Active bath-induced localization and collapse of passive semiflexible polymers

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ABSTRACT

The conformational and dynamical properties of a passive polymer embedded in a bath of active Brownian particles (ABPs) are studied by Langevin dynamics simulations. Various activities and ABP concentrations below and above the critical values for motility-induced phase separation (MIPS) are considered. In a homogeneous ABP fluid, the embedded polymer swells with increasing bath activity, with stronger swelling for larger densities. The polymer dynamics is enhanced, with the diffusion coefficient increasing by a power-law with increasing activity, where the exponent depends on the ABP concentration. For ABP concentrations in the MIPS regime, we observe a localization of the polymer in the low-density ABP phase associated with polymer collapse for moderate activities and a reswelling for high activities accompanied by a preferred localization in the high-density ABP phase. Localization and reswelling are independent of the polymer stiffness, with stiff polymers behaving similarly to flexible polymers. The polymer collapse is associated with a slowdown of its dynamics and a significantly smaller center-of-mass diffusion coefficient. In general, the polymer dynamics can only partially be described by an effective (bath) temperature. Moreover, the properties of a polymer embedded in a homogeneous active bath deviate quantitatively from those of a polymer composed of active monomers, i.e., linear chains of ABPs; however, such a polymer exhibits qualitatively similar activity-dependent features.

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I. INTRODUCTION

Active matter exhibits remarkable cooperative and collective phenomena, such as swarming and active turbulence of bacteria¹⁻¹³ and activity-induced phase separation of synthetic Janus-swimmers, 13-22 which are absent in passive counterparts. In large-scale simulations of active Brownian particles (ABPs)^{15,16,23}—self-propelled (hard-sphere-type) spherical colloids-motility-induced phase separation (MIPS) has been found and phase diagrams have been determined for systems in two^{21,22,24} and three dimensions.^{20,21,24,25} Here, activity yields a separation of the active fluid into a dense and dilute phase.

Mixtures of active and passive particles (PPs) show even more intriguing effects. Hydrodynamic and steric interactions yield an enhanced diffusive motion of passive (colloidal) tracer particles immersed in a bath of active agents.²⁶⁻³⁹ Simulations of two-dimensional (2D) binary mixtures of isometric passive and active particles yield for sufficiently strong activities and active particle densities phase separation and formation of dense passive

clusters, which are encased by layers of active particles. 40-44 Similarly, large athermal passive colloids in a mixture with small active particles reveal an effective depletion-like attraction by the interactions with the small particles and a phase separation. 45 Phase separation can also be achieved by a fixed temperature difference⁴⁶ between two species of particles.⁴⁷ Yet, in contrast to mixtures of ABPs/passive colloids, no encasing active-particle layer seems to appear in this case, which indicates a qualitatively different driving mechanism for the phase separation. Simulations provide evidence of an emergent collective dynamics in phase-separated mixtures of isometric active and passive Brownian particles with a novel steadystate of propagating interfaces.⁴² This emphasizes the tight dynamical coupling between the two types of particles, which certainly depends on the mechanism maintaining their out-of-equilibrium

The presence of both active and passive components is a hallmark of living systems.^{48–52} The motility of microorganisms plays an essential role in maintaining an ecological balance and achieving biomixing of nutrients in aqueous environments. 33,53,54

The enhanced diffusion of a variety of passive particles, such as enzymes, granules, or extracellular products, either by cyclic conformational changes, for example of proteins and other biomolecules (DNA and RNA) during the transcription process fueled by ATP (adenosine triphosphate), or by induced hydrodynamic flows is essential for the proper function of a cell and promotes intercellular signaling and metabolite transports. 55-60 So far, the impact of activity on the properties of the passive components has not yet received the attention it deserves. Simulations of two-component mixtures of polymers at different temperatures yield phase separation.⁶¹ Here, the two temperatures account for, e.g., the activity of hetero- and euchromatin, which could play a role in chromatin separation in the cell nucleus.61-65 There are a variety of other out-of-equilibrium processes in a cell, which merit awareness. Cells exhibit coherent structures—the so-called membraneless organelles or condensates-encompassing and concentrating specific molecules, such as proteins and RNA in the cytoplasm. 66-68 In vivo experiments suggest that active processes, which occur constantly within such organelles, play a role in their formation.^{66,67} Insight into the interplay between equilibrium thermodynamic driving forces and nonequilibrium activity in the process of organelle formation is fundamental to reveal their functional properties and to elucidate their contribution to cell physiology and diseases.

Anisotropic shapes and internal degrees of freedom of passive particles in an active bath yield further effects that are absent in pure passive systems. Ellipsoids embedded in an *Escherichia coli* suspension show an anomalous coupling between the ellipsoid's translational and rotational motion, which is strictly prohibited in thermal equilibrium.³⁷ Passive semiflexible polymers embedded in an active bath of ABPs exhibit novel transient states in 2D,⁶⁹⁻⁷³ where an activity-induced bending of the polymers implies an asymmetric exposure to active particles, with ABPs accumulating in regions of highest curvature, as has been observed for ABPs in confinement.¹⁹ This leads to particular polymer conformations, such as hairpins, structures that are only temporarily stable and dissolve and rebuild in the course of time.

