Electronic Supplementary Information (ESI)

Number density distribution of solvent on a substrate: A transform theory for atomic force microscopy

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Further verification tests of HPA transform

To check the validity of the transform theory, we conduct computational validation tests of the transform theory by using a sophisticated integral equation theory, one-dimensional Ornstein-Zernike equation[1] coupled with both hypernetted-chain closure and Verlet-Choudhury-Ghosh bridge function.[2] In the main text, we prepared Tables 1-3 (model systems 1-18) for the verification tests, however, the number of the model systems are not sufficient. In the supplementary information, we prepare other model systems (see Tables S1 and S2).

Table S1 Parameters of the model systems S1-S6 (all $\varepsilon_{BS}/k_BT = 0$).

model system #	$\rho_0 d_S$	d_P/d_S	ε_{SS}/k_BT	ε_{PS}/k_BT	ε_{BS}/k_BT	g_{CP}
S1	0.7	3	1	0	0	3.30
S2	0.7	6	1	0	0	3.51
S3	0.7	3	1	1	0	4.38
S4	0.7	6	1	1	0	4.65
S5	0.7	3	1	2	0	5.70
S6	0.7	6	1	2	0	6.04

Table S2 Parameters of the model systems S7-S12 (all $\varepsilon_{BS}/k_BT = 2$).

model system #	$\rho_0 d_S$	d_P/d_S	ε_{SS}/k_BT	ε_{PS}/k_BT	ε_{BS}/k_BT	g_{CP}
S7	0.7	3	1	0	2	3.30
S8	0.7	6	1	0	2	3.51
S9	0.7	3	1	1	2	4.38
S10	0.7	6	1	1	2	4.65
S11	0.7	3	1	2	2	5.70
S12	0.7	6	1	2	2	6.04

In the model systems S1-S6, the cylindrical substrate is (weakly) solvophobic, meanwhile in the model systems S7-S12, the cylindrical substrate is (weakly) solvophilic. Here, ρ_0 is the bulk number density of the small spheres, d_S is the diameter of the small sphere, d_P is the diameter of the model probe, ε_{SS} is the attractive parameter between the two small spheres, ε_{PS} is the attractive parameter between the model probe and the small sphere, ε_{BS} is the attractive parameter between the cylindrical substrate and the small sphere, k_B is the Boltzmann constant, T is the absolute temperature, g_{CP} is the normalized contact number density of the small spheres on the model probe.

In Figs. S1 and S2, the results obtained from Tables S1 and S2, respectively, are shown. The reproducibilities of HPA transform in the model systems S1-S12 are almost the same with that obtained in the model systems 1-12 (Tables 1 and 2) in the main text (see Figs. 3-6). That is, HPA transform can reproduce the number density distribution semi-quantitatively also in these cases.

