2. Molecular Dynamics: Modelling

November 8, 2010

Overview

Pair Potentials and Forces

Multi-Centered Molecules

2.1. Pair Potentials and Forces

Question: What indicates a high attraction force between two bodies?

a) a steep descent of the potential,

b) a steep ascent of the potential,

c) a high positive value of the potential,

d) a high negative value of the potential,

e) a slow descent of the potential,

f) a slow ascent of the potential.

Remark: As can be seen from the examples of last tutorial, negative forces are attraction forces and positive forces are repulsion forces.

Answer: b) If there's a steep ascent, there is a strong negative force according to $F = -\nabla U \Rightarrow$ high attraction.

Pair Potentials and Forces

Name	potential	force	attractive(-) / repulsive(+)
Hard Sphere	$\infty \quad \forall r \leq d$ $0 \quad \forall r > d$	$0 \quad r \neq d$ $\infty \quad r = d$	+
Soft Sphere	$\epsilon \cdot \left(\frac{\sigma}{r}\right)^n$	$\frac{n \cdot \epsilon}{r} \cdot \left(\frac{\sigma}{r}\right)^n$	+
Van der Waals	$-4\epsilon \cdot \left(\frac{\sigma}{r}\right)^6$	$\frac{-24\epsilon}{r} \cdot \left(\frac{\sigma}{r}\right)^6$	-
Lennard-Jones-12-6	$4\epsilon \cdot \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right)$	$\frac{24\epsilon}{r} \cdot \left(2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right)$	+ -

Pair Potentials and Forces – Homework Exercise

Example: Softsphere-, Van-der-Waals- and Lennard-Jones-Potential for Helium (He)

Helium is an inert gas, so it can be modelled very well with the single-center Lennard-Jones potential with parameters

- $\epsilon = 10.2$
- $\sigma = 2.28$

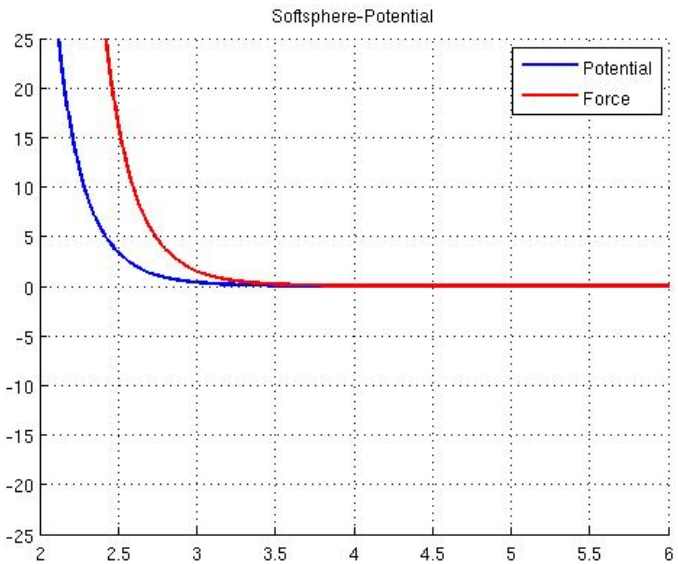

Figure: Softsphere-Potential

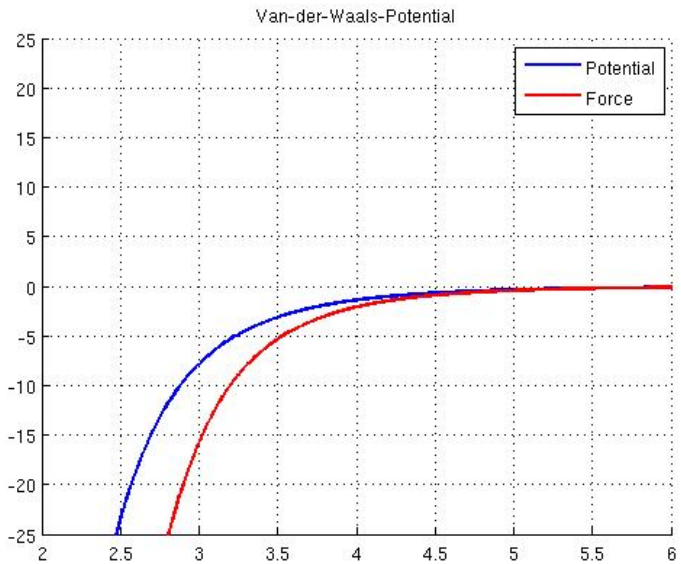

Figure: Van-der-Waals-Potential

Helium is an inert gas, so it can be modelled very well with the single-center Lennard-Jones potential with parameters

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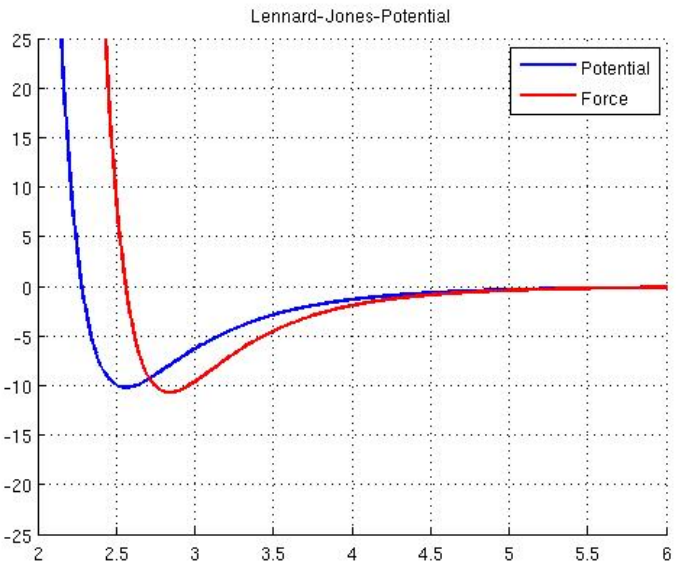
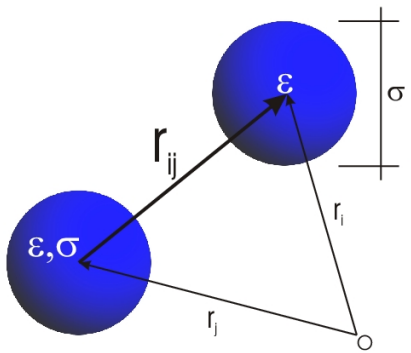


Figure: Lennard-Jones-Potential

- Hard-sphere model not integratable
- Differences: model repulsive and / or attractive potentials
- All potentials decrease quickly $\Rightarrow$ so called short-range potentials (decrease faster in r than $\frac{1}{r^d}$ (d: Dimension)

2.2. Multi-Centered Molecules

- Up to now: assumption, that molecules are spheres and can be modelled by one Lennard-Jones-Center
- sensible for inert gases (He, Ar, Kr, etc...), Methan (CH_4)
- Force on molecule i: $\vec{F}_i = \sum_{j \neq i} \vec{F}_{ij}$



But how about elongate molecules (e.g. Ethan(C_2H_6), Carbon-Dioxyd (CO_2))?