

Supplementary Information

Structural and dynamical equilibrium properties of diffusing hard board-like particles in parallel confinement

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S1. Simulation settings

Table 1: Translational and rotational diffusion coefficient at infinite dilution of the HBPs studied in this work.

W^*	$D_T^{tra} D_0^{-1}$	$D_W^{tra} D_0^{-1}$	$D_L^{tra} D_0^{-1}$	$D_T^{rot} \tau$	$D_W^{rot} \tau$	$D_L^{rot} \tau$
1	$2.2 \cdot 10^{-2}$	$2.2 \cdot 10^{-2}$	$3.1 \cdot 10^{-2}$	$1.1 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$2.3 \cdot 10^{-2}$
8	$9.4 \cdot 10^{-3}$	$1.4 \cdot 10^{-2}$	$1.5 \cdot 10^{-2}$	$3.5 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$	$6.3 \cdot 10^{-4}$

Table 2: Details of systems with prolate hard board-like particles and DMC simulations settings with correspondent acceptance rates.

$\{W^* = 1, L^* = 12\}$							
N	L_x/T	L_y/T	h/T	$dt_{MC,1}/\tau$	\mathcal{A}_1	$dt_{MC,2}/\tau$	\mathcal{A}_2
1200	~ 63.3	~ 63.3	25	10^{-5}	0.998	10^{-2}	0.934
1800	~ 63.3	~ 63.3	37	10^{-5}	0.998	10^{-2}	0.934
2400	~ 63.3	~ 63.3	49	10^{-5}	0.998	10^{-2}	0.934

Table 3: Details of systems with dual-shaped hard board-like particles and DMC simulations settings with correspondent acceptance rates.

$\{W^* \sim 3.46, L^* = 12\}$							
N	L_x/T	L_y/T	h/T	$dt_{MC,1}/\tau$	\mathcal{A}_1	$dt_{MC,2}/\tau$	\mathcal{A}_2
1200	~ 117.7	~ 117.7	25	10^{-5}	0.999	10^{-2}	0.970
1800	~ 117.7	~ 117.7	37	10^{-5}	0.999	10^{-2}	0.970
2400	~ 117.7	~ 117.7	49	10^{-5}	0.999	10^{-2}	0.970

Table 4: Details of systems with oblate hard board-like particles and DMC simulations settings with correspondent acceptance rates.

$\{W^* = 8, L^* = 12\}$							
N	L_x/T	L_y/T	h/T	$dt_{MC,1}/\tau$	\mathcal{A}_1	$dt_{MC,2}/\tau$	\mathcal{A}_2
1200	~ 178.9	~ 178.9	25	10^{-5}	0.999	10^{-2}	0.978
1800	~ 178.9	~ 178.9	37	10^{-5}	0.999	10^{-2}	0.979
2400	~ 178.9	~ 178.9	49	10^{-5}	0.999	10^{-2}	0.979

S2. Slabs definition

In Tables 5, 6, 7 are reported all the sizes of each slab we used for the calculation of all the dynamical properties of the suspensions in confinement.

Table 5: Definition of the slabs used for the computation of the dynamical properties of the HBPs in parallel confinement, for systems with $h = 25T$.

slab label	Δx	Δy	Δz
$l_{\omega,bot}, 25T$	$[0, L_x]$	$[0, L_y]$	$[0, 3.5T]$
$l_{1,bot}, 25T$	$[0, L_x]$	$[0, L_y]$	$[3.5T, 6.5T]$
$l_{2,bot}, 25T$	$[0, L_x]$	$[0, L_y]$	$[6.5, 9.5T]$
$l_{3,bot}, 25T$	$[0, L_x]$	$[0, L_y]$	$[9.5T, 12.5T]$
$l_{3,top}, 25T$	$[0, L_x]$	$[0, L_y]$	$[12.5T, 15.5T]$
$l_{2,top}, 25T$	$[0, L_x]$	$[0, L_y]$	$[15.5T, 18.5T]$
$l_{1,top}, 25T$	$[0, L_x]$	$[0, L_y]$	$[18.5T, 21.5T]$
$l_{\omega,top}, 25T$	$[0, L_x]$	$[0, L_y]$	$[21.5T, 25T]$