In this article, we consider the properties of semiflexible polymers embedded in a three-dimensional (3D) ABP fluid. Compared to 2D systems, the additional spatial dimension removes constraints on the ABPs' degrees of freedom and 2D-characteristic transient states are no longer present. We analyze the conformational and transport properties of the passive polymers as a function of bath density and activity. Specifically, we consider a homogeneous bath (no MIPS or clusters) and compare the polymer properties with those in a phase-separated fluid (MIPS). As for mixtures of active and passive colloids, in the homogeneous phase, we find an enhanced diffusive motion of the polymer—an anomalous diffusion at short times and an activity-driven diffusive motion at long times. Flexible polymers swell and semiflexible polymers shrink at smaller activities, and semiflexible polymers swell at larger activities similar to flexible polymers. An equivalent behavior is obtained for dry active polymers composed of ABP monomers (ABPO) exposed to colored noise.^{74–77} However, there are significant quantitative differences between the conformational and dynamical characteristics of ABPOs and polymers embedded in the active bath. The latter show a less pronounced dependence on activity. This is not surprising because the active ABP bath does not strictly mimic colored noise, in the sense of an exponentially decaying noise correlation function,⁷⁸ and the bath-induced active motion rather decays faster and correspondingly affects polymer conformations to a less extent.

In the case of the phase-separated active fluid (MIPS), most remarkably, we find an activity-dependent localization of (semiflexible) polymers in the low-fluid-density ABP region. This is accompanied with a collapse of the polymer manifested by a mean-square end-to-end distance comparable to that of a flexible polymer in a passive bath. This also affects the polymer dynamics and the center-of-mass diffusion coefficient is substantially lower than that predicted in the absence of localization. Stronger active noise leads to a dissolution of the polymer in the high-density ABP phase, with a swelling of the polymer and an enhanced dynamics. Interestingly, this behavior is independent of polymer stiffness.

This article is organized as follows: Section II describes the model for the ABP active bath and the polymer. The properties of bare ABP fluids as well as fluid mixtures of passive and active particles are briefly addressed in Sec. III. The results for the conformational and dynamical properties of semiflexible polymers embedded in ABP baths of various concentrations are presented in Sec. IV. Finally, Sec. V summarizes our findings and presents our conclusions.

II. MODEL

A. Active Brownian particle

We consider a three-dimensional system of N_a ABPs in a cubic box of length L_b with periodic boundary conditions. The ABPs are modeled as colloidal particles of mass m, diameter σ , and self-propulsion velocity v_0 along the fixed direction e_i , $i=1,\ldots,N_a$. ^{15,16,79,80} The translational motion of their positions r_i is described by the Langevin equations

$$m\ddot{\mathbf{r}}_i(t) = \gamma [v_0 \mathbf{e}_i(t) - \dot{\mathbf{r}}_i(t)] + \mathbf{F}_i(t) + \mathbf{\Gamma}_i(t), \qquad (1)$$

with the translational friction coefficient γ and the forces F_i on particle i by excluded-volume interactions between ABPs and monomers of a polymer [cf. Eq. (8)]. The change in the propulsion directions, e_i , is given by

$$\dot{\mathbf{e}}_i(t) = \mathbf{\Xi}_i(t) \times \mathbf{e}_i(t). \tag{2}$$

 Γ_i and Ξ_i are Gaussian and Markovian stochastic processes with zero mean and the second moments

$$\langle \Gamma_{\alpha i}(t) \Gamma_{\beta j}(t') \rangle = 2\gamma k_B T \delta_{\alpha \beta} \delta_{ij} \delta(t - t'),$$
 (3)

$$\langle \Xi_{\alpha i}(t) \Xi_{\beta j}(t') \rangle = 2D_R \delta_{\alpha \beta} \delta_{ij} \delta(t - t'),$$
 (4)

with the temperature T, the Boltzmann constant k_B , the rotational diffusion coefficient D_R , and the Cartesian coordinates $\alpha, \beta \in \{x, y, z\}$. Equation (4) yields the correlation function of the propulsion direction, ^{15,81}

$$\langle \mathbf{e}_i(t) \cdot \mathbf{e}_j(0) \rangle = e^{-2D_R t} \delta_{ij}.$$
 (5)

For a three-dimensional colloid in a fluid, the thermal translational, $D_T = k_B T/\gamma$, and the rotational, D_R , diffusion coefficients are related according to $D_T/\sigma^2 D_R = 1/3.^{81}$

