Title

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Todo list

Chapter 1

Theoretical exercises

1.1 Exercise 1

opgaven maken

1.2 Exercise 2

1.2.1 a

$$U = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]. \tag{1.2.1}$$

Take the derivative to r and put to zero for $r = r_{\text{min}}$

$$\left. \frac{\partial U}{\partial r} \right|_{r = r_{\text{min}}} = 4\varepsilon \left[-12 \frac{\sigma^{12}}{r_{\text{min}}^{13}} + 6 \frac{\sigma^{6}}{r_{\text{min}}^{7}} \right] = 0. \tag{1.2.2}$$

This solves to

$$r_{\text{min}} = \sqrt[6]{2}\sigma. \tag{1.2.3}$$

Putting this in U gives

$$U\left(r = r_{\text{min}}\right) = -\varepsilon. \tag{1.2.4}$$

1.2.2 b

D_e is the depth of the potential well. A Taylor-expansion of the potential around $l = l_0$ gives

$$v(l) = D_e \left[1 - \exp\left(-a(l - l_0)\right)\right]^2 \tag{1.2.5a}$$

$$\approx a^2 D_e (l - l_0)^2 + \mathcal{O}\left((l - l_0)^3\right). \tag{1.2.5b}$$

So at small deviations from l_0 the Morse potential is approximately equal to a harmonic potential $v(l) = k/2(l - l_0)^2$ with $k = 2a^2 D_e$. At distances away from the equilibrium the Morse potential deviates from the harmonic potential as the Morse potential approaches the potential depth D_e asymptotically.

Figuur van morse potential, taylor series en harmonic unit erop zetten

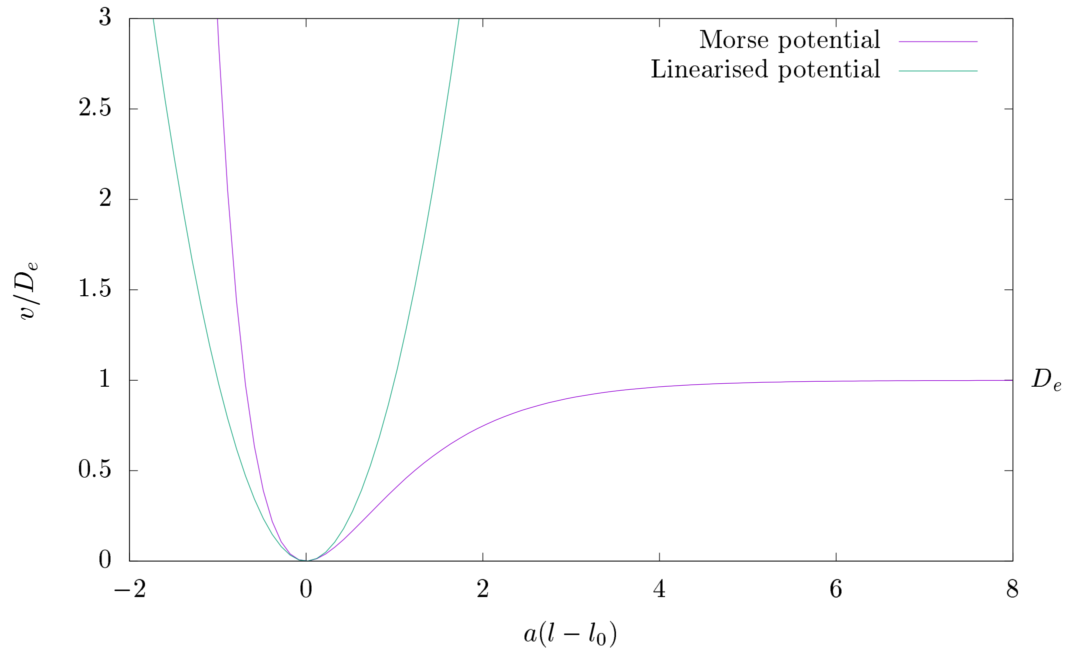


Figure 1.1

1.3 Exercise 3

The characteristic frequency ω of a harmonic spring with two masses is given by (?, ?)

$$\omega = \sqrt{\frac{k}{\mu}} \tag{1.3.1}$$

with k the spring constant and $\mu = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)$ the reduced mass. $1\,\mathrm{N/m} = 1.4393\,\mathrm{kcal\,mol^{-1}\,\AA^{-2}}$

frequencies door rekenen en gebruiken omega = c*golfgetal

1.4 Exercise 4

In a N dimensions the amount of periodic images is given by $3^N - 1$.

beetje uitleg geven

Chapter 2

Molecular Dynamics of a Simple Liquid

choose 1 of the master exercises

2.1 Exercise 1

maken, mass: special == 1 -> mass = 1, special != 1 –> distribution 1

2.2 Exercise 2

2.2.1 a

1.2 is voorbij cut-off, no repulsion when r>rmin

2.2.2 b

maken

2.3 Exercise 3

2.3.1 a

slides

2.3.2 b

T = eps/kb, getallen invullen, slides, p = eps/sigma$\hat{3}$

2.3.3 c

sigma/characteristic time

2.4 Exercises 4

sommatie van impulsen moet 0 zijn, Vcm = sum(mi vi)/sum(mi), vi = vi - Vcm, geimplementeerd in loop starting at r. 235.

