

# BD Exercises: Solution

February 06, 2026

**Note:** Please be fair and acknowledge good work when you see it. If a solution isn't entirely correct but demonstrates a solid understanding and correct approach, you can award 70-80% of the points, even if the final answer is wrong. Conversely, if the final answer is correct but the reasoning and steps are not clearly explained, consider deducting 20-30% if the calculations are unclear. However, if solutions are missing or significantly off-topic, you should consider awarding very few points or none at all.

**PLEASE PROVIDE A DESCRIPTION OF HOW YOU AWARDED YOUR POINTS!**

Maximum marks: 70

## Answers

### 1. Verification of the Einstein Diffusion Equation

The Einstein diffusion relation for Brownian motion is

$$D = \frac{k_B T}{\gamma},$$

which predicts a linear dependence of the diffusion coefficient  $D$  on temperature  $T$ , inverse friction  $\gamma^{-1}$ , and inverse mass  $m^{-1}$ .

- **Step 1: Dependence on friction coefficient**

The diffusion coefficient was computed for  $\gamma^{-1} = 0.1, 0.3, 0.6, 1.0$ , while keeping the mass  $m = 1$  and  $k_B T = 1.0$  fixed.

The resulted data for the  $\gamma^{-1}$  vs  $D$  is pasted below.

0.1	0.0998
0.3	0.2993
0.6	0.5982
1.0	0.9954

**Marking Criteria:** Numbers given are the approximate values and need not to be exactly the same. For all the four correct values give full marks.

[2.5 marks]

- **Step 2: Dependence on temperature**

Simulations were performed at temperatures  $k_B T = 1, 2, 3, 7$ , with fixed  $\gamma^{-1} = 0.1$  and  $m = 1$ . The plot shown in Figure 2 (t\_vs\_d.png) demonstrates a linear increase of the diffusion coefficient with temperature.

The resulted data for the  $k_B T$  vs  $D$  is pasted below.

1.0	0.0998
2.0	0.1996
3.0	0.2993
7.0	0.6985

**Marking Criteria:** Numbers given are the approximate values and need not to be exactly the same. For all the four correct values give full marks.

[2.5 marks]

- **Step 3: Dependence on mass**

The diffusion coefficient was evaluated for particle masses  $m = 1, 2, 3, 6$ , while keeping  $k_B T = 1.0$  and  $\gamma^{-1} = 0.1$  fixed.

The resulted data for the  $k_B T$  vs  $D$  is pasted below.

1.0	0.0998
2.0	0.0499
3.0	0.0333
6.0	0.0166

**Marking Criteria:** Numbers given are the approximate values and need not to be exactly the same. For all the four correct values give full marks.

[2.5 marks]

- **Step 4: Discussion**

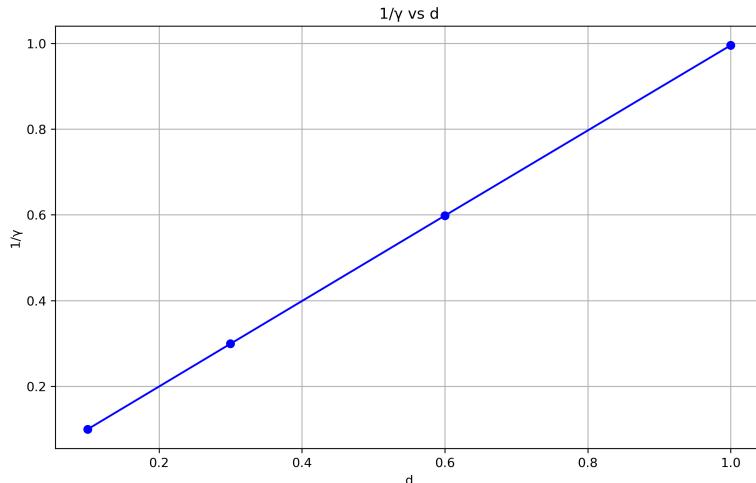


Figure 1: Diffusivity is plotted as a function of  $\gamma^{-1}$ .