B. Passive polymer

A polymer is modeled as a bead-spring chain of N_m monomers, with monomers of the same size and mass as ABPs. Their equations of motion are given by Eq. (1) without the active force, i.e., $v_0=0$. The forces $F_k=-\partial U/\partial r_k$ $(k=1,\ldots,N_m)$ comprise contributions from potentials by bonds, U_l , bending, U_b , and excluded-volume interactions, U_{ex} , i.e., $U=U_l+U_b+U_{ex}$, with the potentials

$$U_{l} = \frac{k_{l}}{2} \sum_{k=1}^{N_{m}-1} (|\mathbf{R}_{k}| - l)^{2},$$
 (6)

where $\mathbf{R}_k = \mathbf{r}_{k+1} - \mathbf{r}_k$ is the bond vector connecting neighboring monomers, k_l is the spring constant, and l is the rest length of a bond,

$$U_b = \frac{k_b}{2} \sum_{k=1}^{N_m - 2} (\mathbf{R}_{k+1} - \mathbf{R}_k)^2, \tag{7}$$

with the bending constant k_b , and

$$U_{ex}(r) = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} + \frac{1}{4} \right], & r < r_{c} = \sqrt[6]{2}\sigma, \\ 0, & r > r_{c}, \end{cases}$$
(8)

with r being the distance between particles and ϵ being the interaction strength.

The equations of motion (1) are integrated with a velocity Verlet-type scheme.⁸² The procedure to solve Eq. (2) is described in Refs. 81 and 83.

C. Parameters

In the simulation, we measure energies in units of the thermal energy k_BT , lengths in units of the equilibrium bond length $\sigma = l$, and time in units of $\tau = \sqrt{m\sigma^2/(k_BT)}$. The activity of the ABPs is characterized by the Péclet number

$$Pe = \frac{v_0}{\sigma D_P},\tag{9}$$

and the ratio $\Delta=D_T/(\sigma^2D_R)=1/3$ is used. Explicitly, we choose $\gamma=50\sqrt{mk_BT/\sigma^2}$, which yields the rotational diffusion coefficient $D_R=0.06/\tau$. This choice of the friction coefficient ensures overdamped motion on time scales $t\gg 1/\gamma$. To prevent bond stretching and an activity-dependent overlap between ABPs and monomers, respectively, we set $k_l=(5+Pe)\times 10^3k_BT/\sigma^2$ and $\epsilon=(Pe+1)k_BT$, which implies bond-length variations smaller than 3% of the equilibrium value l and a nearly Pe-independent nearest-neighbor distance. The density of ABPs is measured in terms of the global packing fraction $\phi=\pi\sigma^3N/(6L_b^3)$, with L_b being the length of the cubic simulation box. We study a single polymer with $N_m=20$ monomers; hence, length L=19l in a system of size $L_b=22\sigma$ for the ABP packing fractions $\phi\approx0.13,0.27$, and 0.53.

In the integration of Eqs. (1) and (2), the time step $\Delta t = 5 \times 10^{-4} \tau$ is applied. For every Péclet number, simulations are performed for 10^8 time steps, corresponding to the total time $T_t = 5 \times 10^4 \tau$ —or $T_t D_R = 3 \times 10^3$ —and up to eight realizations are considered.

III. PROPERTIES OF ACTIVE-PASSIVE MIXTURES

A remarkable feature of an active fluid is MIPS, which for ABPs in 3D leads to a phase separation into a dense and a dilute fluid phase above a critical density and Péclet number. 20,21,24,25 Here, the Péclet number (9) needs to exceed the value $Pe\approx30$, and the packing fraction needs to exceed the value $\phi\approx0.35$ for $Pe\lesssim300.^{20,42}$ Simulations of pure ABP fluids with the current setup confirm these results. Figure 1 illustrates the coexistence of a high-density and low-density fluid region.

The presence of passive particles (PPs) in isometric mixtures with ABPs changes the critical Péclet number as well as the critical overall packing fraction (ABPs + PPs) for MIPS. 42,43 Simulations of 2D mixtures yield a shift of these critical quantities to larger values. However, the studies of Ref. 42 suggest that the critical packing fraction of ABPs for MIPS in mixtures is independent of the concentration of PPs and needs to exceed the critical ABP value in the absence of PPs. Our current studies on 3D mixtures confirm these observations.

To illustrate the effect of the active bath on the properties of PPs (monomers) in a mixture, we analyze their diffusive behavior. Figure 2 presents the mean-square displacement (MSD) $\langle \Delta r_i^2(t) \rangle = \langle (r_i(t) - r_i(0))^2 \rangle$ of PPs and ABPs in mixtures for various fractions N_p/N of PPs, where N_p is the number of PPs and $N=N_p+N_a$ is the total number of particles, and various Péclet numbers at the overall packing fraction $\phi=0.53$. Note that a pure ABP fluid is

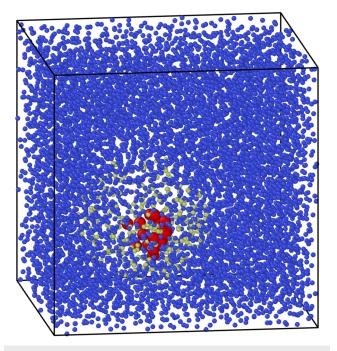


FIG. 1. Simulation snapshot of a polymer (red) immersed in bath of ABPs (blue, green) at the Péclet number Pe=100. The size of the ABPs is reduced to illustrate the density inhomogeneity and for visibility of the polymer. The polymer is localized in the "bubble" of the low-density MIPS phase. The ABPs inside the spherical bubble of radius 5.5σ with the polymer center-of-mass as center are colored in green (see movie M1 of the supplementary material for illustration).

