Introduction to Computational Physics

Matthias Jamin

(To be discussed on Friday, 18.7. and Monday, 21.7.)

EXERCISE 10.1: **Quantum Mechanical Anharmonic Oscillator**

Since the wave function is known to vanish exponentially at large $|x|$, it is sufficient to start the integration of the DEQ at a finite x_0. To achieve an accuracy of roughly 10^{-9} for the bound state energies, $x_0 = -6$ is large enough.

Now, since the wave function is either symmetric (even principal quantum number n), or anti-symmetric (odd n), either $\psi'(x)$ (even n) or $\psi(x)$ (odd n) vanish at $x = 0$. Thus we have the following equations

$$\left.\frac{\psi'(x,E)}{\psi(x,E)}\right|_{x=0} \;=\; 0 \qquad \text{even } n\,; \qquad \left.\frac{\psi(x,E)}{\psi'(x,E)}\right|_{x=0} \;=\; 0 \qquad \text{odd } n\,,$$

where the normalisation cancels, and from which the bound state energies E_n can be calculated as the roots of the equations.

Finally, the normalisation condition

$$\int\limits_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx \;=\; 1$$

can be used in order to normalise the initial condition $\psi'(x_0)$ correctly.

My Fortran implementation of the program is given in `Ex10.1.f`, and a plot of the first three wave functions can be found in `psi.ps`. The energies for the first three levels are explicitly given in the program. The program has to be run for each $n = 0,\,1,\,2$ separately.

EXERCISE 10.2: **Fourier Transform**

The solution of the differential equation for the Duffing oscillator is provided in the Mathematica program `Ex10.2.m`. From this solution, tables of function values can be generated with the Mathematica function `Table[]`, which can then be analysed with the Mathematica function `Fourier[]` for the discrete Fourier transform.