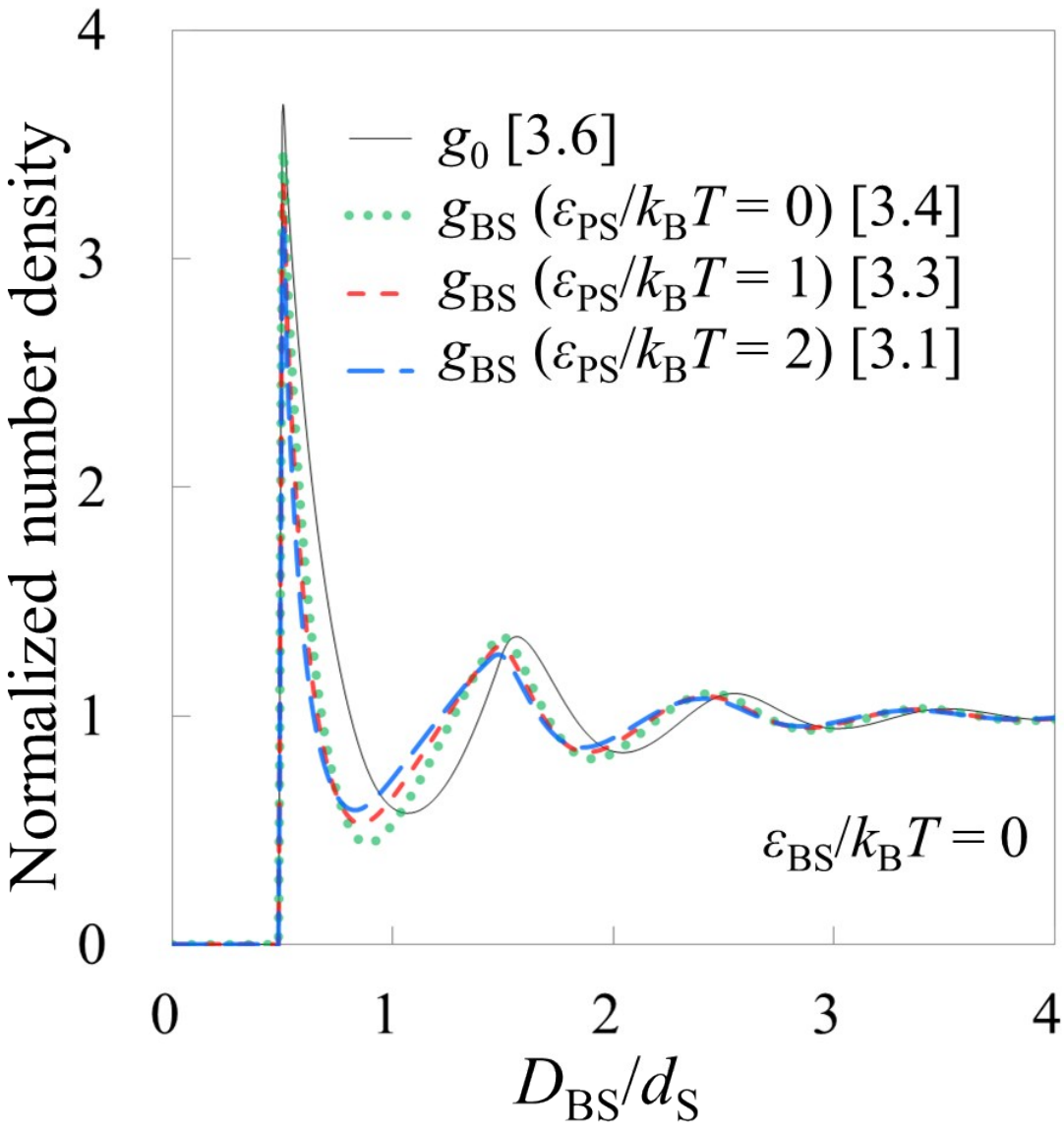

Fig. S1 Results from the model systems S1-S6. The normalized number density calculated by 1D-OZ-HNC-VCG being g_0 is the benchmark structure of the verification test, which is shown by the solid line. The normalized number density calculated through HPA transform being g_{BS} is compared with g_0. g_{BS}s for the model systems S1 (S2), S3 (S4), and S5 (S6) are shown by the dotted, short-dashed, and long-dashed lines, respectively. g_{BS}s for the model systems S1 and S2 are collectively shown in one line, because the shapes obtained from these model systems are identical. g_{BS}s for the model systems 'S3 and S4' and 'S5 and S6' are also shown in the same manner. Values in the brackets represent the maximum values of the respective normalized number densities.