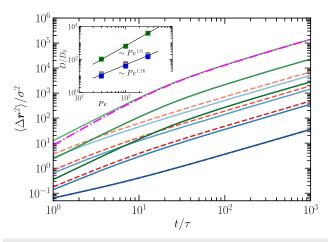


FIG. 2. Mean-square displacement of APBs (green) and PPs (blue, red) in an active bath with the average particle packing fraction $\phi=0.53$, the PP fractions $N_p/N=0.3$ (red, dashed) and 0.5 (blue), and the Péclet numbers Pe=0.01, 30, 100, and 300 (dark to bright). The magenta dashed-dotted line indicates the MSD of an ABP with the rotational diffusion coefficient $D_R=0.06/\tau$ and the effective Péclet number Pe=48.7. The MSD for Pe=0.01 is identical for all considered cases. Inset: long-time active diffusion coefficients for ABPs (green) and passive particles in the active bath for $N_p/N=0.3$ (red), 0.4 (cyan), and 0.5 (blue) as a function of the Péclet number. The ABP diffusion coefficients are independent of the fraction N_p/N . The solid lines indicate power-laws with the exponent 1.60 (ABPs) and 1.16 (PPs), respectively. $D_0=0.006\sigma^2/\tau$ is the diffusion coefficient of the particles in the passive system.

phase-separated for this packing fraction. Yet, the ABP concentrations $N_p/N=0.3,0.4$, and 0.7, in our considered mixtures, are too small to exhibit MIPS. Evidently, the passive-particle dynamics is activity enhanced, with MSDs increasing with increasing bath activity, *Pe.* However, the enhancement is significantly smaller than that of ABPs. As for the latter, we obtain a short-time super-diffusive behavior, which turns into an active diffusion for long times. However, the exponent in the super-diffusive regime is significantly smaller than 2, the value of ABPs in dilute systems.¹⁵

The magenta line in Fig. 2 indicates a fit of the MSD of the ABPs at Pe = 300 by the expression¹⁵

$$\left\langle \Delta \mathbf{r}^2(t) \right\rangle = \frac{\sigma^2 P e^2}{2} \left(2D_R t + \exp(-2D_R t) - 1 \right) \tag{10}$$

of an ABP in a dilute system. This expression yields a crossover from an active ballistic short-time motion to a long-time diffusive MSD at $2D_R t \approx 1$ with the diffusion coefficient $D = \sigma^2 D_R P e^2/6.^{15}$ Since the rotational diffusion is an independent stochastic process, the ABPs in the mixtures follow the predicted crossover. However, the ABP dynamics is significantly slowed down. As indicated by the fit, the extracted effective Péclet number Pe = 48.7 is significantly smaller than that of an ABP in dilute solution, Pe = 300, since the interactions between ABPs and PPs reduce the ABP swim velocity. Moreover, the inset of Fig. 2 reveals a power-law increase in the active diffusion coefficient, D, with the exponent 1.6 smaller than the theoretical value 2. In addition, the short-time dynamics is super-diffusive but not ballistic. These facts reflect the influence of the finite

overall particle density on the ABP dynamics. Noteworthy, the ABP properties are independent of the actual composition of the mixture at the constant packing fraction ϕ .

The activity-dependence of the passive-particle diffusion coefficient $D \sim Pe^{1.16}$ is even weaker than that of the ABPs (Fig. 2). Moreover, an increasing fraction of passive particles reduces the value of D for the considered range of Pe; the diffusion coefficients at $N_p/N=0.3$ are approximately 30% larger than those at $N_p/N=0.5$, independent of Pe.

In contrast to the ABPs, the PPs show no persistent motion. The calculation of the PP velocity correlation function yields a nearly instantaneous decay of the correlation function, roughly as for particles exposed to white-noise. Nevertheless, PPs show a crossover from a short-time super-diffusive behavior to long-time diffusion, which is clearly governed by interactions with ABPs. The activity-enhanced dynamics at larger Pe leads to a shift of the crossover to shorter times by approximately a factor of two between Pe = 300 and 30 for any fraction of passive particles. This reflects that the PP dynamics induced by the bath is significantly different from that of self-propelled particles, despite qualitatively similar features.

IV. PASSIVE POLYMER IN ACTIVE BATH

A. Polymer conformational properties

The polymer properties strongly depend on the ABP concentration. Particular effects appear for concentrations above the critical value for MIPS, $\phi \approx 0.34$, and $Pe \lesssim 300$ (cf. Fig. 3). Since we focus on a single short polymer with $N_m = 20$, the monomer concentration plays a negligible role for the overall concentration of particles in the system.