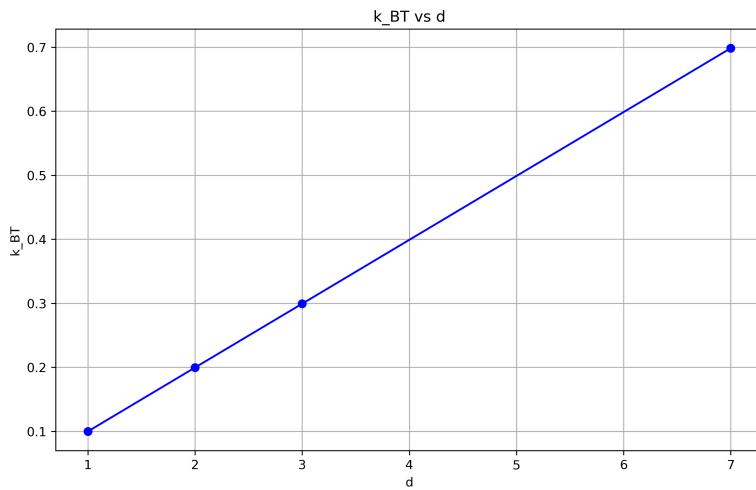


Figure 2: Diffusivity has been shown as the function of temperature.

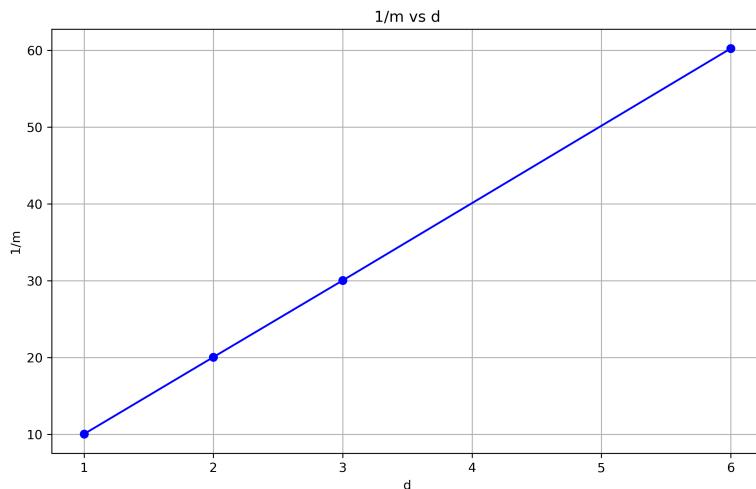


Figure 3: Diffusivity is plotted as a function of mass  $m$ .

From Figures 1-3, the following relations are observed:

$$D \propto \gamma^{-1}, \quad D \propto k_B T, \quad D \propto m^{-1}.$$

All three dependencies are approximately linear within numerical uncertainty, thereby validating the Einstein diffusion equation for the simulated system.

**Marking Criteria: For each plots give 1/2 marks and for the explanation give 1 marks. The explanation should be similar to the above given example.**

[2.5 marks]

## 2. Dumbbell-Shaped Patchy Particle System

- **Step 1: Constructing a dumbbell-shaped molecular template**

The dumbbell-shaped molecule consists of three atoms: - One central hard-core atom (core) - Two patch atoms located on opposite ends of the core

The complete .mol file is provided below:

```

# Dumbbell-shaped molecule template

3 atoms          # Total number of atoms in the molecule

# ----- COORDINATES -----
# Format: atom_index  x  y  z (in reduced LJ units)
Coords
1 1.0 1.0 1.0    # Core atom at the center
2 1.0 1.0 1.5    # Patch atom on +z direction (bond length 0.5)
3 1.0 1.0 0.5    # Patch atom on -z direction (bond length 0.5)

# ----- ATOM TYPES -----
# Format: atom_index  type
Types
1 1    # Core atom
2 2    # Patch atom
3 2    # Patch atom

```

**Justification:** - The molecule is symmetric along the z-axis to form a dumbbell shape. - The central core atom (type 1) is bonded to both patch atoms (type 2) with fixed bond length 0.5 LJ units.

