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E1 Coupled harmonic oscillators

Oscillatory motion is common in physics. Here we will consider coupled harmonic oscillators. Fourier transformation of the time-dependence can be used to reveal the vibrational character of the motion and normal modes provide the conceptual framework for understanding the oscillatory motion.

You will be asked to solve a few computational problems. The first three is about the discrete Fourier transform and you will make use of the fast Fourier transform (FFT) technique, a computationally very efficient way of performing discrete Fourier transformations. In the fourth problem you will determine the vibrational frequencies for a triatomic linear molecule, carbondioxid, by solving Newton's equation of motion using the velocity Verlet algorithm. Finally, as an extra exercise you are asked to determine the normal modes for the triatomic linear molecule.

You should solve the problems using the c language. For your convenience you can find a set of programs and README files at the homepage for the course. We provide plotting programs both using matlab and python.

1 Coupled harmonic oscillators

Consider three harmonically coupled particles. The mass of each particle is m and the springs are identical with a spring constant κ. We denote the displacements from the equilibrium positions with u_i, i=1,2,3 and v_i for the corresponding velocities. The system is anchored to the walls and we introduce the coordinates u_0 and u_4 with $u_0 = u_4 = 0$.

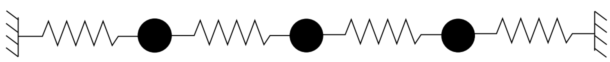

Figure 1: System of three coupled harmonic oscillators with fixed boundary conditions.

The Hamiltonian for the system is given by

$$\mathcal{H} = \sum_{i=1}^{3} \frac{mv_i^2}{2} + \sum_{i=0}^{3} \frac{\kappa}{2}(u_{i+1} - u_i)^2$$

and the corresponding equation of motion can be written as

$$m\frac{d^2}{dt^2}u_i(t) = \kappa \left[u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)\right] , \quad i = 1, 2, 3$$

This is a set of three coupled second order ordinary differential equations. These can be solved using a stepping procedure in time. One popular method is the velocity Verlet algorithm

$$u_i(t+\Delta t) = u_i(t) + v_i(t)\Delta t + \frac{1}{2}a_i(t)\Delta t^2$$
$$v_i(t+\Delta t) = v_i(t) + \frac{1}{2}[a_i(t) + a_i(t+\Delta t)]\Delta t$$

where Δt is the timestep and $a_i = d^2q_i/dt^2$ is the acceleration for particle i. In this case we have

$$a_i(t) = \frac{\kappa}{m}\,[u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)]$$

One step in the velocity Verlet algorithm can be coded in an efficient way as

$$v_i(t+\Delta t/2) = v_i(t) + \frac{1}{2}a_i(t)\Delta t$$
$$u_i(t+\Delta t) = u_i(t) + v_i(t+\Delta t/2)\Delta t$$
`calculate new accelerations/forces`
$$v_i(t+\Delta t) = v_i(t+\Delta t/2) + \frac{1}{2}a_i(t+\Delta t)\Delta t$$

which only requires the storage of positions and velocities at one time point.

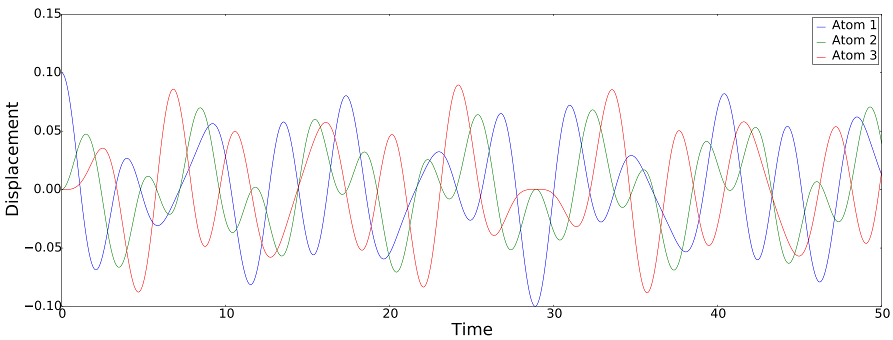

Figure 2: The time-dependent displacements for the three particle system.