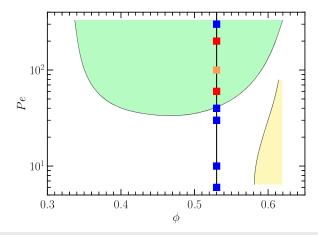


FIG. 3. Illustration of the phase diagram of active Brownian particles in three dimensions as a function of the Péclet number and the packing fraction. The shaded areas indicate the liquid–gas (light green) and the crystal–gas (light yellow) coexistence regimes.^{20,81} Symbols represent the considered Péclet numbers for the simulations of a passive polymer in the active bath. Blue squares indicate swollen polymer conformations comparable to a non-localized polymer and red/orange squares shrunk polymers during localization with a minimum size at Pe = 100 (orange).

1. Low ABP concentration regime—Homogeneous fluid

In the low-concentration regime, we consider the ABP packing fractions $\phi = 0.13$ and $\phi = 0.27$, the ABP fluid is homogeneous and isotropic (cf. Fig. 3). As illustrated in Fig. 4 for the polymer meansquare end-to-end distance $\langle \mathbf{R}_e^2 \rangle = \langle (\mathbf{r}_N - \mathbf{r}_1)^2 \rangle$, the active bath generates a swelling of the polymer with the increasing Péclet number, where the swelling is more pronounced at higher ABP concentrations. At small Pe, the interactions with the ABPs seem to result in a small shrinkage of the polymer, an effect that appears also for polymers composed of ABP monomers (ABPOs) in the presence of excluded-volume interactions.^{84–86} Qualitative, the conformational properties are similar to those of ABPOs.74,77 However, ABPOs swell stronger and reach asymptotically the value $\langle \mathbf{R}_e^2 \rangle / L^2 \approx 0.4$ in the limit $Pe \to \infty$, ⁷⁶ a value slightly smaller than the theoretically predicted value 1/2, ⁷⁴ whereas here $\langle R_e^2 \rangle / L^2 \approx 0.2$ for $\phi = 0.27$. Hence, qualitatively a passive polymer in an active bath exhibits the same conformational properties as an ABPO, however, to a less extent.

2. High ABP concentration regime-MIPS

At high concentrations, we consider $\phi = 0.53$, the ABPs exhibit MIPS associated with strong density differences above a critical Péclet number (Figs. 1 and 3). Most remarkable, the active bath leads to a polymer localization in the bubble of the low-density ABP phase over a certain range of Péclet numbers (red/orange squares in Fig. 3). This is quantified by the fraction of ABPs in a spherical volume centered at the polymer center-of-mass. Figure 5 presents distribution functions of the packing fraction ϕ_a of ABPs within a sphere of radius $R=5.5\sigma$ —the radius is much larger than the radius of gyration $R_g \approx 2.7\sigma$ of the flexible polymer in dilute solution-for various Péclet numbers. (The result is independent of R, as an analysis for spheres of radii $R = 5.5 \pm 2$ shows.) At Pe = 10, the fluid is homogeneous, and the peak in $P(\phi_a)$ corresponds to the average packing fraction. With increasing Pe (Pe = 40), the maximum shifts to larger packing fractions and the distribution function broadens. ⁸⁷ For Pe = 100, the distribution function exhibits a peak at

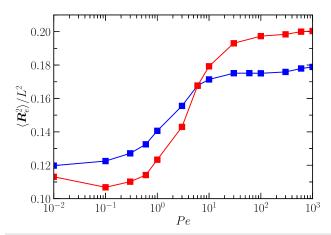


FIG. 4. Mean-square end-to-end distance of a flexible polymer as a function of Péclet number for the ABP packing fractions $\phi=0.13$ (blue) and $\phi=0.27$ (red).

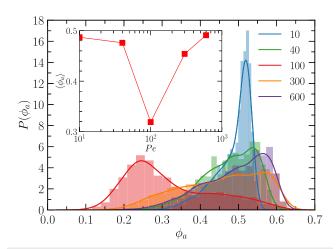


FIG. 5. Distribution function of the local ABP packing fraction within a sphere of radius $R=5.5\sigma$ centered at the polymer center-of-mass position for the indicated Péclet numbers Pe=10–600. Inset: mean value of the local packing fraction as a function of the Péclet number. The average packing fraction is $\phi=0.53$.

 $\phi_a \approx 0.23$, with a broad tail toward higher ϕ_a . This reflects a preferred localization of the polymer in the low-density ABP spatial region (Fig. 6). At higher Péclet numbers, phase localization switches and the polymer is dissolved in the high-density ABP phase, as indicated by the peak at $\phi_a \approx 0.6$ for Pe = 300 and 600. The inset of Fig. 5 illustrates the substantial drop in the average ABP packing fraction in the vicinity of the polymer at Pe = 100. Figure 6 shows various snapshots of polymers in the low- and high-density ABP phase.

