

Active-parameter polydispersity in the 2d ABP Yukawa model

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The most commonly studied kind of parameter polydispersity is that of varying particles size. This paper investigates by simulations the effects of introducing polydispersity in other parameters of the two-dimensional Active Brownian Particles model with Yukawa pair interactions. Polydispersity is introduced separately in the translational and rotational diffusion coefficients, as well as in the persistence speed v_0 . Uniform and binary parameter distributions are considered in both the homogeneous and the motility-induced phase-separation (MIPS) phases. We find only minute changes in the structure and dynamics upon the introduction of parameter polydispersity, even for situations involving up to 50% polydispersity. The reason for this is not clear. An exception is the case of v_0 polydispersity for which the average radial distribution function shows significant changes in the MIPS phase with increasing polydispersity. Even in this case, however, the dynamics is only modestly affected. As a possible application of these findings, we suggest that the temporal introduction of polydispersity into single-component active-matter models characterized by a very long equilibration time, i.e., a glass-forming active system, may be used to equilibrate the system efficiently by particle swaps.

I. INTRODUCTION

Active matter includes fluids of self-propelled particles like bacteria, birds, or insect flocks [1–7]. An example of the intriguing features of active matter – relating to the fact that time-reversal invariance is broken – is motility-induced phase separation (MIPS), the fact that a purely repulsive system may phase separate into high- and low-density phases [4, 8–13].

There is currently a considerable interest in passive polydisperse systems, in particular deriving from the use of polydispersity for SWAP-equilibrating models of supercooled liquids [14]. An obvious question in this respect is: how different are the dynamics of the different particles [15–17]? Polydispersity is also relevant for active matter models because for a biological system one cannot expect all constituents to be identical [18–21]. Thus Castro *et al.* recently showed that the MIPS phase gets suppressed with the introduction of a spread of persistence speeds in the Active Brownian Particles (ABP) model [22].

This paper presents a systematic study of the effects of polydispersity in the ABP model in two dimensions. The particles interact via the Yukawa (screened Coulomb) pair potential [23, 24]; polydispersity is introduced by varying the three activity parameters controlling the motion of the individual particles. We find a surprisingly small effect of even quite high polydispersity (up to 50%) when the 0parameters vary under the constraint of constant average. This applies to both continuous and binary polydispersity and is in sharp contrast to the usually observed large effects of introducing size polydispersity (in both passive and active matter).

II. THE 2D ABP YUKAWA SYSTEM

The Yukawa pair potential [23, 25] is defined [26] by

$$v(r) = \frac{Q^2\sigma}{r} \exp\left(-\frac{r}{\lambda\sigma}\right). \quad (1)$$

Here σ is a length parameter, λ is dimensionless, and the “charge” Q has dimension square root of energy. Throughout the paper $\lambda = 0.16$ and $Q = 50$, while $\sigma \equiv 1$ defines the unit of length and thus the unit of particle density.

If \mathbf{r}_i is the position vector of particle i , the ABP equations of motion in two dimensions are [27]

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$$\dot{\mathbf{r}}_i = \mu \mathbf{F}_i + \boldsymbol{\xi}_i(t) + v_0 \mathbf{o}_i(t). \quad (2)$$

Here, μ is the mobility (velocity over force), $\mathbf{F}_i(\mathbf{R}) = -\nabla_i U(\mathbf{R})$ is the force on particle i in which $\mathbf{R} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$ is the configuration vector and $U(\mathbf{R})$ the potential-energy function, $\boldsymbol{\xi}_i(t)$ is a Gaussian random white-noise vector, and v_0 is the so-called persistence speed. The vector $\mathbf{o}_i(t) = (\cos \theta_i(t), \sin \theta_i(t))$ is a stochastic unit vector in which the change of the angle $\theta_i(t)$ is given by a Gaussian white noise term with magnitude defining the rotational diffusion coefficient D_r , i.e.,

$$\langle \dot{\theta}_i(t) \dot{\theta}_j(t') \rangle = 2D_r \delta_{ij} \delta(t - t'). \quad (3)$$

The magnitude of the white-noise velocity vector $\boldsymbol{\xi}_i(t)$ defines the translational diffusion coefficient D_t ,

$$\langle \xi_i^\alpha(t) \xi_j^\beta(t') \rangle = 2D_t \delta_{ij} \delta_{\alpha\beta} \delta(t - t') \quad (4)$$

in which α, β are spatial x, y, z indices and i, j are particle indices. The mobility μ is taken to be unity throughout, i.e., is regarded as a material constant, while the remaining model parameters D_r , D_t , and v_0 are allowed to vary from particle to particle. This introduces three kinds of polydispersity. In each case the average of the parameter in question is kept constant. For any varying parameter X the polydispersity δ is conventionally defined [28] as $\delta \equiv \sqrt{\langle X^2 \rangle - \langle X \rangle^2} / \langle X \rangle$ in which the sharp brackets denote an average.

