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

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MOLECULAR DYNAMICS SIMULATIONS DETAILS

We considered systems of particles interacting via the Lennard-Jones (LJ) and Yukawa (Ykw) pair potentials:

$$\varphi_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \tag{1}$$

$$\varphi_{\mathrm{Ykw}}(r) = A\frac{e^{-k_D r}}{r}, \tag{2}$$

where ε and σ are the energy and length scale of the interaction, respectively; A and k_D are parameters which where chosen as $A = 1$, $k_D = \lambda_D^{-1} = 1$. Corresponding coupling and screening parameters are $\Gamma = A(ak_BT)^{-1}$ and $\kappa = a\lambda_D^{-1}$, respectively. Here λ_D is the Debye length, $a = (3/4\pi n)^{1/3}$ is the Wigner-Seitz radius, where $n = N/V$ is the numerical density, k_B is the Boltzmann constant and T is the temperature.

We have studied 3D and 2D fluids consisting of $N = 4000$ ($N = 4900$ in 2D case) particles in an NVT ensemble with a Nose–Hoover thermostat. The initial state of the system was a cubic lattice (a square in 2D case) with a size $L = 10$ ($L = 70$ in 2D case) with periodic boundary conditions with Maxwell distribution of velocities. The cutoff radius of interaction was chosen as $r_{\mathrm{cut}} = 7.5n^{-1/d}$, where $n = N/V$ is the numerical density and d is the space dimension. The mass m, length σ, and energy ε were normalized to unity.

The interatomic potential with machine learning (ML-IAP) for liquid aluminum [1] was also considered:

$$\varphi_{\text{ML-IAP}}(r) = \varphi_{\mathrm{ref}}(r) + \sum_{i=1}^{N} E^i_{\mathrm{SNAP}}, \tag{3}$$

where E_{ref} denotes a reference potential and E^i_{SNAP} is the total energy of atom i relative to the atoms in its neighborhood, governed by the spectral neighbor analysis potential method (SNAP) [2]. Ziegler-Biersack-Littmark (ZBL) potential [3] is used as a reference potential. The SNAP energy for each atom is calculated using a linear combination of the bispectrum components $\mathbf{B}^i$

$$E^i_{\mathrm{SNAP}} = \boldsymbol{\beta} \times \mathbf{B}^i, \tag{4}$$

where $\boldsymbol{\beta}$ are linear coefficients and $\mathbf{B}^i$ are descriptors of the local environment of atom i. Obtained using machine learning coefficients [4] $\boldsymbol{\beta}$ were used in this work.

Simulations of liquid Al were performed in a three-dimensional face-centered cubic box with dimensions of $Lx = Ly = Lz = 10a$, where a is lattice constant, with mass density $\rho = 2.7\mathrm{g/cm}^3$. The remaining simulation details including number of particles, thermostating and boundary conditions follow previously established setup.

Moreover, we considered liquid iron using Embedded atom model (EAM). The general form of this potential can be expressed as:

$$E_i = \sum_i F(\rho_i) + \frac{1}{2}\sum_i \sum_{j\neq i} \varphi_{\mathrm{p}}(r_{ij}), \tag{5}$$

where $F_i(\rho_i)$ denotes the embedding energy for atom i, a function of the local electron density ρ_i. This local density is computed as a superposition of the contributions from all neighboring atoms j:

$$\rho_i = \sum_{j\neq i} \rho(r_{ij}). \tag{6}$$

In these expressions, $\varphi_{\rm p}(r_{ij})$ represents the pairwise potential between atoms i and j, separated by a distance r_{ij}. The specific functional forms for $F(\rho)$, $\rho(r)$, and $\varphi_{\rm p}(r)$ employed in this work are those established in the corresponding paper [5].

The mass density $\rho = 10 g/cm^3$ was used in the simulations for liquid iron. The remaining simulation parameters correspond to those employed for liquid iron.

Simulations of fluids of particles interacting via the Lennard-Jones and Yukawa potentials were performed using the numerical time step $\Delta t = 5 \times 10^{-3}\sqrt{m\sigma^2/\varepsilon}$. For ML-IAP and EAM potentials in liquid aluminum and iron the time step $\Delta t = 5$ fs was chosen. All simulations where performed with the LAMMPS package [6] for 5×10^4 time steps, where the first 5000 were used for system relaxation.

Table I. 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
		κ	Γ
Yukawa	3D	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

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[2] A. Thompson, L. Swiler, C. Trott, S. Foiles, and G. Tucker, Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials, Journal of Computational Physics **285**, 316 (2015).