The localization of the polymer in the bubble of the dilute ABP region severely affects its conformations. Figure 7 displays the mean square end-to-end distance of semiflexible polymers of various persistence lengths and Péclet numbers. An increasing activity leads to a swelling of flexible ($k_b = 0$) and a shrinkage of semiflexible polymers $(k_b = 2, 10)$, as for ABPOs.⁷⁴ Above $Pe \approx 10$, even passive semiflexible polymers swell with increasing Pe similar to flexible polymers.⁷⁴ However, due to localization in the low-density ABP regime, the polymer shrinks for $Pe \gtrsim 40$, assumes a minimum at $Pe \approx 100$, and reswells for larger Péclet numbers. The shrinkage appears as soon as the ABPs phase separate at $Pe \approx 34$ and is most pronounced for Pe = 100. Noteworthy, polymers of all considered stiffnesses shrink and reswell in a similar manner. The apparent asymptotic mean square end-to-end distance for $Pe \to \infty$, $\langle \mathbf{R}_e^2 \rangle / L^2 \approx 0.3$, is larger than the values in Fig. 4 for the lower ABP concentrations. Hence, the active bath implies qualitatively similar features as those observed for ABPOs, namely, swelling of flexible polymers and shrinkage and reswelling of semiflexible polymers; yet, in addition, it induces a polymer localization over a certain range of Péclet numbers by MIPS.

Two-dimensional mixtures of ABPs and PPs at Pe = 100 exhibit an increased concentration of PPs in the ABP depleted phase of the phase-separated mixture. ⁴² The same physical mechanism may apply for ABP/polymer and ABP/PP mixtures, although the density of the ABP/PP mixture is much higher in the studies of Ref. 42 and the Péclet-number dependence has not be studied, i.e.,

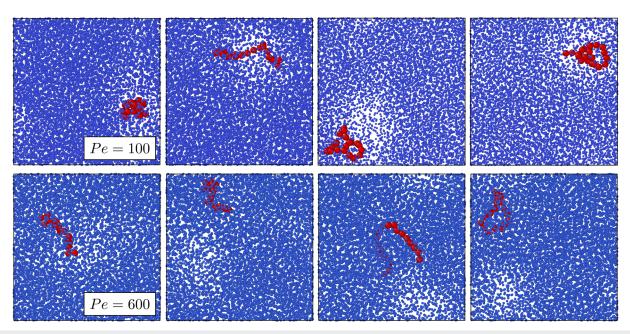


FIG. 6. Snapshots illustrating the localization of the polymer in the dilute (top, Pe = 100) and dense (bottom, Pe = 600) ABP phase, respectively, at various times. The average packing fraction is $\phi = 0.53$ (see movies M1 and M2 of the supplementary material for illustration).

it is not clear whether a higher density of PPs in the ABP rich phase would be obtained at high Péclet numbers. Interestingly, the polymers approximately assume the same size as a flexible polymer in dilute solution. This is surprising since polymers in a homogeneous active bath of the density of the dilute regime ($\phi = \phi_a \approx 0.32$, Fig. 5) are substantially swollen as shown in Fig. 4. Thus, segregation is not the only reason for the strong polymer shrinkage. The polymer is highly dynamic and rapidly explores the low-density ABP bubble.

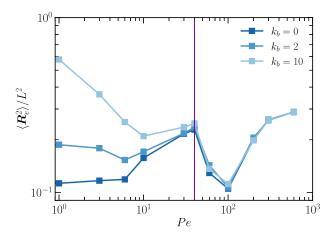


FIG. 7. Mean square end-to-end distance of semiflexible polymers of length L=19I as a function of Pe. The ABP fluid density is $\phi=0.53$, and the stiffness parameters of the bending potential are indicated in the legend. The purple line at Pe=40 approximately indicates the critical Péclet number for MPIS (cf. Fig. 3).

Yet, it is most of the time localized inside that bubble. The ABPs in the high-density phase seem to repel the polymer, which may ultimately be responsible for its strong shrinkage. Only beyond a certain Péclet number, the active forces are strong enough to overcome the activity-induced confinement.

B. Polymer dynamical properties

1. Low ABP concentration regime—Homogeneous fluid

The results for the polymer center-of-mass dynamics at ABP packing fractions below the critical value $\phi \approx 0.34$ are displayed in Fig. 8. The active bath implies an enhanced dynamics with a Pe-dependent short-time super-diffusive regime [Fig. 8(a)], yet with an exponent smaller than 2, and long-time diffusion with an activity-amplified diffusion coefficient. As for the passive particles in the active bath, the crossover to the diffusive regime shifts to shorter times with increasing Pe.