We simulated 10000 particles of the 2d Yukawa system with interactions cut off at 4.5σ . The time step used was $\Delta t = 0.0625 \langle D_t \rangle / \langle v_0 \rangle^2$. Each simulation involved $2 \cdot 10^7$ time steps. The code employed was RUMD [29], modified to deal with polydispersity in particle-activity parameters. Parameters corresponding to both the homogeneous ($D_t = 1.0$, $D_r = 0.8$, $v_0 = 25$) and the MIPS phase ($D_t = 1.0$, $D_r = 0.2$, $v_0 = 25$) were simulated.

III. PARAMETER POLYDISPERSITY IN THE HOMOGENEOUS PHASE

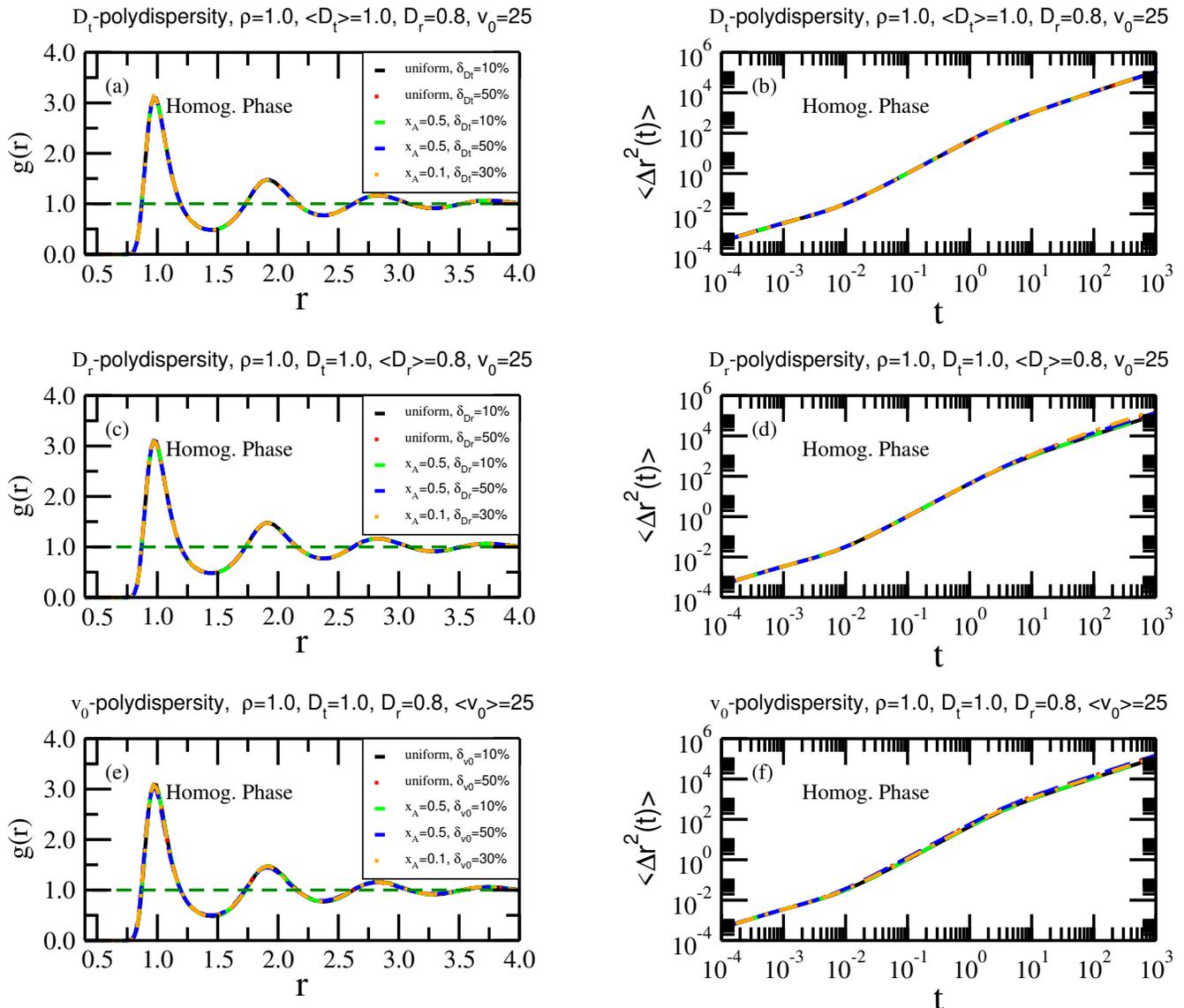


FIG. 1. Structure and dynamics in the homogeneous phase for uniformly polydisperse systems (black and red curves for 10% and 50% polydispersity) and binary systems. Green represents 10%, orange 30%, and blue 50% polydispersity. (a), (c), and (e) show the average radial distribution functions (RDFs), $g(r)$, for systems with polydispersity in the D_t , D_r , and v_0 parameters. (b), (d), and (f) show the corresponding results for the mean-square displacement as a function of time, $\langle \Delta r^2(t) \rangle$. In all cases there is little effect of polydispersity.

We first consider the effect of active-parameter polydispersity on the structure and dynamics in the homogeneous phase. The left column of Fig. 1 shows the (average) radial distribution functions (RDFs) for different degrees of polydispersity: uniform parameter distributions of 10% and 50% polydispersity and binary parameter distributions of 10%, 30%, and 50% polydispersity in D_t (top), D_r (middle), and v_0 (bottom). The right column of Fig. 1 shows the (average) mean-square displacement (MSD) as a function of time for the same situations. In all cases we see little effect of polydispersity. This is not trivial because the individual particles conform to different equations of motion and indeed move differently, as is clear from the next figure.