**Marking Criteria:** Students are supposed to check just the distance of the patches from the core, such that patches are supposed to be inline with the core and with each other forming dumbbell shaped, while origin of the dumbbell can be placed anywhere, e.g., at 0.0,0.0,0.0. If correct give full marks.

[5.0 marks]

- **Step 2: Phase behavior**

If reported temperature is ( $k_B T < 0.15$ ) and the system exhibits liquid-like chain-forming behavior, as shown in Figure 4, give **3 marks**.

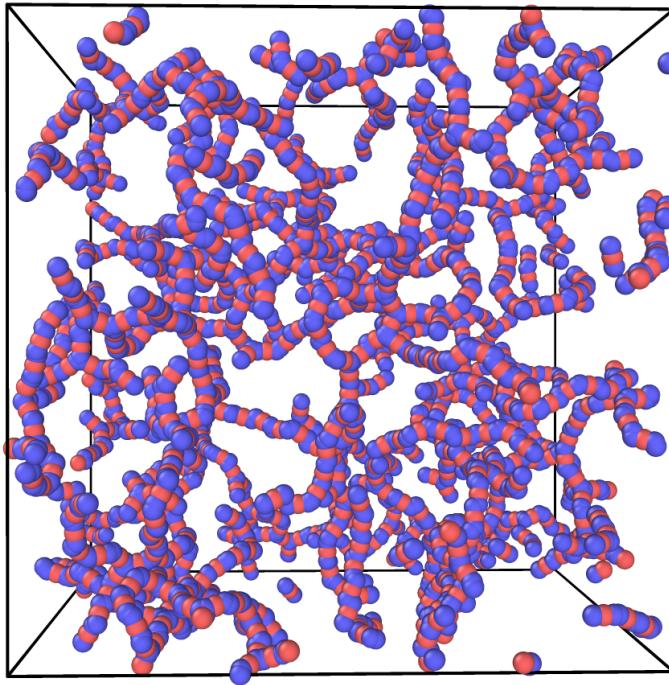


Figure 4: Liquid state defined by the chain like structure.

Core and patch particles are clearly distinguishable by color and size (**2 marks**). The corresponding temperature at which stable chains are observed is reported.

**Marking Criteria: If temperature is reported give 3 marks. If patches and particles are distinguishable by their color and sizes give 2 marks.**

[**5.0 marks**]

- **Step 3: Stability discussion**

The chain structures are metastable and persist over long simulation times at lower temperatures.

At low temperatures, thermal motion is insufficient to break directional patch bonds, leading to metastable chains.

At higher temperatures, thermal fluctuations dominate, resulting in chain breakup which leads system to the lowest potential energy state, which has more than one bond per patch ( where a chain can have only one bond per patch). Compared to globular structures observed at  $k_B T = 1.0$ , chain phases are stabilized by directional interactions and anisotropic bonding and therefore not an equilibrium structure, especially at higher temperatures.

**Marking Criteria: If the explanation isn't entirely correct but demonstrates a solid understanding and correct approach, you can award 70-80% of the points.**

[**5.0 marks**]

### 3. Viscosity of a Lennard–Jones Fluid Using the Green–Kubo Method

- **Step 1: Simulation time modification and density control**

To simulate a Lennard–Jones fluid at the target number density

$$\rho = \frac{N}{V} = 0.1,$$

the simulation box dimensions and lattice parameters were adjusted accordingly.  $V$  can be calculated from the box size specified in the LAMMPS input file.

The relevant section of the modified LAMMPS input file is shown below. To ensure numerical stability, the integration time step was chosen such that

$$dt \leq 0.001.$$

**Example:**

```
variable dt equal 0.00001
timestep 0.00001
```

**Reason or Justification:** At larger time steps, particles that are initially placed close to one another, particularly due to periodic boundary conditions-can experience large repulsive forces, leading to numerical instability and poor energy conservation. To allow the system to relax smoothly from the initial configuration, a smaller time step ( $dt = 10^{-5}$ ) was employed during the early stages of the simulation. This choice ensures stable integration of the equations of motion and prevents unphysical particle overlaps during equilibration.