The extracted long-time activity-enhanced diffusion coefficients are depicted in Fig. 8(b). They increase in a power-law manner with the increasing Péclet number, with an exponent depending on the ABP concentration. The exponents, 1.30 and 1.38, are larger than those of passive particles in the active bath (Fig. 2) but are smaller than the value 2.0 (black line) of ABPOs in dilute solution. The exponents, qualitatively similar to ABPOs, however with significant quantitative differences in terms of activity-dependence and magnitude, as reflected by the variance with diffusion coefficients of ABPOs (black line in Fig. 8). This can be considered as a consequence of a finite and short lived cooperative motion of an ABP and

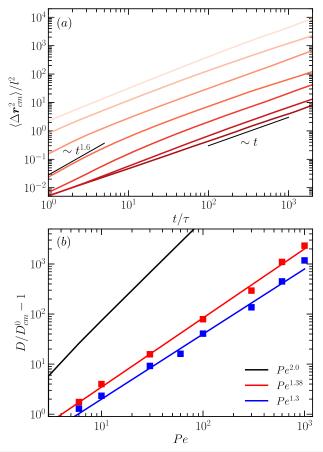


FIG. 8. (a) Center-of-mass mean-square displacement as a function of time of a flexible polymer in an ABP bath of packing fraction $\phi=0.27$ for the Péclet numbers Pe=1, 3, 10, 30, 100, 300, and 600 (dark to light). The black lines indicate (fitted) power-law dependencies. (b) Diffusion coefficients extracted from the long-time diffusive regime for the ABP packing fractions $\phi=0.13$ (blue) and 0.27 (red). Symbols indicate simulation results, and the corresponding solid lines are power-law fits with the exponents displayed in the legend. The black line denotes the active diffusion coefficient of an ABPO in dilute solution for the same D_R . D_{cm}^0 is the diffusion coefficient of the polymer in a passive bath with $\phi=0.27$.

a monomer. ABPs push against monomers for a short time before the slide past of them, which implies an effectively smaller Péclet number and an effective active noise different from strict colored nose.

Diffusion of a polymer in a passive bath is determined by the bath temperature, and the dissipation–fluctuation relation applies. The existence of a comparable effective temperature and relation is *a priori* not evident, and various contradicting cases have been presented and discussed for active systems.^{17,88–91} The center-of-mass MSD of a passive polymer with inertia in a white-noise bath is given by⁹²

$$\left\langle \Delta \mathbf{r}_{cm}^{2}(t)\right\rangle =\frac{6D_{e}}{\gamma}\left(\gamma t-1+e^{-\gamma t}\right),\tag{11}$$

with the diffusion coefficient $D_e = k_B T_e / (N_m \gamma)$, the temperature T_e , and the total friction γN_m . Equation (11) shows a universal time-dependent function with the argument γt , multiplied by a

temperature-dependent factor. The MSDs of Fig. 8(a) cannot be reproduced by Eq. (11) for an activity-independent friction coefficient, as the short-time power-law changes with activity and the crossover to diffusion shifts to shorter times with increasing Pe. Hence, the overall polymer dynamics cannot be described by an effective temperature, in general. However, in the diffusive regime, $t/\tau \gtrsim 10^2$, the active diffusion coefficient can be related to a temperature T_e , and with $D=D_e$ follows $T_e \sim Pe^\alpha$, with $\alpha=1.30$ and 1.38 for the packing fractions $\phi=0.13$ and 0.27, respectively. The power-law relation is rather trivial and no conclusions on the underlying stochastic process can be drawn and, hence, on the existence of an effective temperature.

2. High ABP concentration regime-MIPS

The phase separation of the ABPs and the associated localization of the polymer in the low-density phase affect the polymer dynamics. Figure 9(a) displays polymer center-of-mass

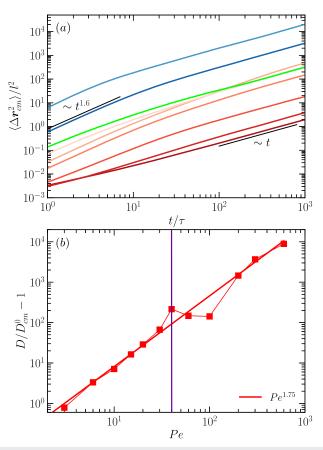


FIG. 9. (a) Center-of-mass mean-square displacement as a function of time of a flexible polymer in an ABP bath of packing fraction $\phi=0.53$ for the Péclet numbers Pe=1,3,10,30,40,60 (red, dark to light); 100 (lime), 300; and 600 (blue, dark to light). The black lines indicate (fitted) power-law dependencies. (b) Diffusion coefficients extracted from the long-time diffusive regime. Symbols indicate simulation results with the thin solid line as a guide for the eye. The thick solid line indicates the fitted power-law increase $Pe^{1.75}$. The purple line at Pe=40 approximately indicates the critical Péclet number for MIPS (cf. Fig. 3).

mean-square displacements for various Péclet numbers. As for the lower ABP densities, the MSD exhibits an activity-dependent sub-diffusive short-time regime with the time dependence $t^{1.6}$ followed by diffusion at longer times. Remarkably, the MSD curve for $Pe = 10^2$ shows a slow-down of the polymer dynamics compared to that for somewhat smaller and larger Pe, which is related to the localization of the polymer in the low-density ABP bubble (Fig. 5). Although the local polymer dynamics is rather fast, the long-time behavior is determined by the diffusive dynamics of the low-density ABP bubble. The center-of-mass diffusion coefficients displayed in Fig. 9(b) emphasize the changes of the polymer dynamics in the vicinity and above the critical Péclet number for MIPS. For Pe = 40, close to the MIPS transition, we find an enhanced polymer dynamics compared to the "average" trend revealed by the power-law $Pe^{1.75}$. Here, larger density fluctuations seem to result in an additional active noise leading to a faster dynamics. At $Pe \approx 10^2$, the polymer diffuses, at least part time, with the low-density ABP bubble, which moves significantly slower due to collective effects. The dissolution of the polymer for activities $Pe \gtrsim 2 \times 10^2$ in the high ABP-density region results in an enhanced diffusion. The activity dependence, $Pe^{1.75}$, is similar for Pe < 30 and $Pe \gtrsim 10^2$, since the average ABP concentrations in the vicinity of the polymer are comparable as reflected in Fig. 5.

