Homework and Solutions

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Chapter 2

Homework 2.1

Consider a one-dimensional harmonic oscillator of mass, *m*, and spring constant of *k* that follows Hooke's law, $F = -kx$, in an isolated system (E = const.). Then the Newton's second law becomes the second-order ordinary differential equation as:

$$a(t) = -\frac{k}{m}x(t)$$

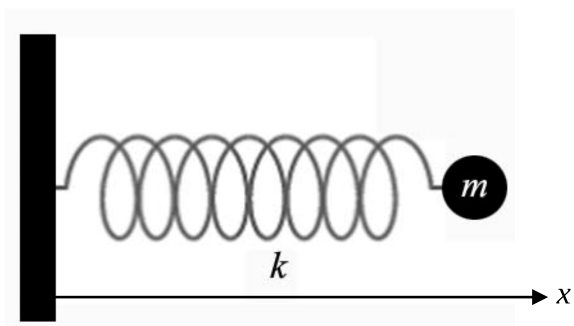
Let us assume that the spring is fixed at one side and is ideal with zero mass. Given oscillator frequency of $\omega = (k/m)^{1/2} = 1$ and initial conditions of $x_0 = 5$ and $v_0 = 0$, find and discuss the following:

- Analytical solution for ball positions with time

- Numerical solution for ball positions with time by taking the first two terms in the Taylor series expansion (the first-order Euler method) with $\Delta t = 0.2$ for 10 timesteps
- Compare the two methods above on a position-time plot and discuss what will happen if the numerical calculation proceeds further for more timesteps and how to improve its accuracy
- Write down the potential expression for the system

Solution 2.1

Model



An ideal ball-spring system in one dimension.

Analytical solution:

$$F = -kx = ma\,,\ 0 = -kx = ma \text{ at equilibrium}$$

This second-order differential equation has the general solutions as:

$$v(t) = v_0 \cos(\omega t) - \omega x_0 \sin(\omega t) = -5\sin(t)$$

$$x(t) = x_0 \cos(\omega t) + \frac{v_0}{\omega}\sin(\omega t) = 5\cos(t)$$

Numerical solution:

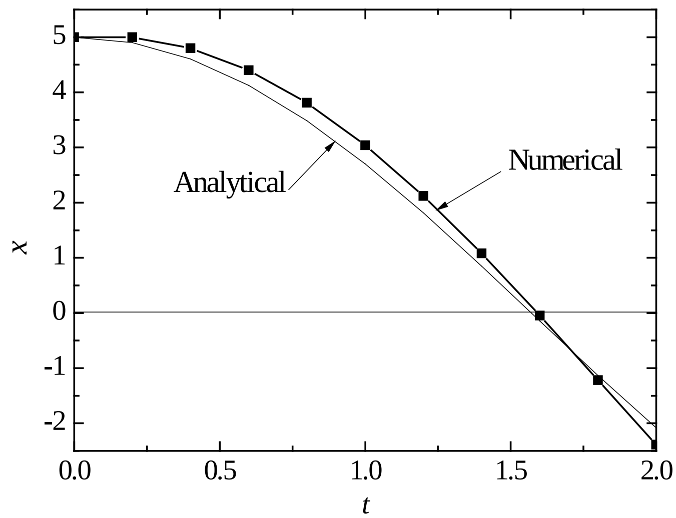
$$v(t+\Delta t) = v(0) + a(0)\Delta t\ ,\ \ldots..$$

$$x(t+\Delta t) = x(0) + v(0)\Delta t\ ,\ \ldots..$$

$$-kx = ma\ ,\ \ k/m = 1 \rightarrow\ a = -x$$

Numerical calculation for one-dimensional harmonic oscillator

t	Δt	x	$a=-x$	v
0.0	-	$x_0 = 5$	a_0 = -5	$v_0 = 0$
0.2	0.2	$x_1 = x_0 + v_0\Delta t$ = 5 + 0 = 5	a_1 = -5	$v_1 = v_0 + a_0\Delta t$ = 0 - 1 = -1
0.4	0.2	$x_2 = x_1 + v_1\Delta t$ = 5 - 0.2 = 4.8	a_2 = -4.8	$v_2 = v_1 + a_1\Delta t$ = -1 - 1 = -2
0.6	0.2	$x_3 = x_2 + v_2\Delta t$ = 4.8 - 0.4 = 4.4	a_3 = -4.4	$v_3 = v_2 + a_2\Delta t$ = -2 - 0.96 = -2.96
0.8	0.2	$x_4 = x_3 + v_3\Delta t$ = 4.4 - 0.592 = 3.808	a_4 = -3.808	$v_4 = v_3 + a_3\Delta t$ = -2.96 - 0.88 = -3.84
1.0	0.2	$x_5 = x_4 + v_4\Delta t$ = 3.808 - 3.84(0.2) = 3.04	a_5 = -3.04	$v_5 = v_4 + a_4\Delta t$ = -3.84 - 3.808(0.2)= -4.6016
1.2	0.2	$x_6 = x_5 + v_5\Delta t$ = 3.04 - 4.6016(0.2) = 2.12	a_6 = -2.12	$v_6 = v_5 + a_5\Delta t$ = -4.6016 - 3.04(0.2)= -5.2096
1.4	0.2	$x_7 = x_6 + v_6\Delta t$ =2.11968 - 5.2096(0.2) = 1.07776	a_7 = -1.07776	$v_7 = v_6 + a_6\Delta t$ = -5.2096 - 1.07776(0.2) =-5.63354
1.6	0.2	$x_8 = x_7 + v_7\Delta t$ = =1.07776 - 5.63354(0.2) = -0.04895	a_8 = 0.04895	$v_8 = v_7 + a_7\Delta t$ = -5.63354 - 1.07776(0.2) = -5.84909
1.8	0.2	$x_9 = x_8 + v_8\Delta t$ =-0.04895 - 5.84909(0.2) =-1.21876	a_9 = 1.21876	$v_9 = v_8 + a_8\Delta t$ = -5.84909 + 0.04895(0.2) = -5.8393
2.0	0.2	$x_{10}= x_9 + v_9\Delta t$ = -1.21876 - 5.8393(0.2) = -2.38662	a_{10} = 2.38662	$v_{10} = v_9 + a_9\Delta t$ = -5.8393 + 1.21876(0.2) = -5.59555