[3] The Stopping and Range of Ions in Matter, in *Treatise on Heavy-Ion Science* (Springer US, Boston, MA, 1985) pp. 93–129.

[4] S. Kumar, H. Tahmasbi, K. Ramakrishna, M. Lokamani, S. Nikolov, J. Tranchida, M. A. Wood, and A. Cangi, Training scripts and input data sets: Transferable Interatomic Potential for Aluminum from Ambient Conditions to Warm Dense Matter (2023).

[5] A. B. Belonoshko, R. Ahuja, and B. Johansson, Quasi– *Ab Initio* Molecular Dynamic Study of Fe Melting, Physical Review Letters **84**, 3638 (2000).

[6] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, Journal of Computational Physics **117**, 1 (1995).

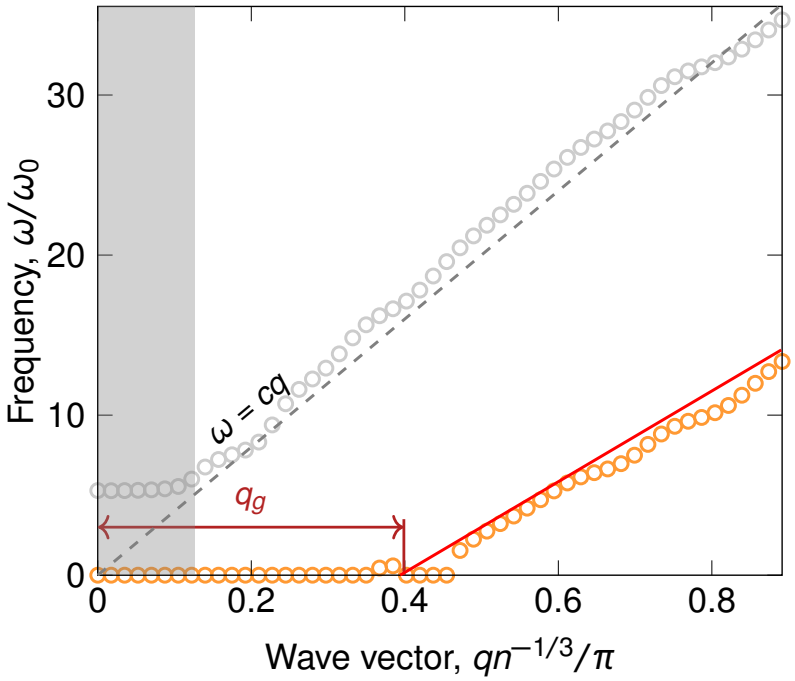

Figure 1. Dispersion relations $\omega_{L,T}(q)$ for a 3D Lennard-Jones fluid at density $n = 1$ and temperature $T = 5$. Transverse (ω_T) and longitudinal (ω_L) modes are represented by orange and gray circles, respectively. The gray and red lines depict the theoretical asymptotic curves $\omega = cq$. 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).

Table II. Minimum values of q_g and corresponding slopes for studied systems

Potential	Dimension	Density	Value of q_g near the MP, q_0	$\left(\frac{\mathrm{d}D}{\mathrm{d}q_g}\right)_{q_0}$
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		κ		
	3D	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	

