THE VIBRATIONS OF MOLECULES II
THE CARBON DIOXIDE MOLECULE

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This is the computational document, co2run.mcd. You should have the written instructions for this program at hand while you are using the program. The written instructions are in a file called co2ins.mcd (a Mathcad document).

$m_1 := 16 \quad m_2 := 12 \quad k := 200$

First set the values of the atomic weights (g/mole) and the force constant k.

$$B_{11} := \frac{1}{2}\cdot m_1 \cdot \frac{(m_1 + m_2)}{(m_2 + 2\cdot m_1)} \qquad B_{12} := \frac{m_1^2}{m_2 + 2\cdot m_1}$$

Next, calculate the quantities to be used in the differential equation.

$$d_1 := B_{12} - \frac{4\cdot B_{11}^2}{B_{12}} \qquad d_2 := 2\cdot B_{11} - \frac{B_{12}^2}{2\cdot B_{11}}$$

$$e_1 := \frac{2\cdot k\cdot B_{11}}{B_{12}} \qquad e_2 := \frac{k\cdot B_{12}}{2\cdot B_{11}}$$

d_1, d_2, e_1 and e_2 are groups of constants

$d_1 = -12 \quad d_2 = 6.857 \quad e_1 = 350 \quad e_2 = 114.286$

$$Q := \begin{bmatrix} 2 \\ 0 \\ 0 \\ 3 \end{bmatrix}$$

This column vector contains the initial values of the coordinates and velocities in the order:

initial Q_1

initial Q_1' (Derivative)

initial Q_2

initial Q_2' (Derivative)

$$D(t,Q) := \begin{bmatrix} Q_1 \\ \frac{e_1 \cdot Q_0 - k \cdot Q_2}{d_1} \\ Q_3 \\ \frac{e_2 \cdot Q_0 - k \cdot Q_2}{d_2} \end{bmatrix}$$

This vector describes the differential equation to the Mathcad software in this order

Q_1' (First Derivative)

Q_1'' (Second Derivative)

Q_2' (First Derivative)

Q_2'' (Second Derivative)

Since we do not know the first derivatives (Q_i') we put in Q1 and Q3 in their places. The second derivative expressions (Q_i'') are those given in the instructional document.

$z := rkfixed(Q, 0, 100, 2048, D)$

The rkfixed Mathcad function solves the differential equation numerically at a series of points, time in our case.

$z =$

	0	1	2	3	4
0	0	2	0	0	3
1	0.049	1.932	-2.746	0.184	4.486
2	0.098	1.738	-5.126	0.431	5.555
3	0.146	1.441	-6.934	0.717	6.04
4	0.195	1.072	-8.026	1.01	5.835
5	0.244	0.67	-8.336	1.275	4.913
6	0.293	0.271	-7.878	1.479	3.324
7	0.342	-0.088	-6.745	1.591	1.197
8	0.391	-0.379	-5.1	1.59	-1.278
9	0.439	-0.582	-3.154	1.464	-3.865
10	0.488	-0.686	-1.142	1.215	-6.309
11	0.537	-0.696	0.702	0.854	-8.362
12	0.586	-0.624	2.168	0.408	-9.811

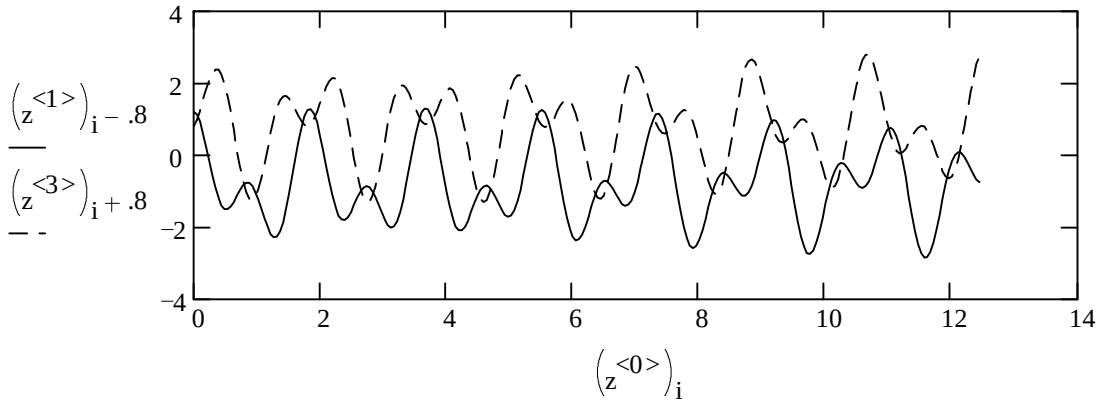
The numerical solution appears in a table, see left, with the following columns:

0 time
1 Q (Position)
2 Q_1' (Derivative)
3 Q_2 (Position)
4 Q_2' (Derivative)

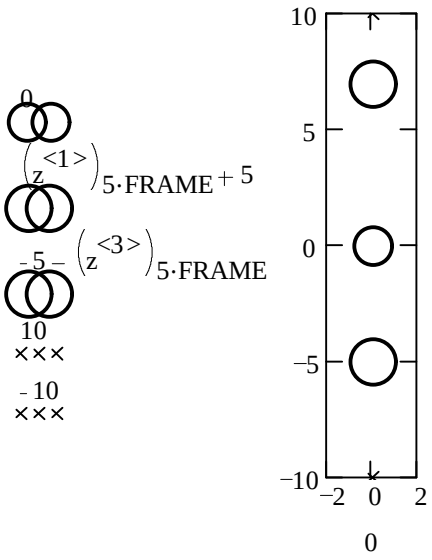
We now plot the first 256 points. The upper plot is Q_1 and the lower plot is Q_2.

$i := 0..255$ $S_i := \left(z^{<1>}\right)_i$

S_i is used below in the Fourier transform of Q_1



The chart below can be animated. See the instructions.



The graph below shows the Fourier transform of Q_1.

$c := fft(S)$ $N := last(c)$ $N := 128$ $j := 0..N$