effective potentials in one dimension from OUPs simulation and the Fox theory, Eq. (42), between two active particles with the parameters \( \tau^{(1)} \) and \( D_a^{(1)} \) (as labeled) with \( \tau^{(2)} = 0.1 - \tau^{(1)} \) and \( D_a^{(2)} = 9.6 - D_a^{(1)} \), such that \( \tau = 0.05 \) and \( D_a = 4.8 \) (the results are invariant under exchanging the labels 1 and 2). Here we consider only particles with at least one pair of equal parameters (\( \tau^{(2)} = \tau^{(1)} \) or \( D_a^{(2)} = D_a^{(1)} \)), such that the results only depend on \( |\Delta D_a| \) or \( |\Delta \tau| \), respectively (equivalent parameter values are shown in brackets). The case of all parameters being equal is labeled as “ep”. The Fox theory predicts the same result (ep) in all cases. We consider a system (a) without and (b) with thermal noise; note the different scale on the vertical axes.

The nature of this term can be understood from Eq. (39), the persistence times \( \tau^{(1)} \) and \( \tau^{(2)} \). The persistence times \( \tau^{(1)} \) and \( \tau^{(2)} \) are the same as in Fig. 1 (left).

or \( D_a^{(2)} = 0 \) with \( I_1^{(2)} = 1 \). Both definitions result in the same \( E_n^{(v)} \) for an active-passive mixture with arbitrary \( \tau^{(v)} \) and \( D_a^{(v)} \) only if the term \( \Delta D_a \Delta E_n(r) \) is present.

In the following, we restrict ourselves to the one-dimensional case, where the one-component theory is highly accurate \cite{38,39}. Solving Eq. (42) we obtain the most general form

\[
\beta u_{\nu}(x) = \int_{-\infty}^{x} ds \frac{d\beta u(s)}{ds} E_2^{(\nu)}(s) - \ln \left( D_a \left| E_2^{(\nu)}(x) \right| \right)
\]

of the effective potential for a symmetric bare potential with \( \lim_{x \to \infty} u(x) = 0 \). For two different species, it is not possible to carry out the integral in general, even if \( I_1^{(v)} = I_1^{(\mu)} = 0 \). If, in addition, both species either have the same active diffusivity \( D_a^{(v)} = D_a^{(\mu)} \) or characteristic functions \( I_1^{(v)} = I_1^{(\mu)} \), one recovers an effective potential similar to the single-component result in Eq. (38) with \( \nu = 1 \), replacing \( \tau^{(v)} \to \tau \) or \( D_a^{(v)} \to D_a \), respectively, with the appropriate average parameter.

It is straightforward to generalize the above discussion to higher spatial dimensions. However, we would face the following complications: (i) the exact effective potentials can be written in a form similar to Eq. (42) only if \( I_1^{(v)} = 0 \), in addition to \( I_1^{(v)} = I_1^{(\mu)} = 0 \), we assume \( D_a^{(v)} = D_a^{(\mu)} \) or \( \tau^{(v)} = \tau^{(\mu)} \); (ii) we have no rigorous proof that the underlying assumption \( J_1 = J_2 \) holds for \( d > 1 \); (iii) already for two particles of the same species, empirical corrections of the effective potential are required and the quantitative agreement with computer simulation becomes worse with increasing dimensionality \cite{38}.

D. Model calculations in one dimension

To test the generalized theory we consider a soft-repulsive bare potential \( u(x) = x^{-12} \) between two particles and perform computer simulations of active
OUPs [38], evolving according to Eq. (11), as a benchmark for the effective potentials predicted from Fox’s approach. Since we focus on the one-dimensional case, we can also make quantitative statements about whether the accuracy of the single-component theory [38, 47] is maintained if the difference in activity increases. We checked that the qualitative behavior is not altered when an additional thermal-noise vector is added to Eq. (11) and a quantitative comparison to the simulation data is thus analogous to the single-component case [38]. An exemplary direct comparison of these two systems is made in Fig. 4.