In Fig. 2 we show the result for the position of the three different particles as function of time. We gave then used the initial conditions $q_1(0) = 0.1$ and $q_2(0) = q_3(0) = v_1(0) = v_2(0) = v_3(0) = 0$. In Fig. 3 the corresponding time-dependence of the kinetic and potential energies are shown as well as the sum, the total energy. It can be seen that the total energy is very well conserved. We also show the corresponding power spectra (see appendix A) in Fig. 4. Three clear peaks for positive and negative frequencies are seen. These corresponds to the normal mode frequencies (see below). The data in Figs 2 - 4 are obtained using the c program Task 4, which you find at the homepage.

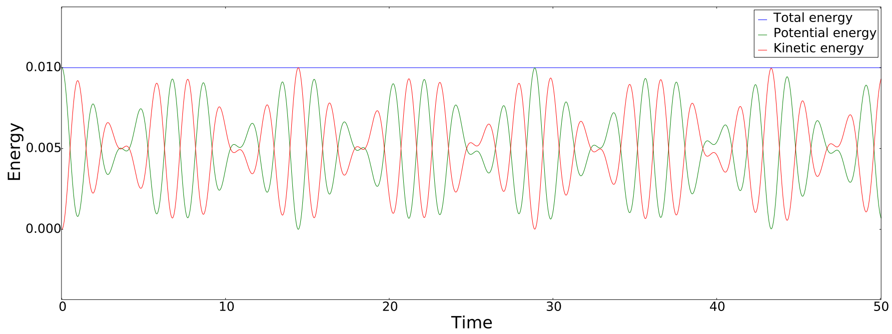

Figure 3: The time-dependence of the potential, kinetic and total energies for the three particle system.

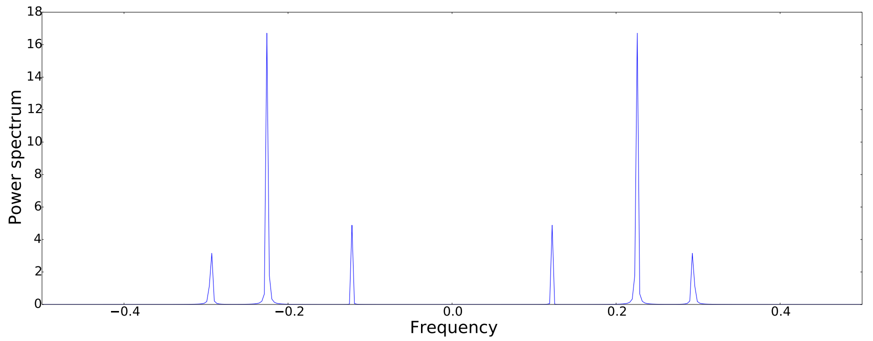

Figure 4: The power spectrum for the three particle system.

Task

To get used to the discrete Fourier transform consider the time-dependent signal

$$h(t) = a \cos (2\pi f t + \phi)$$

Some basic properties of the discrete Fourier transform is given in the appendix A.

1. The program, Task 1, determines the discrete Fourier transform of the above time-dependent signal using a=1, Φ=0, $f = 2$, Δt=0.1, and N=250. and computes the corresponding power spectrum P_n for $n = 0, 1, \ldots, (N-1)$. Run the program and plot the result for $h(t)$ and P_n. Do you understand the spectrum? (0p)

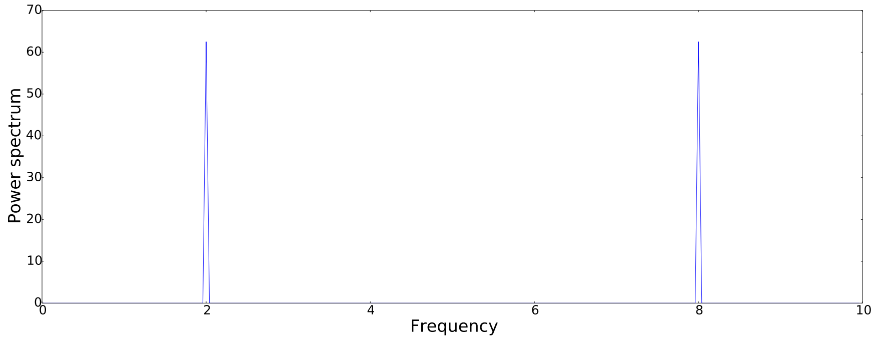

Figure 5: Power spectrum.