**Marking Criteria:** For the reported value of time step give 3 marks and for the justification give 2 marks

[5.0 marks]

- **Step 2: Box sizes and density control**

The relevant section which led to the successful run is pasted below,

```
region           box block 0 23 0 23 0 23
create_box       1 box
lattice          fcc 0.5
```

**Marking Criteria:** Here students should note that the correct value is strictly not as same as shown in this example. The real test is whether students are able to find the relevant part which is causing problem, which has been pasted above.

**Reason or Justification:** Due to periodic boundary condition the atoms can overlap as the box size is not the exact (integer) multiple of the lattice constant calculated for the given density and lattice structure (in case fcc). However, one of the simplest way is change the box size slightly within the range of lattice constant unless system stop blowing up.

In practical applications, due to the complexity associated with exact calculations, it is often more effective to adjust model parameters rather

than pursue an exact solution, provided that the adjusted approach adequately captures the essential physical behavior of the system.

**Marking Criteria:** In this question, students are supposed to check just the relevant section as specified in the box regardless of values. 3 marks for the specification and 2 marks for the justification.

[5.0 marks]

- **Step 3: Density dependence of viscosity**

The shear viscosity was computed for densities

$\rho = 0.05, 0.1, 0.3, 0.4, 0.5$  using the Green–Kubo formalism.

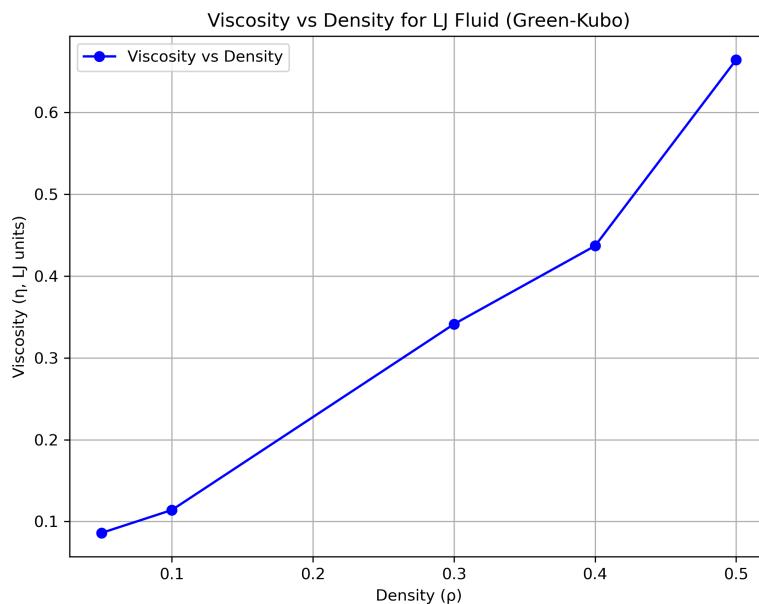


Figure 5: Viscosity as a function of density.

Figure-5 shows that viscosity increases monotonically with density.

This trend is physically reasonable, as higher densities lead to stronger interparticle interactions and enhanced momentum transport.

**Marking Criteria:** Minimum three state-points in the plot must be shown, for the full marks.

[5.0 marks]

- **Step 4: Conversion of viscosity from LJ to SI units**

**(a) Derivation of the factor** In Lennard–Jones (LJ) reduced units, viscosity is expressed in terms of the fundamental LJ units of mass  $m$ , energy  $\epsilon$ , and length  $\sigma$ . The dimensional form of viscosity is

$$[\eta] = \frac{\text{mass}}{\text{length time}}.$$

In LJ units, the characteristic time scale is defined as

$$\tau = \sigma \sqrt{\frac{m}{\epsilon}}.$$

Therefore, the LJ unit of viscosity can be written as

$$\eta_{\text{LJ}} = \frac{m}{\sigma\tau} = \frac{m}{\sigma^2} \sqrt{\frac{\epsilon}{m}} = \frac{\sqrt{m\epsilon}}{\sigma^2}.$$

