Dynamical anomalies and structural features of Active Brownian Particles characterised by two repulsive length scales

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In this work we study a two-dimensional system composed by Active Brownian Particles (ABPs) interacting via a repulsive potential with two-length-scales, a soft shell and a hard-core (see Fig. 1.a).

$$V(r) = \epsilon\left(\frac{\sigma}{r}\right)^n + \frac{1}{2}\varepsilon_s\left\{1 - \tanh\left[k_0\ (r - \sigma_s)\right]\right\}, \quad (1)$$

Here, ϵ is the energy related to the hard core, ϵ_s and σ_s are the height and width of the repulsive shoulder, respectively, n affects the stiffness of the repulsive core and k_0 determines the steepness of the shoulder decay. Throughout this work, we have chosen to establish the following parameters: $n = 14$ and $k_0 = 10/\sigma$ as in ref[1], and $\sigma_s = 2.5\sigma$. In order to study the time evolution of the system we have used the open source code LAMMPS[2]; when dealing with the $N = 2^{14}$ systems, we have used a modified version of UAMMD[3] (Universally Adaptable Multiscale Molecular Dynamics). Each simulation has been reiterated until the system attains steady state, which we assume arrives when there are no further significant changes in potential energy and overall phase behaviour. The level of activity is measured via the Peclet number, defined as

$$\text{Pe} \equiv \frac{3\,v_p\,\tau_r}{\sigma} = \frac{3\,|F_a|\,D_t}{k_B\,T\,D_r\,\sigma}, \quad (2)$$

where $v_p = |F_a|D_t/k_BT$ is the velocity propulsion of the active particles and $\tau_r = 1/D_r$ the reorentation time.

Depending on the ratio between the strength of the soft shell barrier, ϵ_s and the activity, we find two regimes: If this ratio is much larger or smaller than 1, the observed behaviour is comparable with ABPs interacting via a single length-scale potential. If this ratio is similar to 1, the two length-scales are relevant for both structure and dynamical properties. On the structural side, when the system exhibits a motility induced phase separation, the dense phase is characterised by new and more complex structures compared with the hexatic phase observed in single length-scale systems (see Fig 1.b). On the dynamical side, as far as we are aware, this is the first representation of an anomalous dynamics in active particles (see Fig 1.c).

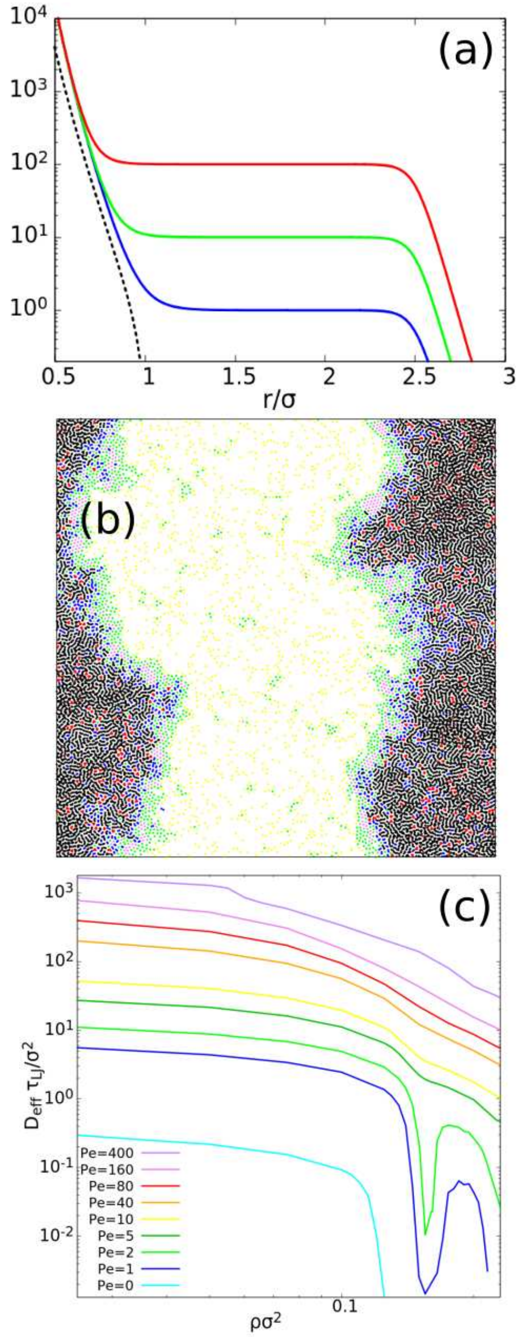

Fig. 1. (a) Shoulder interaction potential for $\epsilon_s/\epsilon = 1$ (blue), $\epsilon_s/\epsilon = 10$ (green) and $\epsilon_s/\epsilon = 100$ (red) and Weeks-Chandler-Andersen (black). (b) Snapshot for a system with $\epsilon_s/\epsilon = 10$, $\rho\,\sigma^2 = 0.150$ and $Pe = 500$. (c) Effective diffusion of the particles as a function of density for different degrees of activity.

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