2. It is more convenient to plot P_n for $n = N/2, \ldots, (N-1), 0, \ldots, (N/2-1)$. Why? This is done by the program Task 2. Run the program and plot the result for $h(t)$ and P_n. Do you understand the frequency scale on the x-axis. What are the minimum and maximum frequencies? Change to $N = 258$ and $N = 260$, respectively, and plot in both cases $h(t)$ and P_n. Can you comment on your results? (0p)

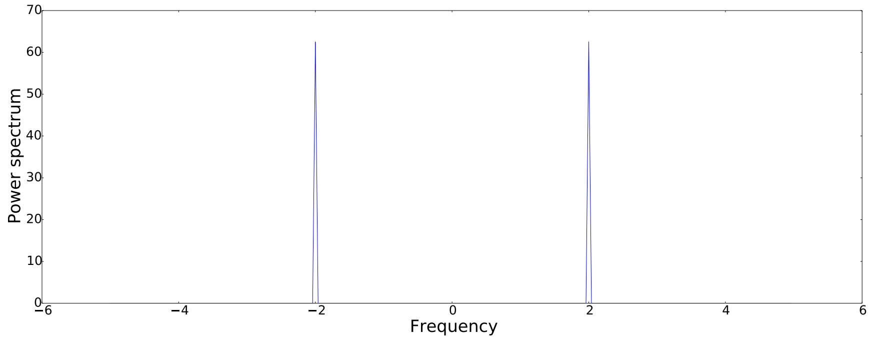

Figure 6: Power spectrum, shifted.

3. Consider now the signal

$$h(t) = a_1 \cos(2\pi f_1 t + \Phi_1) + a_2 \cos(2\pi f_2 t + \Phi_2)$$

with $a_1 = a_2 = 1$, $\Phi_1 = \Phi_2 = 0$, $f_1 = 2$, $f_2 = 6$, and $\Delta t = 0.1$, $N = 250$. Fourier transform $h(t)$ and plot P_n for $n = N/2, \ldots, (N-1), 0, \ldots, (N/2-1)$. Do you understand the result? What is the problem with the present signal $h(t)$. Can you modify the sampling in time domain so that you get a more correct representation of the power spectrum? (1p)

Next consider the motion of a three-particle system with free boundary conditions (see Fig. 7). The two end particles, each of mass m are bound to the central particle, with mass M, with two springs, each with spring constant κ. Consider the motion only in one dimension.

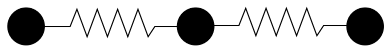

Figure 7: System of three coupled harmonic oscillators with free boundary conditions.

4. Apply the model to the triatomic molecule CO_2. The spring constant for carbondioxid is $\kappa = 1.6$ kN/m. Derive the coupled set of equation of motions and solve them numerically using the velocity Verlet algorithm. Use "metal"-units (see appendix B). Choose an appropriate time-step Δt based on conservation of the total energy. At the home page you find a c program Task 4, that solves this problem using fix boundary conditions. Fourier analyse the trajectories and try to determine the normal mode frequencies. Compare with the experimental data for CO_2. (3p)

2 Normal modes

2.1 Three coupled oscillators

Consider again the three coupled harmonic oscillators in Fig. 1. The Hamiltonian, now expressed in terms of the momenta p_i and coordinates q_i, is

$$\mathcal{H} = \sum_{i=1}^{3} \frac{p_i^2}{2m} + \sum_{i=0}^{3} \frac{\kappa}{2}(q_{i+1} - q_i)^2$$

with the corresponding Hamilton's equation of motion

$$\begin{aligned} \dot{q}_i &\equiv \frac{\partial \mathcal{H}}{\partial p_i} = \frac{p_i}{m} \\ \dot{p}_i &\equiv -\frac{\partial \mathcal{H}}{\partial q_i} = \kappa(q_{i+1} - 2q_i + q_{i-1}) \end{aligned}$$