Hence, the conversion factor from LJ viscosity units to SI units (Pa·s) is

$$\eta_{\text{SI}} = \eta_{\text{LJ}} \frac{\sqrt{m\epsilon}}{\sigma^2}.$$

[2.5 marks]

**(b) Final conversion factor** The LJ parameters are mapped to physical units as follows:

$$\begin{aligned}\sigma &= 1 \times 10^{-10} \text{ m}, \\ \epsilon &= k_B T, \quad T = 300 \text{ K}, \\ k_B &= 1.380649 \times 10^{-23} \text{ J K}^{-1}, \\ m &= 12 \text{ amu}, \quad 1 \text{ amu} = 1.660539 \times 10^{-27} \text{ kg}.\end{aligned}$$

First, convert the mass into SI units:

$$m = 12 \times 1.660539 \times 10^{-27} = 1.99265 \times 10^{-26} \text{ kg}.$$

Next, compute the energy scale:

$$\epsilon = k_B T = 1.380649 \times 10^{-23} \times 300 = 4.14195 \times 10^{-21} \text{ J}.$$

Now evaluate  $\sqrt{m\epsilon}$ :

$$\sqrt{m\epsilon} = \sqrt{(1.99265 \times 10^{-26})(4.14195 \times 10^{-21})} = \sqrt{8.25 \times 10^{-47}} = 9.08 \times 10^{-24}.$$

Finally, divide by  $\sigma^2$ :

$$\frac{\sqrt{m\epsilon}}{\sigma^2} = \frac{9.08 \times 10^{-24}}{(1 \times 10^{-10})^2} = 9.08 \times 10^{-4} \text{ Pa} \cdot \text{s}.$$

$$1 \eta_{\text{LJ}} = 9.1 \times 10^{-4} \text{ Pa} \cdot \text{s}$$

Thus, the viscosity obtained from LAMMPS in LJ units can be converted to SI units by multiplying it with  $9.1 \times 10^{-4} \text{ Pa} \cdot \text{s}$ .

**Marking Criteria: If the conversion factor is specified with the correct order (which is  $10^{-4}$ ), give full marks.**

[2.5 marks]

#### 4. Liquid–gas coexistence of the Lennard–Jones fluid at temperature $k_B T = 0.7$

- **Step 1: Fitting procedure (slab simulation method)**

The density profile obtained from the slab simulation is shown below. The profile is fitted to extract the coexistence densities of the liquid and gas phases.

