NB: The graded, first version of the report must be returned if you hand in a second time!

H1b: MD simulation – dynamic properties

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November 22, 2018

Task №	Points	Avail. points
Σ		

Introduction

Already in antiquity people studied the effect of particles impinging on other particles. Since then the art has developed ... (*If you like to do so, you may take the opportunity to put the methods in a wider perspective here.*) Here is a random reference.[1]

Task 1

We determined the theoretical lattice parameter ....

Figure 2 shows the potential energy as a function of the lattice parameter. We used a quadratic fit to find the minimum energy, and obtained $V_{\text{eq}} \approx 65.38\,\text{Å}^3$. This corresponds to the equilibrium lattice parameter $a_{\text{eq}} \approx 4.029\,\text{Å}$ at 0 K, which we took as the initial lattice parameter for the following tasks.

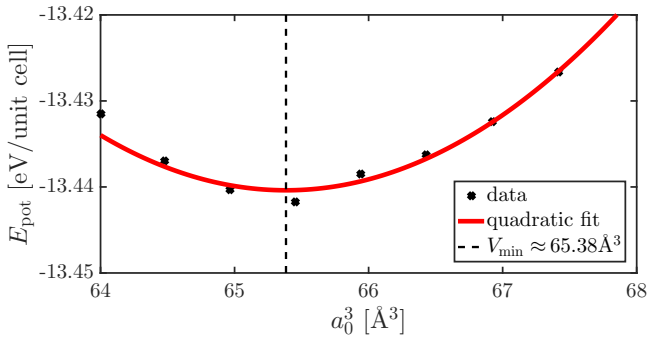

Figure 1: The potential energy per unit cell for aluminum as a function of the lattice parameter cubed.

We find that figure 2 looks similar to the figure 1 in the homework problem file.

Task 5

Equation (82) in MD lecture notes:

$$\Delta_{\text{MSD}}(t) = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt' \frac{1}{N_{\text{atoms}}} \sum_{i=0}^{N_{\text{atoms}}-1} [\mathbf{r}_i(t+t') - \mathbf{r}_i(t')]^2 \tag{1}$$

$$\Rightarrow$$

$$\Delta_{\text{MSD}}(t_k) \approx \frac{1}{N_T - k} \frac{1}{N_{\text{atoms}}} \sum_{j=0}^{N_T-k-1} \sum_{i=0}^{N_{\text{atoms}}-1} \left[\mathbf{r}_i(t_{k+j}) - \mathbf{r}_i(t_j)\right]^2 \tag{2}$$

To determine M, we used mean of ... for t ¿ ...

Task 7

What we did

We calculated the discrete auto-correlation function similarly to the MSD,

$$\Phi_j = \frac{1}{N-j} \sum_{i=0}^{N-j-1} \left\langle v_{i+j} v_i \right\rangle, \tag{3}$$

where $j = 0, 1, \ldots, N-1$ and the average is taken over all atoms. We then preceded to numerically approximate the integral

$$\hat{\Phi}(f) = 2\int_0^\infty \mathrm{d}t\ \Phi(t)\cos(2\pi f t) \approx 2\int_0^{T_s} \mathrm{d}t\ \Phi(t)\cos(2\pi f t) \tag{4}$$

using a trapeziodal method in MATLAB, with a frequency range $f = 0$ to $f = 1/(2\Delta t) = f_{\text{Nyqvist}}$, and frequency steps $\Delta f = 1/T_s$, where T_s is a time at about half the simulation end time. This is to avoid including noisy data in $\Phi(t)$ at later times, where the statistics are poor.

