

Supplementary material: Dependence of the self-diffusion coefficient on the q -gap value in fluids

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Table 1: Chosen states of considered systems.

Potential	Dimension	Density	Temperature
ML-IAP (Al)	3D	2.7 g/cm ³	1560 — 2560 K
EAM (Fe)	3D	3.6 g/cm ³	1812 — 2392 K
LJ	3D	1.00	1.6 — 7.0
		1.10	2.7 — 8.0
		1.20	4.0 — 9.0
		1.30	5.8 — 15.6
		1.40	8.1 — 17.9
		1.60	14.6 — 21.8
		1.80	24.2 — 29.8
		2.00	37.4 — 44.8
	2D	0.80	0.60 — 3.10
		0.85	1.00 — 3.50
		0.90	2.00 — 4.50
Yukawa	3D	κ	Γ
		1.00	217 — 117
		1.25	250 — 110
		1.50	270 — 86
		2.00	440 — 157
		2.50	750 — 305
		3.00	1185 — 665
	2D	1.00	177 — 77
		1.50	250 — 73
		2.00	395 — 112

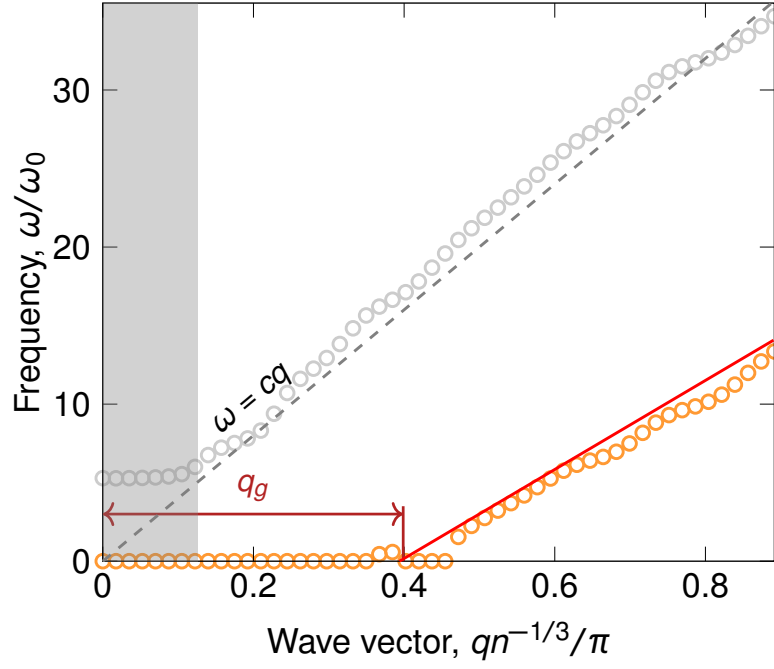


Figure 1: Dispersion relations $\omega_{L,T}(q)$ for a 3D Lennard-Jones fluid at density $n = 1$ and temperature $T = 5$. Transverse (ω_T) and longitudinal (ω_L) modes are represented by orange and gray circles, respectively. The gray and red lines depict the theoretical asymptotic curves $\omega = cq$. The dark gray zone indicates the region where $qn^{-1/3} < 2\pi/L$ and finite-size effects are significant (L being the system size).