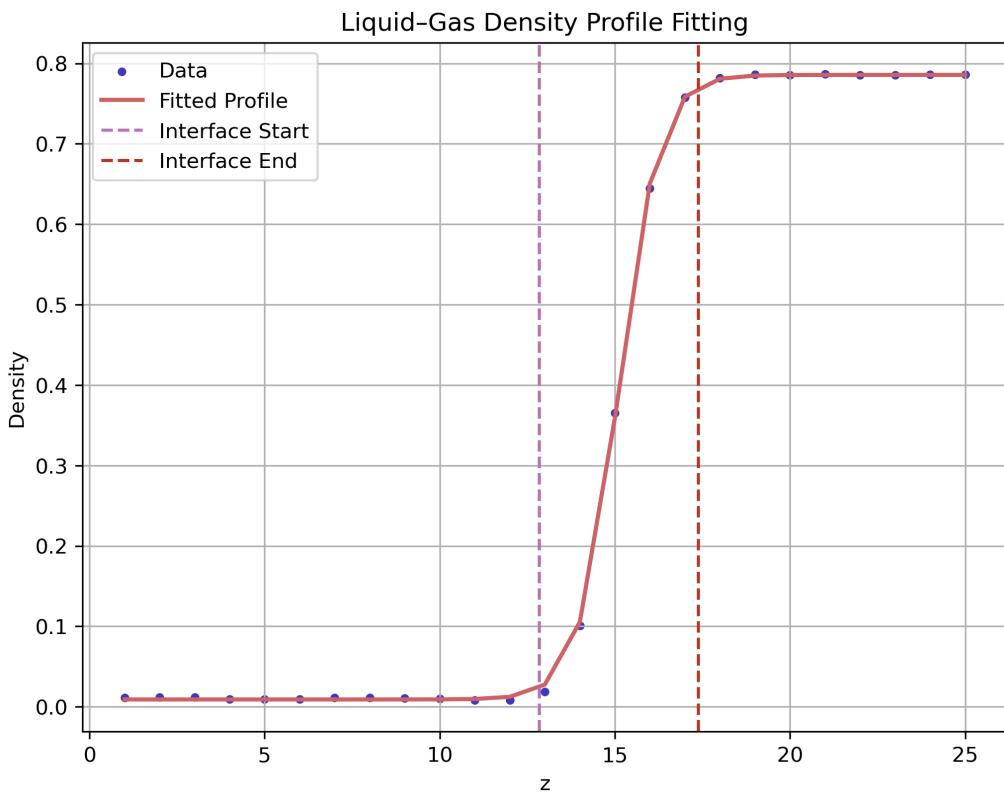


Figure 6: Fitted density profile for the Lennard–Jones fluid at temperature  $k_{\text{B}}T = 0.7$ .

**Marking Criteria:** Students are supposed to attach the plot of coexistence density for the full marks.

[15 Marks]

- **Step 2: Interface evolution with temperature**

The coexistence densities obtained from the simulation are:

- Liquid phase density:  $\rho_l \approx 0.7856$
- Gas (vapour) phase density:  $\rho_g \approx 0.0091$

The vapor phase corresponds to a low-density region. As the temperature increases, the vapour density increases while the liquid density decreases, leading to a reduction in the density contrast between the two phases. Consequently, the liquid-vapor interface becomes more diffuse, and the surface tension decreases with increasing temperature.

**Marking Criteria:** Students are supposed to check only the approximate value and give full marks if it is reasonably close to the given value.

[5 Marks]

## 5. Martini Force-Field Representation of Carbon Nanotubes

- Since we have a chain configuration and each Martini carbon particle represents four real carbon atoms, the effective bond length between two Martini beads is approximately four times the real C–C bond length:

$$d_{\text{Martini}} \approx 4 \times 1.2 \text{ \AA} = 4.8 \text{ \AA}.$$

**Marking Criteria:** If specified value is as same as given above, give full marks.

[2.5 marks]

- On the provided graphene lattice (Fig. 7), Martini beads are placed such that each bead overlays four carbon atoms, forming a coarse-grained lattice that perfectly superimposes the real structure without voids or defects. To do so, there are several ways and each of them are correct answer.

**Marking Criteria:** If students are able to specify any of the diagram as given in the Fig.7 give full marks.

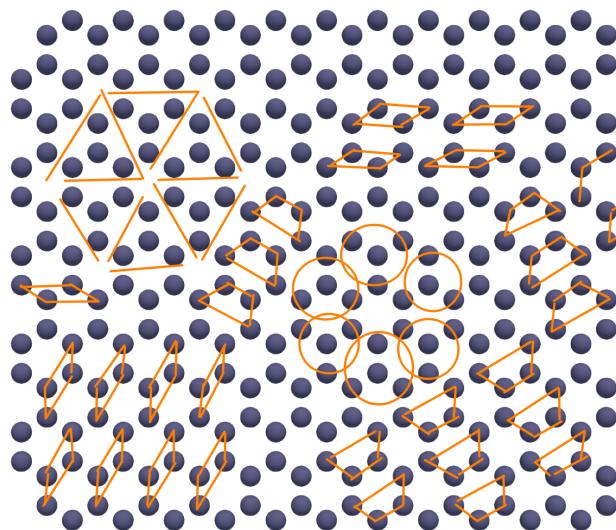


Figure 7: Graphene sheet with coarse grained lattice geometry, where each closed curve or atoms within the curve, represents a single Martini carbon atom.

[2.5 marks]