We would like to emphasize that MSD curves and diffusion coefficients of semiflexible polymers (Fig. 7) are indistinguishable from those of the flexible polymer (Fig. 9) for the presented range of activities. The strong conformational change by the active bath renders stiffness irrelevant.

V. SUMMARY AND CONCLUSIONS

We have performed computer simulations of mixtures of isometric passive colloids and active Brownian particles (ABPs) as well as of a passive polymer embedded in an ABP bath for various ABP packing fractions, ϕ , and activities, Pe. In general, the active bath strongly affects the embedded passive particles, with a pronounced enhancement of their dynamics.

Our simulations of mixtures of isometric passive and active particles at the total packing fraction $\phi = 0.53$ and the fraction of passive particles in the range $N_p/N = 0.3-0.5$ show no large-scale phase separation. For the latter, higher APB concentrations are required. The ABP bath enhances the dynamics of the passive particles, with a 30% faster diffusion for $N_p/N = 0.3$ compared to the ratio N_p/N = 0.5. For any considered ratio N_p/N , the diffusion coefficient of the passive particles increases as $P^{1.16}$ with the increasing Péclet number in the range $3 \le Pe \le 300$. However, the ABP dynamics is independent of the concentration of the passive particles in the considered range, and their active diffusion coefficient increases as Pe^{1.6} with

Our studies of a single polymer in an ABP bath of packing fraction $\phi = 0.13$ and 0.27—both densities are below the critical value for MIPS—and $Pe \lesssim 300$ reveal swelling of the polymer with the increasing Péclet number, which saturates for $Pe \gtrsim 20$. Here, swelling is more pronounced for higher ABP concentrations. As for passive monomers, the dynamics is enhanced and the diffusion coefficient increases in a power-law manner for $1 < Pe \lesssim 10^3$ with an ABP density-dependent exponent.

Remarkably, for the ABP packing fraction $\phi = 0.53$, we find localization of the polymer in the low-density spatial region—in fact, a low-density bubble-of the phase-separated ABP bath at $Pe \approx 10^2$. This separation is accompanied by a collapse of the originally activity-swollen polymer to a value comparable to that of the flexible polymer in the passive bath. Noteworthy, this collapse is independent of polymer stiffness, at least over a significant range of stiffnesses. For larger $Pe \gtrsim 2 \times 10^2$, the polymer is no longer localized and therefore swells again, approaching asymptotically a constant value for large Pe. The localization process also affects the polymer dynamics, and the diffusion coefficient in the localized state is significantly smaller than that predicted in the absence of phase separation.

Quantitatively, the properties of a polymer in an active bath are significantly different from those of a polymer comprised of ABP monomers (ABPO).74,75,77 Common to both is the change of the conformations by swelling and an enhanced dynamics. However, there are major quantitative differences in terms of strength of the obtained effects and the dependence on the (effective) Péclet number. Here, the passive polymers show significantly smaller effects and, in power-laws, smaller exponents. This is a consequence of the far less persistent motion of passive particles in an active bath compared to, e.g., ABP monomers of an ABPO. Ultimately, the active bath does not correspond to a colored-noise external source in this case⁷⁵ due to the only short-time correlated motion of ABPs and monomers, shorter than the characteristic time of the colored noise of the ABPs,

Yet, the bath does not correspond to a thermal bath either, and, strictly speaking, no effective temperature can be introduced. The comparison of the polymer center-of-mass mean-square displacements at $\phi = 0.27$ (Fig. 8) with its theoretical prediction in a thermal bath clearly reveals a more complex dynamics in the active bath. A similar qualitative behavior is displayed by passive particles in an active bath. An effective temperature, T_e , can be introduced to account for the activity dependence of the diffusion coefficient, though with a nonlinear relation between T_e and Pe. Specifically, the concentration-dependent exponent of the latter relation indicates a more complex fluctuation-dissipationlike relation of the active bath than a thermal (white-noise)

Our simulation study is a first step toward the elucidation of the complex interplay between an active bath and embedded polymers or filaments. We hope that they stimulate further investigations, specifically taking into account several polymers, which might show aggregation in the low-density regions of the APB bath.

SUPPLEMENTARY MATERIAL

The supplementary material provides movies of the polymer dynamics in the active bath. Movie M1 illustrates the dynamics for Pe = 100 and M2 illustrates the dynamics for Pe = 600.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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