for $i = 1, 2, 3$. This can also be written on the matrix form

$$\frac{d^2}{dt^2}\mathbf{q}(t) = -\omega_0^2 \, \mathbf{K} \, \mathbf{q}(t)$$

where $\omega_0^2 = \kappa/m$ and

$$\mathbf{K} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$$

is the force constant matrix. If we make the ansatz

$$\mathbf{q}(t) = \mathbf{g} \cos(\omega t + \phi)$$

we get an eigenvalue problem

$$\mathbf{K}\,\mathbf{g} \;=\; \lambda\,\mathbf{g}$$

where $\lambda = \omega^2/\omega_0^2$. The corresponding eigenvalues and normalized eigenvectors are

$$\begin{aligned}
\omega_1 &= \sqrt{2-\sqrt{2}}\,\omega_0 \\
\omega_2 &= \sqrt{2}\,\omega_0 \\
\omega_3 &= \sqrt{2+\sqrt{2}}\,\omega_0
\end{aligned}$$

and

$$\mathbf{g}_1 = \begin{bmatrix} 1/2 \\ 1/\sqrt{2} \\ 1/2 \end{bmatrix} \qquad \mathbf{g}_2 = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{bmatrix} \qquad \mathbf{g}_3 = \begin{bmatrix} 1/2 \\ -1/\sqrt{2} \\ 1/2 \end{bmatrix}$$

respectively. The transformation matrix is then given by

$$\mathbf{G} \equiv [\;\mathbf{g}_1\;\mathbf{g}_2\;\mathbf{g}_3\;] = \begin{bmatrix} 1/2 & 1/\sqrt{2} & 1/2 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/2 & -1/\sqrt{2} & 1/2 \end{bmatrix}$$

This matrix is orthogonal and it diagonalizes the force constant matrix. We can now introduce normal coordinates

$$\mathbf{Q} = \sqrt{m}\;\mathbf{G}^T\;\mathbf{q}$$

with the corresponding inverse relation

$$\mathbf{q} = \frac{1}{\sqrt{m}}\;\mathbf{G}\;\mathbf{Q}$$

and in the same way for the momentum

$$\mathbf{P} = \frac{1}{\sqrt{m}}\;\mathbf{G}^T\;\mathbf{p}$$

and

$$\mathbf{p} = \sqrt{m}\;\mathbf{G}\;\mathbf{P}$$

More explicitly we have

$$\begin{aligned}
Q_1 &= \frac{1}{2}(q_1 + \sqrt{2}q_2 + q_3) \\
Q_2 &= \frac{1}{\sqrt{2}}(q_1 - q_3) \\
Q_3 &= \frac{1}{2}(q_1 - \sqrt{2}q_2 + q_3)
\end{aligned}$$

In matrix form the Hamiltonian can be written as

$$\mathcal{H} = \frac{1}{2m}\mathbf{p}^T\mathbf{p} + \frac{\kappa}{2}\mathbf{q}^T\mathbf{K}\mathbf{q}$$

which can be transformed to

$$\mathcal{H} = \frac{1}{2}\sum_{k=1}^{3}[P_k^2 + \omega_k^2 Q_K^2]$$

and the corresponding equation of motion takes the foorm

$$\frac{d^2}{dt^2}Q_k(t) + \omega_k^2\ Q_k(t) = 0 \quad ; \quad k = 1, 2, 3$$

which explicitly shows that the normal modes are independent modes, uncoupled coordinates. The solution is given by

$$Q_k(t) = Q_k(0)\ \cos\left(\omega_k t\right) + \dot{Q}_k(0)\frac{1}{\omega_k}\ \sin\left(\omega_k t\right)$$

and, hence, the general solution can be written as

$$\mathbf{q}(t) = \frac{1}{\sqrt{m}}\mathbf{G}\mathbf{Q}(t)$$

Task

5. Consider again the three particle system with free boundary conditions in Fig. 7. Assume that the two end particles each have the mass m are bound to the central particle, with mass M, with two springs, each with spring constant κ. Determine analytically the normal mode frequencies. Compare with what you obtained in Task 4. (0p)

2.2 General case - N coupled oscillators

Consider now the general case with N coupled harmonic oscillators

$$\mathcal{H} = \sum_{i=1}^{N}\frac{p_i^2}{2m} + \sum_{i=0}^{N}\frac{\kappa}{2}(q_{i+1} - q_i)^2$$