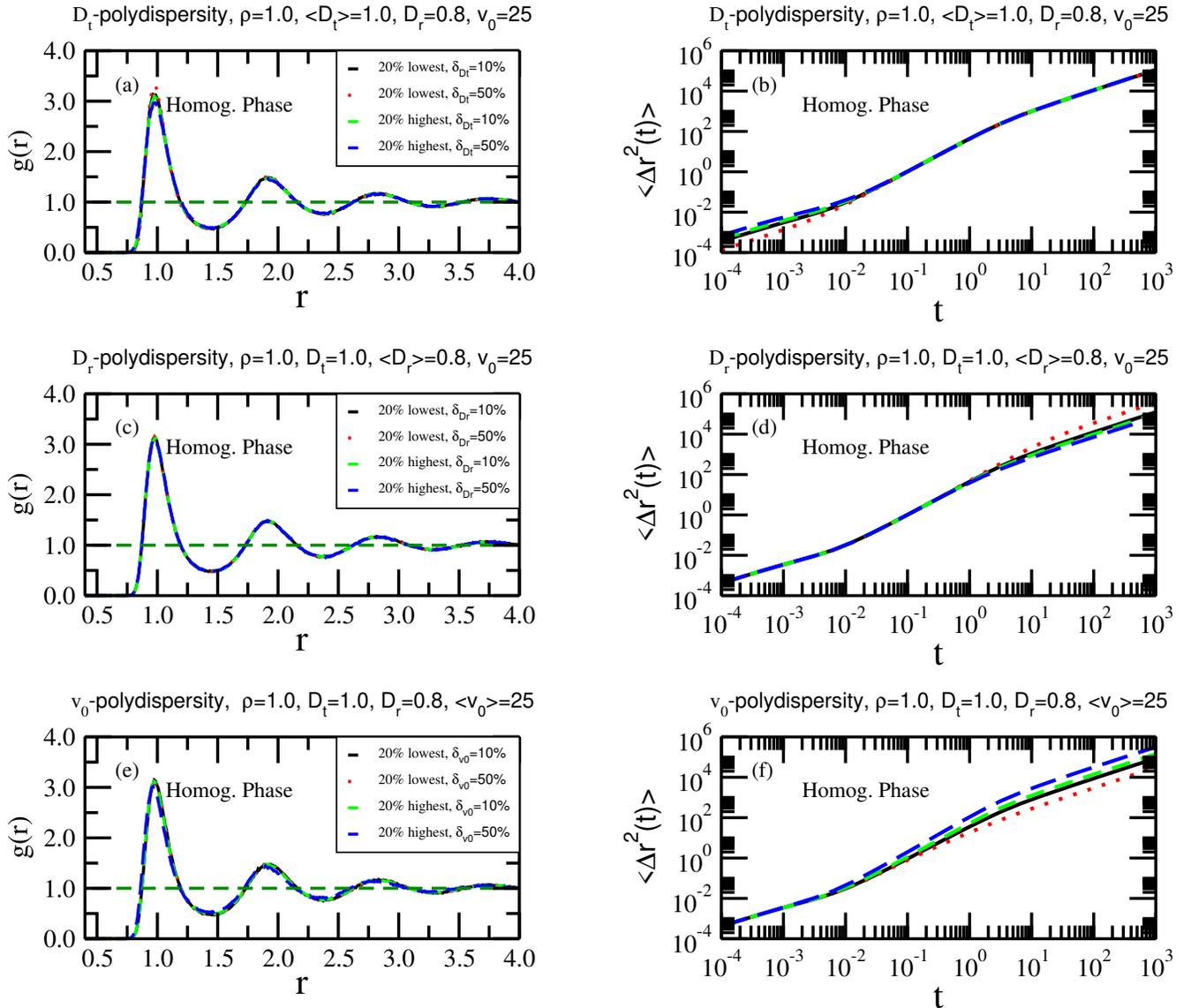


FIG. 2. Role of the 20% lowest (black and red) and 20% highest (green and blue) active-parameter particles in the homogeneous phase of continuously polydisperse systems at 10% and 50% polydispersity. (a), (c), and (e) show RDFs, $g(r)$, for polydispersity in the D_t , D_r , and v_0 parameter, respectively. (b), (d), and (f) show the corresponding results for the mean-square displacement $\langle \Delta r^2(t) \rangle$. For the RDFs there is little difference between the lowest and highest active-parameter particles, while the MSD shows variations that are much larger than those of the overall average (Fig. 1). Interestingly, this variation is seen in the short-time data in the case of D_t polydispersity, but in the long-time data for D_r and v_0 polydispersity.

To illuminate the role of the parameter polydispersity for the individual particles we identified, for the two uniform polydispersities, the particles with the 20% lowest activity parameters and those with the 20% highest parameters. For each of these categories we determined the corresponding RDFs (counting only surrounding particles of the same type) and MSDs. The results are shown in Fig. 2. For the structure (left) there is little difference although one notes that the low D_t particles show a somewhat more pronounced first peak than that of the high D_t particles (upper left). Since D_t in the Langevin-type equation Eq. (2) plays the role of a temperature, this is consistent with the well-known finding for passive systems that lowering the temperature generally leads to a higher first peak of the RDF. For the dynamics, there are clear differences: In the case of D_t polydispersity (upper right), the long-time dynamics is the same while the short-time dynamics is fastest for the highest D_t particles. For D_r polydispersity the opposite is observed: Here the short-time dynamics is the same for the low and high D_r particles while the long-time dynamics is fastest for the particles with low D_r . The rotational diffusion coefficient determines a particle's persistence time such that low D_r corresponds to a large persistence time. In a discrete random-walk picture, this implies longer