For the following discussions, recall the definitions and sign of relative parameters from Eq. (11), where the particle labeled 1 is always considered a member of species \( u \). The most important theoretical statement of Sec. IV C is that either for equal \( D_a^{(1)} = D_a^{(2)} = \bar{D}_a \) or \( \tau^{(1)} = \tau^{(2)} = \bar{\tau} \), the effective potential of the mixture is equal to that of two identical particles with averaged activity parameters. According to Fig. 1, this prediction is indeed confirmed numerically for the latter case, whereas at equal \( D_a \) the effective potential should rather become less attractive with increasing difference \( |\Delta \tau| \). We will return to this point at the end of this section.

If the two species differ in both activity parameters, the theoretical results do no longer depend only on the average values due to the term \( \Delta D_a \Delta E_2(r) \) in Eq. (12). For small differences \( \Delta D_a \) and \( \Delta \tau \), we observe in Figs. 2 and 3 that both theory and simulations predict a deeper minimum of the effective potential when \( \Delta D_a \Delta \tau \) is increased. Further increasing the absolute value of either difference, the theory becomes quantitatively inaccurate. For \( \Delta D_a \Delta \tau < 0 \) the theoretical curves suggest a rapid decline in the effective attraction, while much larger differences between the parameters are required to noticeably shift the numerical curves. For \( \Delta D_a \Delta \tau > 0 \) the theory starts to predict diverging effective potentials, which is qualitatively wrong.

Interestingly, the behavior of the simulation results in the regime \( \Delta D_a \Delta \tau > 0 \) distinctly depends on the parameters that are changed. Fixing \( \Delta \tau < 0 \) and decreasing \( \Delta D_a < 0 \) the curves in Fig. 2b begin to saturate and the deepest minimum is reached for the minimal \( \Delta D_a \) i.e., \( D_a^{(1)} = 0 \). On the other hand, the curve with the deepest minimum in Fig. 4a at constant \( \Delta D_a < 0 \) is found for an intermediate \( \Delta \tau < 0 \), whereas for even smaller \( \Delta \tau \) the trend inverts. This means that for large absolute differences \( |\Delta \tau| \) in the persistence time, i.e., one species becoming more and more passive, there is no significant attraction between two active OUPs (see also Fig. 3).

The special case of a common persistence time \( \tau = \tau^{(1)} = \tau^{(2)} \) of both particles is particularly relevant, since \( \tau \) represents a common rotational diffusion of all species in a mixture of ABPs with different self-propulsion velocities [40]. As noted before, this choice of parameters also yields particularly simple effective potentials, which are equivalent to the single-component results with the averaged diffusivity \( \bar{D}_a \) defined according to Eq. (41). Recall from Fig. 4 that also computer simulation results are well represented by those with \( \bar{D}_a \). Figure 4 nicely confirms for different activity parameters our expectation that for the Brownian mixture under consideration the effective potentials are as accurate as those between identical particles in one spatial dimension [38, 39]. Accordingly, the deviations from the simulation results are most significant for large separations \( r/d \) and increase with increasing average activity \( D_a \).

Another special case, which recently has attracted much interest, is a mixture of an active and a passive Brownian species [22, 23]. Given the prior results, the only way to set up a meaningful theoretical description of such a system is to fix \( D_a^{(1)} = D_a^{(2)} = 1 \), since the persistence times \( \tau^{(2)} = 0 \) of the passive and \( \tau^{(1)} \) of the active species are different by necessity in the OUPs model. Choosing the latter as the free activity parameter, as shown in Fig. 4b, makes it difficult to connect to ABPs, where the activity should rather be tuned by varying the active diffusivity \( D_a^{(1)} \) (depending on the self-propulsion velocity) rather than the (non-Brownian) reorienta-
tion time $\tau^{(1)}$.