The transformation matrix is given by

$$G_{ik} = \sqrt{\frac{2}{N+1}}\sin\left(\frac{ik\pi}{N+1}\right)$$

and the eigenfrequencies by

$$\omega_k = 2\sqrt{\frac{\kappa}{m}}\sin\left(\frac{k\pi}{2(N+1)}\right)$$

The transformed Hamiltonian takes the form

$$\mathcal{H} = \frac{1}{2}\sum_{k=1}^{N}[P_k^2 + \omega_k^2 Q_k^2]$$

and the normal modes

$$\begin{aligned} Q_k &= \sqrt{\frac{2}{N+1}}\sum_{i=1}^{N}\sqrt{m}q_i \sin\left(\frac{ik\pi}{N+1}\right) \\ q_i &= \sqrt{\frac{2}{N+1}}\sum_{k=1}^{N}\frac{Q_k}{\sqrt{m}} \sin\left(\frac{ik\pi}{N+1}\right) \end{aligned}$$

and

$$\begin{aligned} P_k &= \sqrt{\frac{2}{N+1}}\sum_{i=1}^{N}\frac{p_i}{\sqrt{m}} \sin\left(\frac{ik\pi}{N+1}\right) \\ p_i &= \sqrt{\frac{2}{N+1}}\sum_{k=1}^{N}\sqrt{m}P_k \sin\left(\frac{ik\pi}{N+1}\right) \end{aligned}$$

A Discrete Fourier transform

Consider a time-dependent signal $h(t)$ and discretize it according to

$$h_k = h(t_k) \ , \quad t_k = k\Delta t \ , \quad k = 0, 1, \ldots, (N-1)$$

The corresponding discrete Fourier transform is given by

$$H_n = \sum_{k=0}^{N-1} h_k \ e^{-2\pi ikn/N} \ , \quad n = 0, 1, \ldots, (N-1)$$

where the spacing in frequency is

$$\Delta f = \frac{1}{N\Delta t}$$

The discrete inverse transform is given by

$$h_k = \frac{1}{N}\sum_{n=0}^{N-1} H_n \ e^{2\pi ikn/N} \ , \quad k = 0, 1, \ldots, (N-1)$$

and the discrete form of the Parseval's theorem is

$$\sum_{k=0}^{N-1} \mid h_k \mid^2 = \frac{1}{N}\sum_{n=0}^{N-1} \mid H_n \mid^2$$

We define the power spectrum according to

$$P_n = \frac{1}{N} \mid H_n \mid^2$$

An important frequency is the so called Nyquist frequency

$$f_c \equiv \frac{1}{2\Delta t}$$

Only time signals that are bandwidth limited to less than the Nyquist frequency are correctly described by the corresponding power spectrum.

B System of units

The basic units in the SI system for length (L), mass (M), and time (T) are

L:	1 meter (m)
M:	1 kilogram (kg)
T:	1 second (s)

The units for *e.g.* frequency and energy are then derived from these: Hertz (1 Hz = 1 s^{-1}) and Joule (1 J = 1 kgm^2/s^2), respectively, and cannot be chosen independently.

In computational studies it is often convenient to use other system of units, which are more appropriate for the considered length- and time-scales. In atomic scale simulations the so called "metal"-units[1] are often used. The starting point is the basic units

L:	1 Ångström (Å)
T:	1 picosecond (ps)
E:	1 electron volt (eV)

The unit for mass (M) can then not be chosen independently but is given by

$$\mathrm{M} = \mathrm{E}\mathrm{T}^2\mathrm{L}^{-2}$$

or

$$\mathrm{M:}\ \ 1\mathrm{eV}\,\frac{(1\mathrm{ps})^2}{(1\text{Å})^2} = 1.602 \cdot 10^{-23}\ \mathrm{kg} = 9649\ \mathrm{u} = \frac{\mathrm{u}}{1.0364 \cdot 10^{-4}}$$

where u is the atomic mass unit. In these units the mass m of a oxygen atom is

$$m = 15.9994 \cdot 1.0364 \cdot 10^{-4} = 1.658 \cdot 10^{-3}$$

[1]see http://lammps.sandia.gov/doc/units.html)