jumps and therefore a faster long-time diffusive motion. On the short time scale little change of direction is possible, making the value of D_r irrelevant. Consider finally the case of v_0 polydispersity (lower right). Here there is no effect on the short-time dynamics, while the long-time dynamics is fastest for particles with large v_0 . That the short-time dynamics is unaffected is a simple consequence of Eq. (2) in which the v_0 term on the short time scale gives rise to a MSD proportional to t^2 , which is much smaller than the short-time diffusive contribution to the MSD. The faster long-time diffusive dynamics for the high v_0 particles comes about because a higher persistence velocity means larger displacements in one direction before the direction changes, corresponding to longer jumps in a random-walk picture.

How do the results of Fig. 2 relate to the the overall average structure and dynamics results of Fig. 1? The structure is almost the same for low and high active parameter particles for all three types of polydispersity – and independent of the degree of polydispersity – so the RDF findings of Fig. 1 are not surprising. In regard to the MSD, it seems that the variations induced by parameter polydispersity average out resulting in little overall change of the average MSD. Thus in all three cases the black and green curves in Fig. 2, which represent just 10% polydispersity, are close to each other while the red and blue curves (50% polydispersity) move in opposite direction.

IV. PARAMETER POLYDISPERSITY IN THE MIPS PHASE

The existence of a MIPS phase is a unique feature of active matter. This phase should also be investigated in regard to the effects of introducing active-parameter polydispersity. We did this by repeating the above simulations, the only difference being that the average of D_r is now 0.2 instead of the above used 0.8.