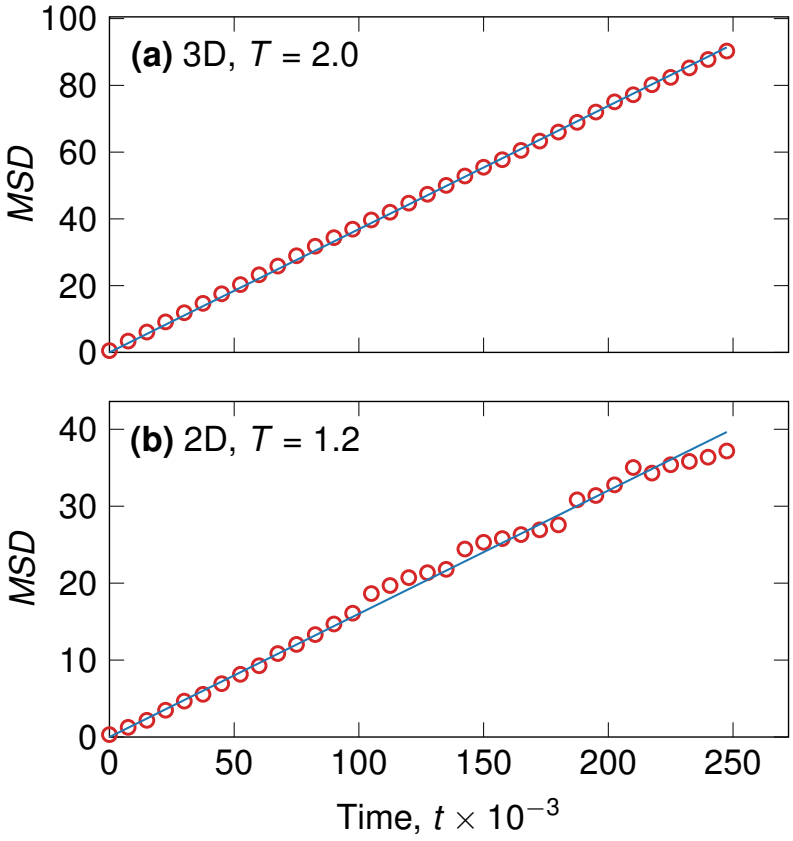

Figure 2. Dependence of the MSD on the time t for the Lennard-Jones potential in three- and two-dimensional cases.

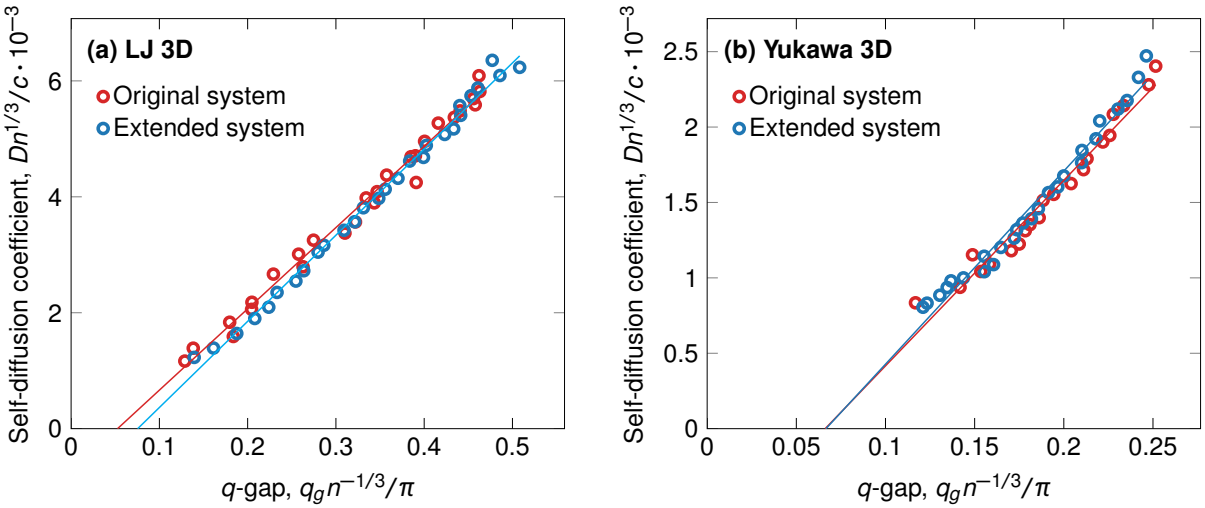

Figure 3. The comparison between $D(q_g)$ relations in extended (blue) and original (red) 3D systems with Lennard-Jones ($n = 1$) and Yukawa ($\kappa = 1$) potentials.

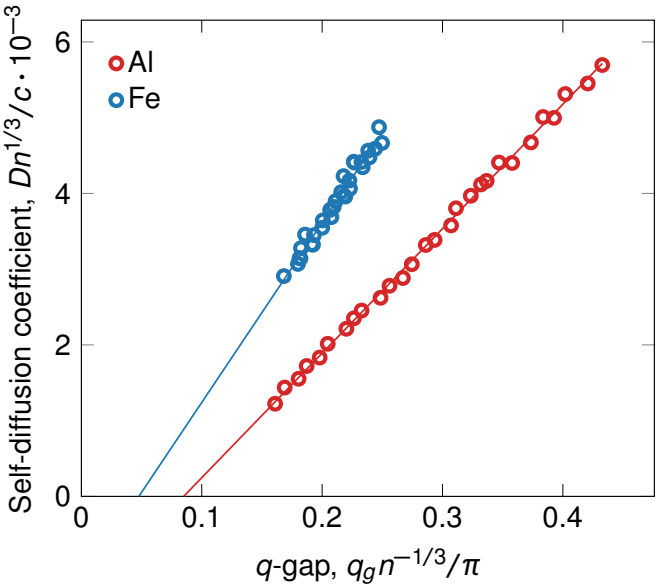

Figure 4. Dependence of the self-diffusion coefficient D on the q-gap width for 3D liquid aluminum at density $\rho = 2.7$ g/cm^3.