Table 6: Definition of the slabs used for the computation of the dynamical properties of the HBPs in parallel confinement, for systems with $h = 37T$.

slab label	Δx	Δy	Δz
$l_{\omega,bot}, 37T$	$[0, L_x]$	$[0, L_y]$	$[0, 3.5T]$
$l_{1,bot}, 37T$	$[0, L_x]$	$[0, L_y]$	$[3.5T, 6.5T]$
$l_{2,bot}, 37T$	$[0, L_x]$	$[0, L_y]$	$[6.5, 9.5T]$
$l_{3,bot}, 37T$	$[0, L_x]$	$[0, L_y]$	$[9.5T, 12.5T]$
$l_b, 37T$	$[0, L_x]$	$[0, L_y]$	$[12.5T, 24.5T]$
$l_{3,top}, 37T$	$[0, L_x]$	$[0, L_y]$	$[24.5T, 27.5T]$
$l_{2,top}, 37T$	$[0, L_x]$	$[0, L_y]$	$[27.5T, 30.5T]$
$l_{1,top}, 37T$	$[0, L_x]$	$[0, L_y]$	$[30.5T, 33.5T]$
$l_{\omega,top}, 37T$	$[0, L_x]$	$[0, L_y]$	$[33.5T, 37T]$

Table 7: Definition of the slabs used for the computation of the dynamical properties of the HBPs in parallel confinement, for systems with $h = 49T$.

slab label	Δx	Δy	Δz
$l_{\omega,bot}, 49T$	$[0, L_x]$	$[0, L_y]$	$[0, 3.5T]$
$l_{1,bot}, 49T$	$[0, L_x]$	$[0, L_y]$	$[3.5T, 6.5T]$
$l_{2,bot}, 49T$	$[0, L_x]$	$[0, L_y]$	$[6.5, 9.5T]$
$l_{3,bot}, 49T$	$[0, L_x]$	$[0, L_y]$	$[9.5T, 12.5T]$
$l_b, 49T$	$[0, L_x]$	$[0, L_y]$	$[12.5T, 36.5T]$
$l_{3,top}, 49T$	$[0, L_x]$	$[0, L_y]$	$[36.5T, 39.5T]$
$l_{2,top}, 49T$	$[0, L_x]$	$[0, L_y]$	$[39.5T, 42.5T]$
$l_{1,top}, 49T$	$[0, L_x]$	$[0, L_y]$	$[42.5T, 45.5T]$
$l_{\omega,top}, 49T$	$[0, L_x]$	$[0, L_y]$	$[45.5T, 49T]$

In the manuscript, we estimated some properties of the systems from HBPs found in slabs, defined here in Tables 5-7. Due to the symmetric nature of the systems investigated, we averaged out the properties obtained from HBPs found in opposite slabs ("top" and "bottom"), with respect to the walls. More specifically, we refer to either the slab at the bottom wall $l_{\omega,bot}$ or the slab at the top wall $l_{\omega,top}$ slabs as l_{ω} in the manuscript; the properties obtained from HBPs found in l_{ω} slabs have been averaged together and are labelled with ω in the manuscript. Similar procedure has been applied for the calculation of the properties with label l_1 , which are obtained as average of properties obtained from $l_{1,bot}$ and $l_{1,top}$ slabs; l_2 as average between $l_{2,bot}$ and $l_{2,top}$ slabs; and l_3 as the average between $l_{3,bot}$ and $l_{3,top}$. The only exceptions are the results obtained in the slabs

corresponding to the bulk region, l_b , which have been found only in systems with $h = 37T$ and $49T$. These slabs are, by definition, much bigger than all the other slabs defined (see Tables 6 and 7), and they have been used as reference for the discussion of the particle dynamics in the proximity of the walls.