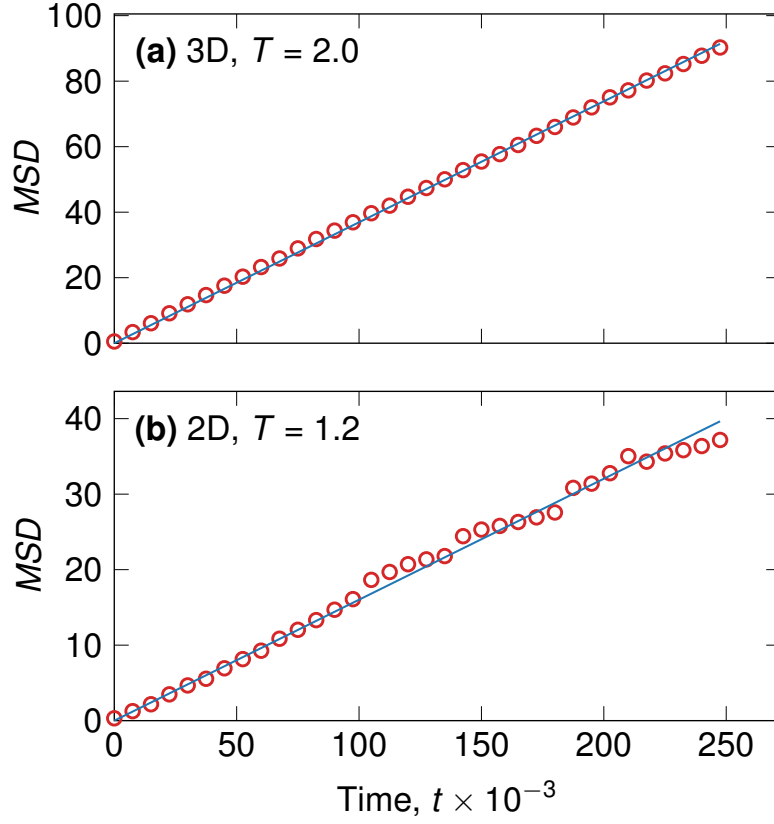


Figure 2: Dependence of the MSD on the time t for the Lennard-Jones potential in three- and two-dimensional cases.

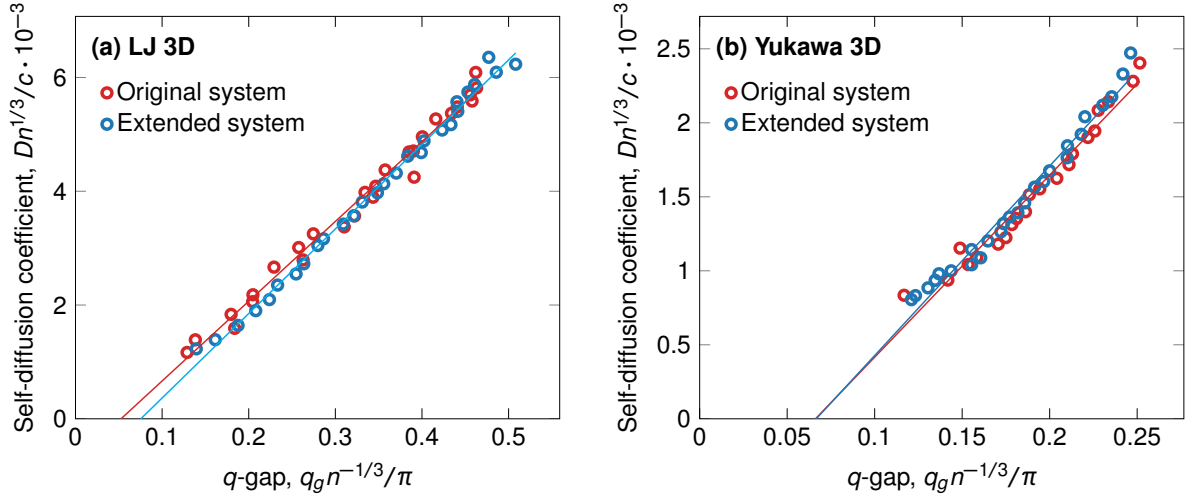


Figure 3: The comparison between $D(q_g)$ relations in extended (blue) and original (red) 3D systems with Lennard-Jones ($n = 1$) and Yukawa ($\kappa = 1$) potentials.

Table 2: Minimum values of q_g and corresponding slopes for studied systems

Potential	Dimension	Density	Value of q_g near the MP, q_0	$\left(\frac{dD}{dq_g}\right)_{q_0}$
ML-IAP (Al)	3D	2.7 g/cm ³	0.078	0.013
EAM (Fe)	3D	3.6 g/cm ³	0.168	0.024
LJ	3D	1.0	0.165	0.0166
		1.1	0.159	0.0142
		1.2	0.157	0.0136
		1.3	0.151	0.0124
		1.4	0.151	0.0110
		1.6	0.169	0.0079
		1.8	0.182	0.0074
		2.0	0.170	0.0062
	2D	0.80	0.172	
		0.85	0.119	
		0.90	0.056	
Yukawa	3D	κ		
		1.00	0.115	0.015
		1.25	0.105	0.027
		1.50	0.123	0.042
		2.00	0.106	0.052
		2.50	0.130	0.058
		3.00	0.111	0.098
	2D	1.00	0.090	
		1.50	0.097	
		2.00	0.129	