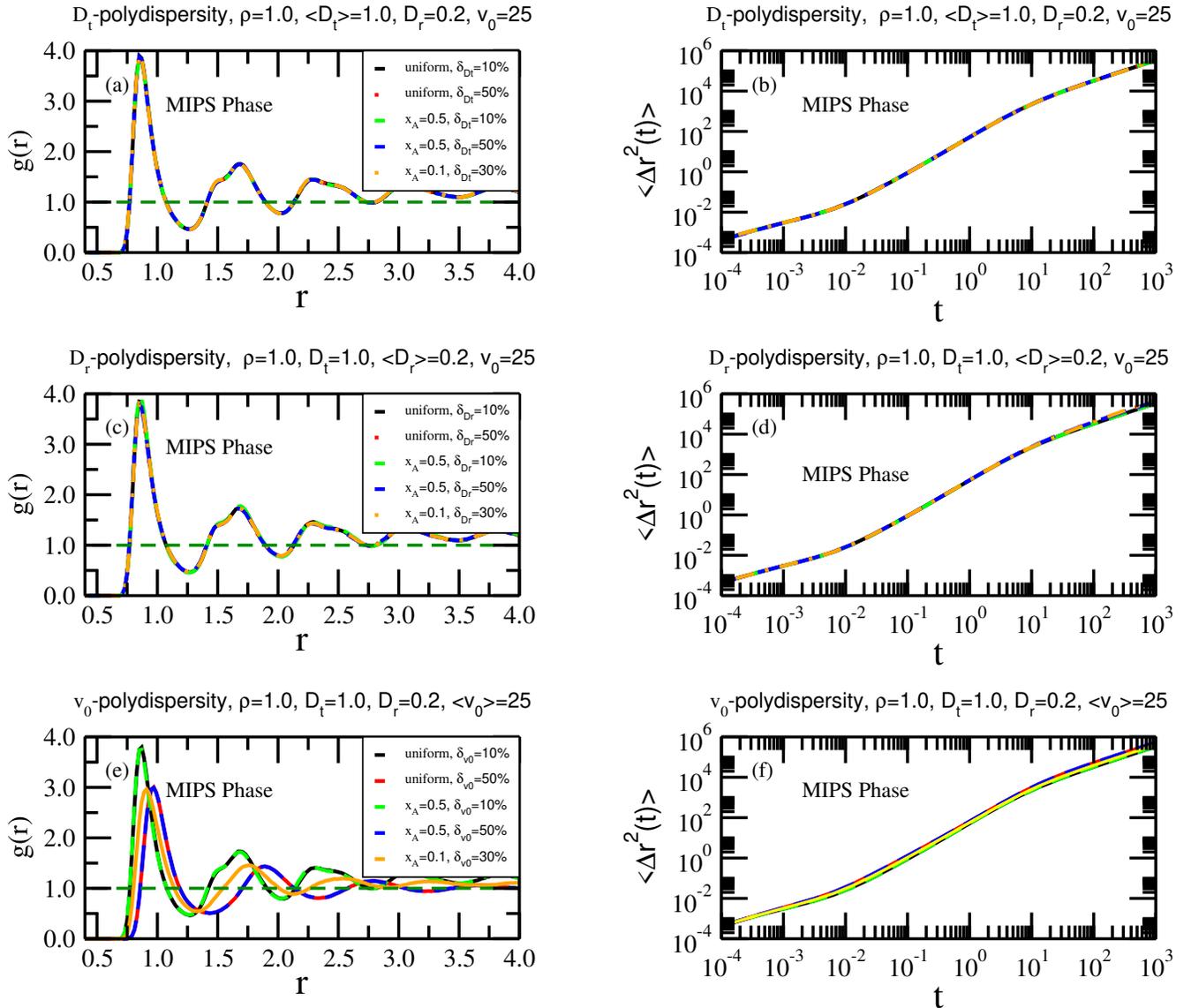


FIG. 3. Structure and dynamics in the MIPS phase for uniformly polydisperse systems (black and red curves) and binary systems (green, blue, and orange curves). (a), (c), and (e) show the average RDFs, $g(r)$, for systems of 10%, 30%, and 50% polydispersity in the D_t , D_r , and v_0 parameters, respectively. (b), (d), and (f) show the corresponding results for the mean-square displacement $\langle \Delta r^2(t) \rangle$. There is little effect of introducing polydispersity in the D_t and D_r parameters whereas a notable effect of v_0 polydispersity is observed for the RDF, in which case there is also a visible – though much smaller – effect on the dynamics.

The results for the RDFs and MSDs are shown in Fig. 3. In regard to the dynamics, the picture is not much different from that of the homogeneous phase: the MSD is virtually unaffected by the introduction of polydispersity in any of the three parameters. The same applies for the RDF for D_t and D_r polydispersity, whereas v_0 polydispersity strongly affects the RDF (lower left). While not clearly visible, a close inspection reveals that the green RDF and MSD curves cover a black one and that the blue curves likewise cover a red one. The former are for 10% polydispersity in the uniform and binary cases, respectively, while the latter similarly are for 50% polydispersity. We conclude that the introduction of v_0 polydispersity strongly affects the RDF in a way that is independent of the parameter probability distribution. Given that the entire existence of the MIPS phase reflects the active-matter feature of a temporary persistence direction in the particle motion, it is not surprising that introducing v_0 polydispersity has a strong effect on the structure of the MIPS phase.

