Introduction to Computational Physics

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

EXERCISE 10.1: **Quantum Mechanical Anharmonic Oscillator**
Employing the Cash-Karp Runge-Kutta solver for ordinary differential equations, solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\,\psi(x) \;=\; E\,\psi(x)$$

for the anharmonic potential

$$V(x) \;=\; \alpha x^2 + \beta x^4\,,$$

and calculate the first three bound state energies as well as the corresponding wave functions. In convenient units, like in exercise 2.1, the constants are given by:

$$\alpha \;=\; 0.5\,\mathrm{eV\mathring{A}}^{-2}\,, \quad \beta \;=\; 0.25\,\mathrm{eV\mathring{A}}^{-4} \quad \text{and} \quad \hbar^2 \;=\; 7.6199682\,m_e\,\mathrm{eV\mathring{A}}^{2}\,.$$

How can the boundary conditions that $\psi(x)$ vanishes at $\pm\infty$ and the normalisation condition

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

be implemented? (Hint: use the fact that for symmetric potentials, the wave functions has to have defined parity ±1, and that the wave function vanishes exponentially.)

EXERCISE 10.2: **Fourier Transform**
With the help of the Mathematica routines `NDSolve[]` and `Fourier[]`, investigate the frequency spectrum of the *Duffing oscillator*

$$\ddot{x} + k\dot{x} + x^3 \;=\; B\cos t$$

for $k = 0$, 1 as well as $B = 2$, 4, 6, 8, 10, 12, 14, 16. As the initial conditions use $x(0) = 0$ and $\dot{x}(0) = 1$. Study the influence of the range in t used for the Fourier transform as well as the discretisation of the data.