2.5 Exercise 5

2.5.1 a

Trivial

2.5.2 b

N*(N-1)/2

2.6 Exercise 6

r. 348 ff

2.7 Exercise 7

2.7.1 a

position: use L MOD R such that 0<R<L

2.7.2 b

26 (3N̂-1)

2.7.3 c

interaction: use L MOD R such that -L/2<R<L/2 for each of the coordinates separately

2.8 Problem 1

2.9 Problem 2

2.10 Problem 3

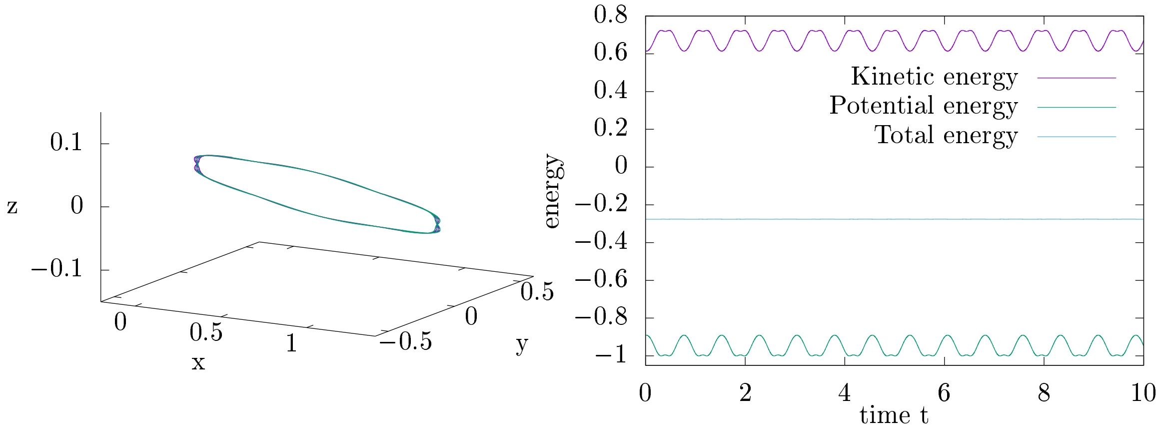


Figure 2.1

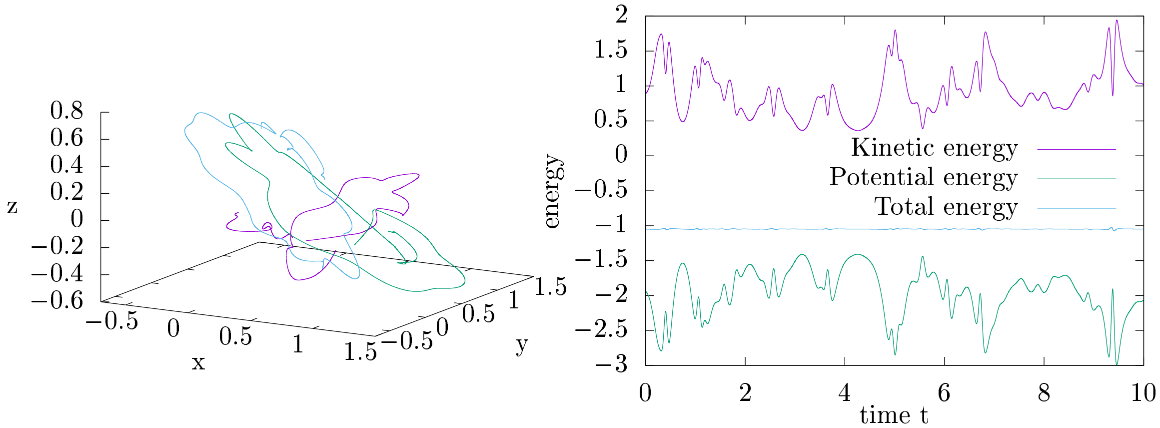


Figure 2.2

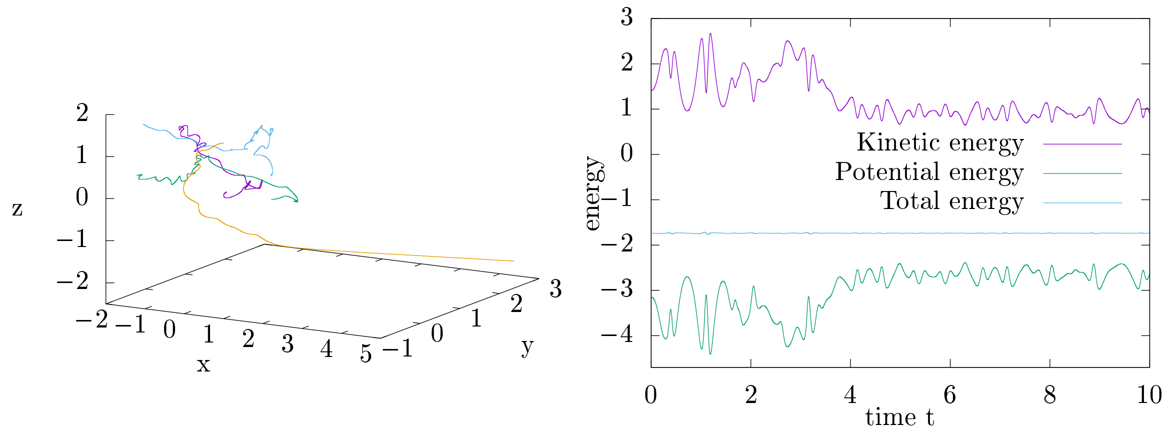


Figure 2.3

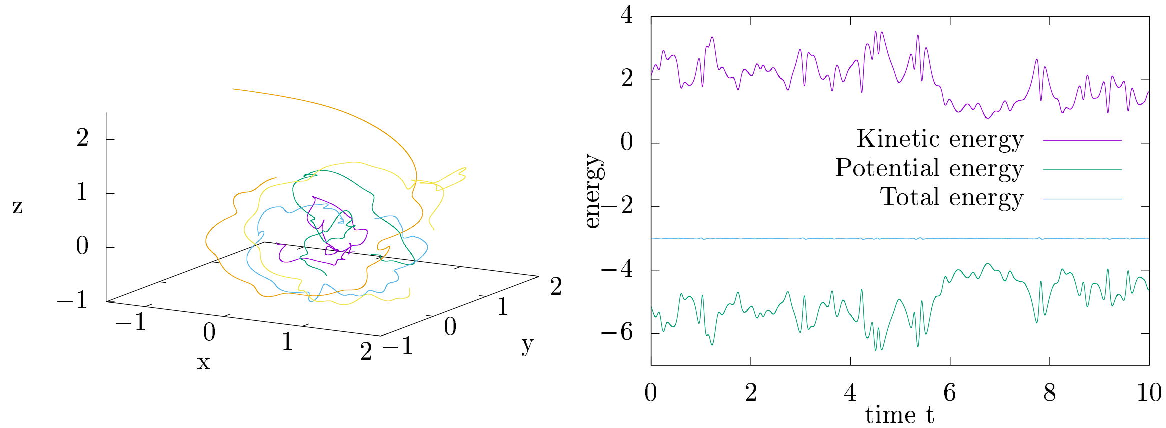
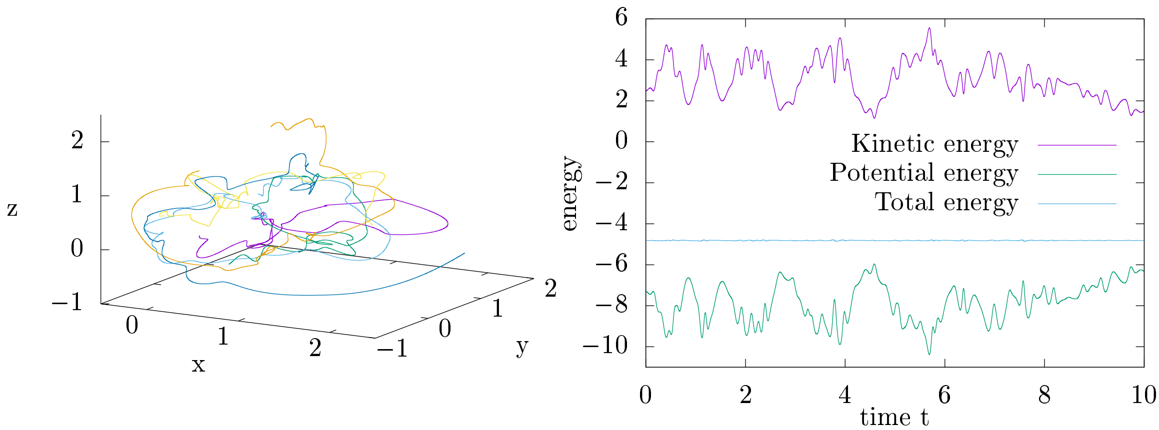


Figure 2.4



z
x
y
energy
time t
Kinetic energy
Potential energy
Total energy

Figure 2.5