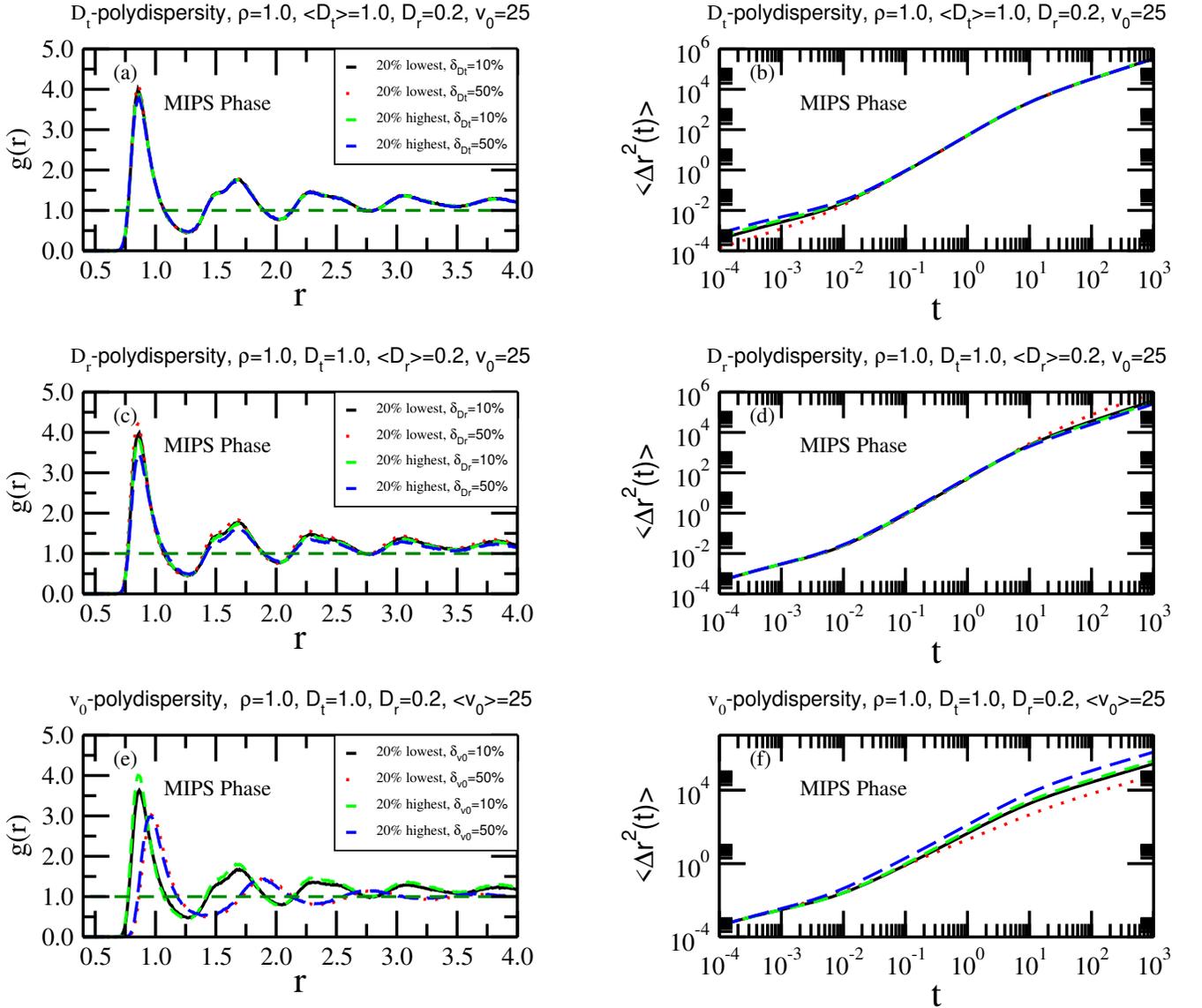


FIG. 4. Role of the 20% lowest (black and red) and 20% highest (green and blue) active-parameter particles in the MIPS phase of continuously polydisperse systems at 10% and 50% polydispersity. (a), (c), and (e) show RDFs, $g(r)$, for polydispersity in the D_t , D_r , and v_0 parameters, respectively. (b), (d), and (f) show the corresponding results for the mean-square displacement $\langle \Delta r^2(t) \rangle$. For the RDFs there is for D_t polydispersity little difference between the lowest and highest active-parameter particles except at the first peak; D_r polydispersity shows a larger but still modest difference, which is most pronounced at 50% polydispersity. The case of v_0 polydispersity shows significant difference between 10% and 50% polydispersity, but for each of these values there is only modest variation between the lowest and highest active-parameter particles' RDF. For the MSD the situation is similar to that observed in the homogeneous phase (Fig. 2): variation is observed in the short-time data for D_t polydispersity, in the long-time data for D_r polydispersity, and (mainly) at intermediate and long times for v_0 polydispersity.