In general, our OUPs simulations indicate that there is no significant effective attraction whenever one of the two particles is passive. Putting aside the difficulties with the equilibration, the numerical curves in Fig. 1 are practically independent of the activity of the second particle. Inspired by Percus’ test particle approach [52], we conjecture that the pair distribution in a two-body system including a passive Brownian particle always reflects the behavior of the bare interaction potential, regardless of the type and magnitude of self propulsion of the other species. This conclusion is also consistent with the behavior of the different curves shown in Figs. 1 and 3a upon increasing $|\Delta \tau|$. As for these sets of parameters, the theoretical effective potentials in Fig. 2 overestimate the effective attraction. However, in this special case with one passive particle the simulation result obtained on the two-body level obviously does not reflect the behavior of the many-body system.

V. CONCLUSIONS

In this paper, we derived the multicomponent generalization of the multidimensional Fox approximation and applied it to pairs of active particles with different persistence times and diffusivities. Our analytic results were compared to an exact solution for harmonic potentials and computer simulations for soft-repulsive interactions in one dimension, which both suggest that our theory is satisfactory at linear order in the persistence times. Explicitly, the formulas (42) with (40) for the effective interaction potentials between two different particles resemble those for two identical particles with average activity parameters plus an additional term depending on their differences. This term is important to make correct qualitative predictions close to equilibrium (or for small differences between the parameters) but also can be identified as the reason for the wrong or even unphysical predictions beyond the low-activity limit. It might be interesting in future work to explore the possibility for an empirical modification of the effective potential in the spirit of the inverse-$\tau$ approximation introduced in Ref. 38.

As for a single component, the predicted effective potentials can be readily implemented in a density functional theory in order to make explicit predictions of the structure and phase behavior [11]. Keeping this in mind, we also stress that the limitations discussed in Sec. V.D if the two particles belong to different species, will eventually only play a minor role on the many-particle level. Here, the effective pair potential between members of the same species will be equally or, most likely, even more relevant. The same is true if one is interested in a mixture in the presence of external forces, which are also single-body quantities. It might thus also constitute a fair approximation to drop the term $\Delta P_a \Delta E_2 (r)$ in Eq. (40), i.e., to simply use the average parameters in any case.

The most obvious application of our effective potentials is also among those of most recent interest. Following the intuition from passive mixtures, the tendency of a two-component system to demix arises from differences in the interactions between the members of each species. In our case the increased effective attraction within the (more) active species can be interpreted as the driving force of the demixing process when its activity is increased. It will thus come to no surprise that an explicit (passive) calculation will predict that the effective equilibrium state of a mixture of two different active species is demixed/phase separated. Of course the problem of demixing is ill-defined in one dimension, but the results discussed here will qualitatively be the same in higher dimensions, although it is a well-known problem of the theory that the effective attraction is overestimated and further empirical corrections are necessary in order to avoid divergences [38].

Considering the problem of active depletion it is not as simple to draw conclusion solely from discussing the effective potentials. The expected attraction between the passive particles does not result directly from the (still passive) effective potential between members of this species. It is still quite likely that the enhancement of the depletion interaction is also captured in our theory and can be implicitly accounted for when studying the full behavior of an effective mixture between an active ideal gas higher effective temperature) and passive colloids. To show this explicitly, another calculation in the spirit of the Asakura-Oosawa model [51] would be necessary. Likewise, all other combinations of different passive potentials in the active mixture can be modeled within our approach, where the effective interactions between members of different species, as studied here, are generally important. As for a single component, an extension of the theory to study dynamical problems is straightforward.

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Appendix A: The multicomponent Fox approximation

We derive of the Fokker-Planck evolution equation of the probability density distribution associated with the stochastic differential equation (1) by employing a generalized Fox approximation [39, 40]. By differentiating with respect to time the probability density distribution [3] associated the stochastic process Eq. (1) we obtain
We first use the Novikov theorem and the explicit form for the noise contribution and is calculated as follows.