We then calculated the powerspectrum according to

$$\begin{aligned}\hat{P}(\omega) &= \lim_{T\to\infty} \frac{1}{T} \left\langle \left| \int_0^T \mathrm{d}t \; v(t) \mathrm{e}^{\mathrm{i}\omega t} \right|^2 \right\rangle \\ &\approx \frac{1}{T} \left\langle \left| \int_0^T \mathrm{d}t \; v(t) \mathrm{e}^{\mathrm{i}\omega t} \right|^2 \right\rangle \\ \implies \quad \hat{P}_k &= \frac{1}{T} \left\langle \left| \frac{T}{N} \sum_{i=0}^{N-1} v_i \exp\left(\mathrm{i}2\pi \frac{ik}{N} \right) \right|^2 \right\rangle = \frac{T}{N} \left\langle |\hat{\boldsymbol{v}}_k|^2 \right\rangle \end{aligned} \tag{5}$$

where the averages is taken over all atoms, and

$$\hat{\boldsymbol{v}}_k = \sqrt{N} \sum_{i=0}^{N-1} \boldsymbol{v}_i \exp\left(\mathrm{i}2\pi \frac{ik}{N} \right) \tag{6}$$

is the discrete Fourier transform of v_i.

When we compare $\hat{\Phi}_k$ and $\hat{P}_k$ in Figure **??**, we find that they are very similar, as, indeed, they should be acording to the Wiener-Khinthchine theorem.

Problem 1

As a starting point we first look at scattering from a hard-sphere potential. We also consider the Lennard–Jones potential, which is depicted in Figure **??**. (*Always refer to Figures in the text.*)

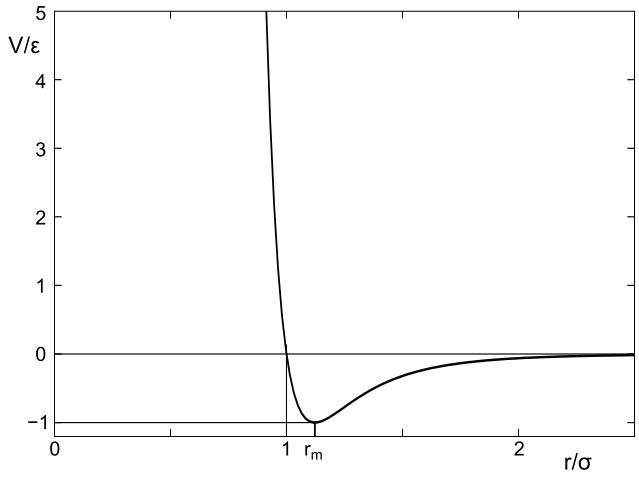

Figure 2: The Lennard–Jones potential. Make sure you label and have units on all axes! Also make sure that labels etc. are legible and that, if you print in black and white, that you use different line styles when required to differentiate between curves. In MATLAB you can export any figure to an .eps file from File → Export... in the Figure window.

Problem 2

In the following we give an example of how to produce a table. Use the code for Table 1 as a template.

Table 1: A dummy table

Col. 1	Col. 2	Col. 3
the	quick	brown
fox	jumps	over
the	lazy	dog

Problem 3

If you find some part of the code particularly interesting you may include it in the text, otherwise it should be included in the appedix. If you do want to include code the following commands will print the text directly, with no LaTeX commands executed:

```
% Hello world ten times in MATLAB
for i = 1 : 10
  fprintf('Hello world %d!\n',i);
end
```

```
# Hello world ten times in Python
for i in range(10):
  print 'Hello world %d!' % i
```

Problem 4

At some point it may be appropriate to include equations. It is done in the following way:

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{7}$$

Do number and reference all your equations.

Concluding discussion

Use your favourite flavor of LaTeX to compile the file:

```
xelatex template.tex
pdflatex template.tex
latex template.tex
```

should all work. If you use `pdflatex` or `xelatex`, included figures need to be in `pdf`, `jpg`, or `png` format. If you want to include eps figures, you can easily convert them to `pdf` using the command

```
ps2pdf -dEPSCrop figure.eps figure.pdf
```

References

[1] Leslie Lamport, *LaTeX: A Document Preparation System*. Addison Wesley, Massachusetts, 2nd Edition, 1994.

A Source Code

Include all source code here in the appendix. Keep the code formatting clean, use indentation, and comment your code to make it easy to understand. Also, break lines that are too long. (Keep them under 80 characters!)