To throw more light on these findings, following the procedure of the homogeneous-phase investigation we identify in Fig. 4 the contributions to structure and dynamics from the lowest (black and red) and highest (green and blue) parameter particles. Compared to the homogeneous case, there is more variation for all three RDFs, in particular for D_r and v_0 polydispersity. In the D_r case, the black and green curves (10% polydispersity) are close and move in the same direction when increasing to 50% polydispersity. Interestingly, the average of black and green, as well as of red and blue, is an almost unchanged RDF (left middle panel of Fig. 3). The v_0 polydispersity case is different: here the 10% polydispersity curves are similar (black and green), but quite different from the 50% polydispersity curves (red and blue). This is consistent with the finding of Fig. 3 (lower left panel) and means that the actual value of v_0 matters little for the structure surrounding a given particle. We believe this is an effect of the strong interparticle

interactions within the MIPS phase that averages out the effect of the individually varying v_0 . At the same time increasing the degree of v_0 polydispersity leads to a considerable broadening of the width of the first peak. Because there is little difference between the low and high v_0 RDFs, the picture is very similar to the overall average picture. In fact, at 50% v_0 polydispersity we find that the system becomes almost homogeneous, which is consistent with the findings of Ref. 30. – In regard to the MSD, the MIPS phase low and high parameter findings are similar to those of the homogeneous phase (Fig. 2).