The first term in Eq. (A1) stems from the deterministic part of the evolution, whereas the second term accounts for the noise contribution and is calculated as follows.

\[
\int D[\{\chi_\alpha\}]P_N[\{\chi_\alpha\}] \left( \prod_\alpha \delta(y_\alpha - x_\alpha(t)) \right) \chi_\beta(t) \\
= - \sum_\gamma \int \left[ \left( \prod_\alpha \delta(y_\alpha - x_\alpha(t)) \right) \frac{\delta x_\gamma(t)}{\delta \chi_\beta(t')} \right] dt' C_{\beta\gamma}(t-t').
\]

(A1)

The formal solution of Eq. (A3) with the initial condition

\[
\left. \left( \frac{\delta x_\gamma(t)}{\delta \chi_\beta(t')} \right) \right|_{t=t'} = \delta_{\beta\gamma}
\]

(A3)

is given (for \(t > t'\)) by the tensor

\[
\frac{\delta x_\gamma(t)}{\delta \chi_\beta(t')} = \left( \exp \int_{t'}^t ds \tilde{\mathbf{f}}'(s) \right)_{\gamma\beta} \Theta(t-t')
\]

\[
\approx \left( \exp(t-t') \tilde{\mathbf{f}}'(t) \right)_{\gamma\beta} \Theta(t-t').
\]

(A5)

In the second step, we expanded the integral in the exponent up to linear order in \((t-t')\) and we introduced \(\tilde{\mathbf{f}}'(t) \approx \tilde{\mathbf{f}}'(x_\alpha(t))\) with the components \(\tilde{\mathbf{f}}'_{\gamma\beta} = D_{\gamma\beta} \partial \beta F_\gamma / \partial x_\beta\). To shorten the notation we indicate the average of a function \(\mathcal{O}(x_\alpha(t))\) as

\[
\langle \mathcal{O}(x_\alpha(t)) \rangle \equiv \int D[\{\chi_\alpha\}]P_N[\{\chi_\alpha\}] \mathcal{O}(x_\alpha(t)).
\]

Now we use Eq. (A3) to rewrite Eq. (A2) as

\[
- \sum_\gamma \frac{\partial}{\partial y_\gamma} f_N \left( \left\langle \prod_\alpha \delta(y_\alpha - x_\alpha(t)) \frac{\delta x_\gamma(t)}{\delta \chi_\beta(t')} \right\rangle \right)
\]

\[
\approx - \sum_\gamma \frac{\partial}{\partial y_\gamma} f_N \left( \left\langle \prod_\alpha \delta(y_\alpha - x_\alpha(t)) \right\rangle \right) \left\langle \tilde{\mathbf{f}}'(t) \right\rangle_{\gamma\beta}^{-1}
\]

(A7)

where \(f_N \equiv \left\langle \prod_\alpha \delta(y_\alpha - x_\alpha(t)) \right\rangle \) and we approximated the average of the product in the in the first line by the product of the averages. Using the explicit correlator and further approximating the average of the exponential with the exponential of the average the integral featuring in Eq. (A7) becomes:

\[
\int_0^t dt' \frac{D_{\alpha\beta}(t)}{\tau_{\alpha\beta}(t)} e^{-\frac{\left\langle \tilde{\mathbf{f}}'(t) \right\rangle_{\gamma\beta}}{\gamma_{\beta}}} \times \left( e^{(t-t') \tilde{\mathbf{f}}'(t)} \right)_{\gamma\beta}^{-1}
\]

(A8)

where we took the small \(\tau_{\alpha\beta}(t)\) limit in the integral. Putting together

\[
\frac{\partial f_N(\{y_\alpha\}, t)}{\partial t}
\]

\[
= - \sum_\beta \frac{\partial}{\partial y_\beta} \left( D_{\beta\gamma}(t) f_N(\{y_\alpha\}, t) \right)
\]

\[
- D_{\alpha\beta}(t) \sum_\gamma \frac{\partial}{\partial y_\gamma} f_N \left( \left\langle \prod_\alpha \delta(y_\alpha - x_\alpha(t)) \right\rangle \right) \left( 1 - \tau_{\alpha\beta}(t) \left\langle \tilde{\mathbf{f}}'(t) \right\rangle_{\gamma\beta}^{-1} \right)
\]

(A9)

Such a formula can be recast under the form (6) given in the main text.

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