Comparison between the analytical and the numerical solutions

for a one-dimensional harmonic oscillator.

Comparison

As the numerical calculation proceeds further for more timesteps, errors due to the truncation in the Taylor series expansion will accumulate (always overshoot the analytical curve since we are taking the slope on the curve). To improve accuracy, higher-order terms in Taylor series expansion should be included for the numerical calculation and timestep should be decreased. Of course, these measures will require more computation time. This is a simple demonstration of how the numerical integration works in practice. Better algorithms such as the velocity Verlet, the Gear, etc. can provide values very close to the exact analytical results.

Potential expression

$$F = -kx$$

$$U = -\int F dx = -\int -kx dx = \frac{1}{2}kx^2$$: Parabolic curve

Homework 2.2

A typical potential curve for most materials looks like the one in Figure 2.5. Referring the curve, explain why most materials expand with increasing temperature.

Solution 2.2

Thermal expansion takes place because the potential curve with lattice constants is asymmetric. When atoms are thermally agitated and vibrate from their equilibrium positions, they face stronger repulsive force closer to each other (to the left in Figure 2.5) because of the Pauli Exclusion Principle. Thus they vibrate less toward left and more toward right and atomic mean positions will shift to right causing thermal expansion.

Homework 2.3

If we increase the average velocities of atoms in a system by two times, by how many times the corresponding temperature will increase in a MD run?

Solution 2.3

$$v_{new} = 2v_{old} = v_{old}\left(\frac{T'}{T}\right)^{1/2}, \quad \therefore T' = 4T$$

Homework 2.4

Predict the positions of the first peak in a diagram of the radial distribution function obtained after a MD run for a simple cubic solid and an FCC solid.

Solution 2.4

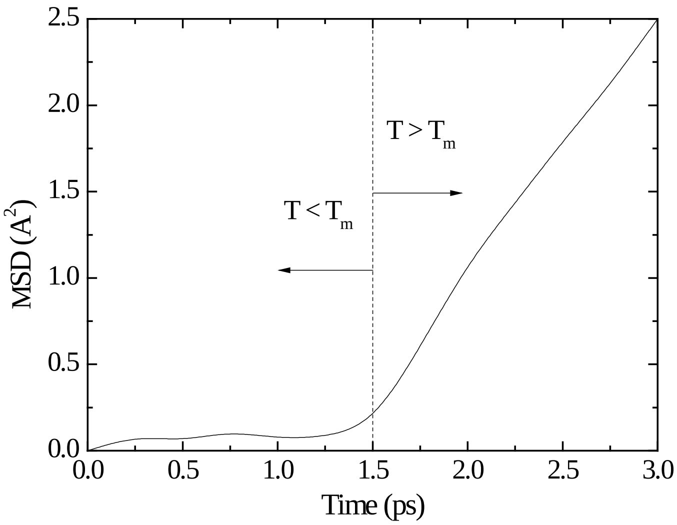
A simple cubic solid will make a peak at equilibrium lattice parameter, a_0, by 6 neighboring atoms. An FCC solid will make a peak at $\sqrt{2}a_0/2$ by 12 neighboring atoms.

Homework 2.5

Draw the general features of the mean square displacement (MSD) function with simulation time when a crystalline solid is melted and becomes a liquid during a MD run and explain its behavior.

Solution 2.5

The following figure schematically shows the general feature of MSD during melting of a solid. At temperature lower than the melting point, the MSD fluctuates slightly but remains at very lower values. When temperature is increased higher than the melting point, melting occurs and the MSD linearly increases with time. Note that atoms in liquid phase no longer stay on their lattice positions. The slope represents the diffusion coefficient, *D* for the liquid.



MSD curve with simulation time when a crystalline solid is melted.