V. ROLE OF THE AVERAGE POTENTIAL ENERGY

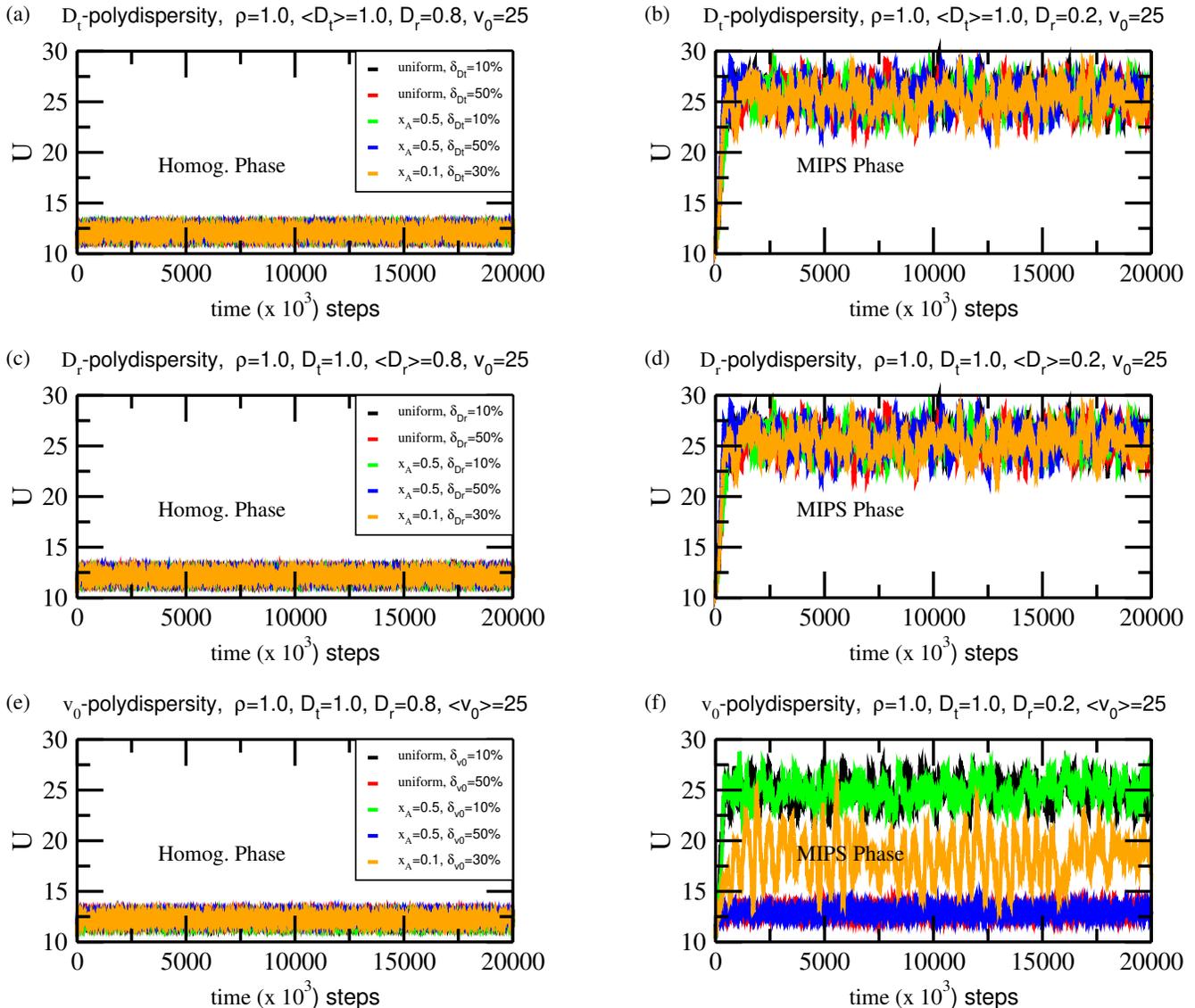


FIG. 5. Average potential energy as a function of time during a steady-state simulations. (a), (c), and (e) show data for the homogeneous phase for systems of 10%, 30%, and 50% polydispersity in the D_t , D_r , and v_0 parameters, respectively. (b), (d), and (f) show the corresponding results for MIPS-phase simulations. Except for the MIPS-phase v_0 polydispersity case, the average potential energy is virtually unaffected by the introduction of polydispersity.

To further illuminate the effect of parameter polydispersity we evaluated the potential energy as a function of time during the simulations (Fig. 5). In the homogeneous phase (left column) polydispersity has little effect on the average potential energy. This is consistent with the finding that in this phase structure and dynamics are virtually unaffected

by the degree of polydispersity (Fig. 1). The same applies for the MIPS phase in the D_t and D_r polydispersity cases. Only in the v_0 polydispersity MIPS case is the structure severely affected (Fig. 3 lower left), which is consistent with the finding that only in this case the average potential energy changes significantly with the degree of polydispersity (Fig. 5 lower right). At increasing v_0 polydispersity the MIPS-phase average potential energy approaches that of the homogeneous phase, which means that the average particle distance increases (the density decreases) with increasing v_0 polydispersity. Indeed, in this case the position of the first peak of the RDF was found to increase toward unity (Fig. 3 lower left), indicating that the MIPS phase gradually fills out the sample area and, eventually, disappears.

In summary, changes in the average potential energy upon introduction of parameter polydispersity correlate with changes of structure and dynamics. This means that the average potential energy is an easy-to-use “thermometer” of changes to the physics.

VI. DISCUSSION

It is well known that introducing size polydispersity into active-matter models by varying the characteristic length of the pair potential has a significant effect on both structure and dynamics [18–21, 31], just as for passive systems [28, 32, 33]. This paper investigated the effects of introducing particle-to-particle variations of other parameters of the 2d ABP model with Yukawa pair interactions. With the exception of v_0 polydispersity in the MIPS phase, we find surprisingly small effects on the structure and dynamics when polydispersity is introduced such that the average of the parameter in question is kept constant. The cause of this is not obvious, but it means that a polydisperse active system in many respects behaves like the homogeneous system of particles with average model parameters, i.e., that a mean-field description applies to a good approximation. We note that a recent study of different Lennard-Jones (passive) systems showed a similar insensitivity to the introduction of energy polydispersity [34], a result that is also still not well understood.

Investigations of other active-matter models should be carried out to determine the generality of our findings. If they are general, the introduction of polydispersity may have applications to instances of non-polydisperse active-matter models for which the system in question is difficult to equilibrate because of extremely long relaxation times [35, 36]. As is well known, passive glass-forming polydisperse liquids may be equilibrated by the SWAP algorithm [14]. Even though detailed balance does not apply for active matter, SWAP may also be applied for equilibrating an active, single-component highly viscous system [37] by proceeding as follows. First introduce polydispersity into one of the active-model parameters. Then, carry out random particle swaps, which according to the above findings will not significantly affect the average structure and dynamics of the system. Finally, remove the artificial polydispersity. Inspired by Ref. 14 we conjecture that this will equilibrate the system more quickly than a long simulation.

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