Supplement: Density Profiles of the Hard-Sphere Fluid at a Planar Hard Wall

Ruslan L. Davidchack[1], Brian B. Laird[2], and Roland Roth[3]

[1] *Department of Mathematics, University of Leicester, Leicester, LE1 7RH, United Kingdom*

[2] *Department of Chemistry, University of Kansas, Lawrence, KS 66045, United States*

[3] *Institut für Theoretische Physik, Universität Tübingen, D-72074 Tübingen, Germany*

The file `hswall.zip` contains files `hswall`xyz`.dat` with data for the density profile $\rho(z)$ of the hard-sphere fluid at a planar hard wall with bulk density approximately equal to $0.xyz\,\sigma^{-3}$. Below is the table of the files, the values of the bulk density ρ, (with digit(s) in parentheses indicating the 95% confidence intervals), excess volume per unit area, $v_{\rm ex}$, and the surface free energy γ.

File name	Bulk density, σ^{-3}	Excess volume, σ	Surface Free Energy, kT/σ^2
`hswall052.dat`	0.05151651(2)	0.461248(16)	0.0275661(5)
`hswall102.dat`	0.10191620(8)	0.42642(3)	0.0583160(14)
`hswall194.dat`	0.1944023(4)	0.36954(6)	0.126051(7)
`hswall305.dat`	0.3046652(6)	0.31192(7)	0.230187(18)
`hswall387.dat`	0.3866741(9)	0.27509(8)	0.32841(3)
`hswall485.dat`	0.4845311(13)	0.23686(9)	0.47529(5)
`hswall547.dat`	0.5473725(18)	0.21534(11)	0.59084(7)
`hswall638.dat`	0.6380515(23)	0.18736(12)	0.79380(12)
`hswall701.dat`	0.700782(3)	0.17008(14)	0.96789(17)
`hswall751.dat`	0.750543(3)	0.15715(14)	1.1282(2)
`hswall792.dat`	0.792318(4)	0.14669(15)	1.2811(3)
`hswall829.dat`	0.829100(4)	0.13746(16)	1.4314(3)
`hswall857.dat`	0.856919(5)	0.13037(17)	1.5556(3)
`hswall884.dat`	0.883720(5)	0.12320(17)	1.6848(4)
`hswall907.dat`	0.906527(5)	0.11656(17)	1.8017(4)
`hswall926.dat`	0.926326(5)	0.10973(18)	1.9082(4)
`hswall938.dat`	0.938164(6)	0.10447(19)	1.9734(5)

In each file `hswall`xyz`.dat`, the first column gives the value of the z coordinate in units of σ, z_i, $i = 1, 2, \ldots$, the second column is the average density ρ_i in the interval $[z_i - 0.01, z_i + 0.01]$ in

units of σ^{-3}, and the third column gives the estimated 95% confidence interval in the values ρ_i. The density $\rho(z) = 0$ for $z < 0.5\,\sigma$.

Note that, the excess volume at zero density, $v_{\rm ex}(\rho = 0) = 1/2$. Also, the adsorption can be easily obtained from the excess volumes given above using the relation $\Gamma = -\rho v_{\rm ex}$.