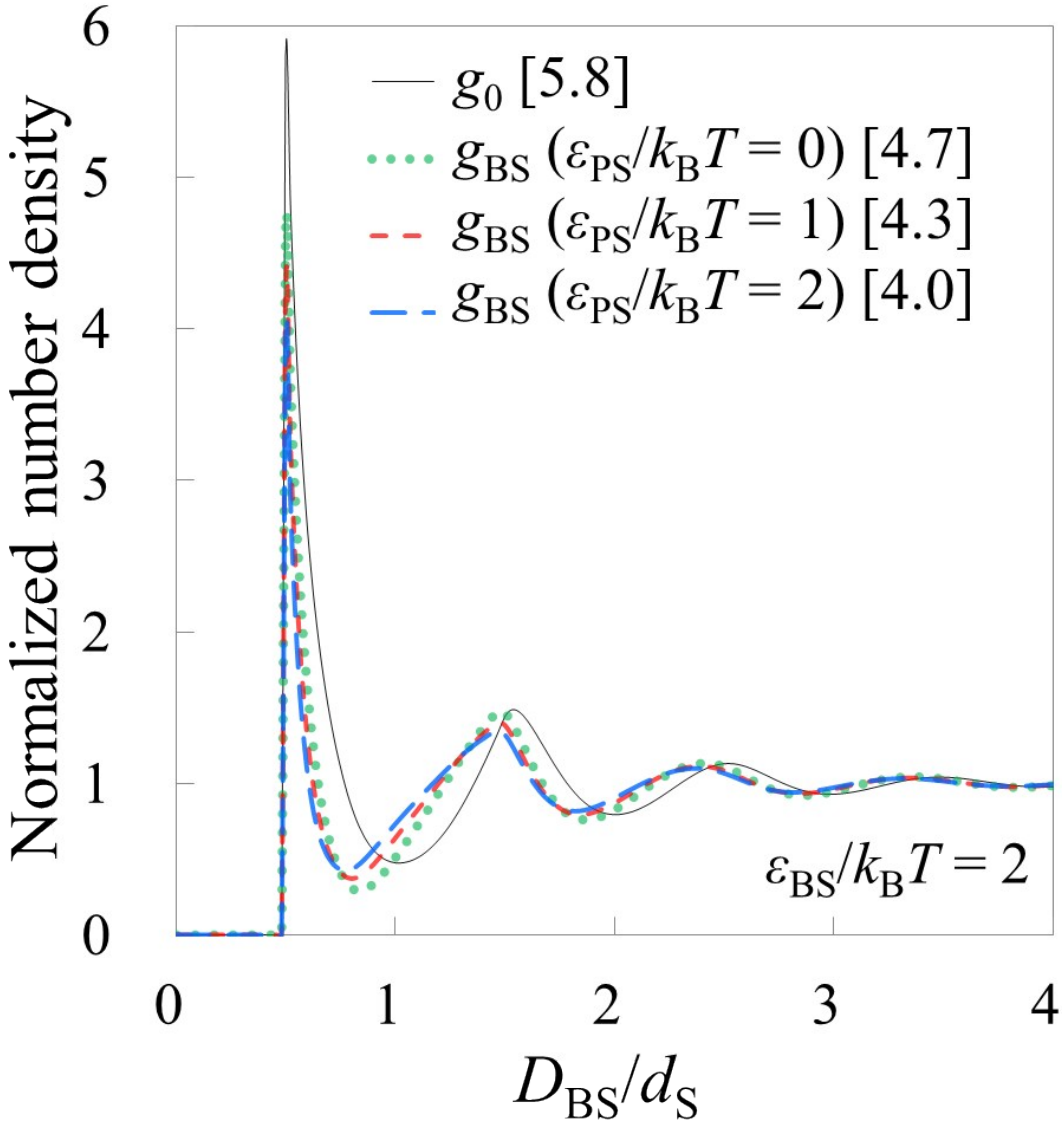

Fig. S2 Results from the model systems S7-S12. The normalized number density calculated by 1D-OZ-HNC-VCG being g_0 is the benchmark structure of the verification test, which is shown by the solid line. The normalized number density calculated through HPA transform being g_{BS} is compared with g_0. g_{BS}s for the model systems S6 (S7), S8 (S9), and S10 (S11) are shown by the dotted, short-dashed, and long-dashed lines, respectively. g_{BS}s for the model systems S6 and S7 are collectively shown in one line, because the shapes obtained from these model systems are identical. g_{BS}s for the model systems 'S8 and S9' and 'S10 and 11' are also shown in the same manner. Values in the brackets represent the maximum values of the respective normalized number densities.

References

1 J.-P. Hansen and I. R. McDonald, Theory of Simple Liquids, Academic Press, London, 1986.
2 N. Choudhury and S. K. Ghosh, *J. Chem. Phys.*, 2002, **116**, 8517–8522.