Introduction to Computational Physics

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(To be discussed on Friday, 23.5. and Monday, 26.5.)

EXERCISE 2.1: **Root Finding (Newton-Raphson)**
With your implementation of the Newton-Raphson algorithm, or the ones given in C/C++, FORTRAN on the CP web-page, calculate the bound state energy levels of the square-well potential. These where given as the roots of the following equations:

$$\begin{aligned} \text{Even}: \quad \alpha(E)\sin(\alpha(E)a) - \beta(E)\cos(\alpha(E)a) &= 0\,, \\ \text{Odd}: \quad \alpha(E)\cos(\alpha(E)a) + \beta(E)\sin(\alpha(E)a) &= 0\,, \end{aligned}$$

with $\alpha(E) = \sqrt{2mE/\hbar^2}$ and $\beta(E) = \sqrt{2m(V_0 - E)/\hbar^2}$.
For the constants use: $V_0 = 10\,\text{eV}$, $a = 3\,\text{Å}$, $m = m_e$ and $\hbar = 7.6199682\,m_e\,\text{eVÅ}^2$.

EXERCISE 2.2: **More Root Finding**
Find the two roots of the function $f(x)$ already investigated in exercise 1.3a):

$$f(x) \;=\; 3x^2 + \ln((\pi - x)^2)/\pi^4 + 1\,.$$

(Hint: since the roots lie very close to π, apply a suitable transformation to make the algorithm more stable.)

EXERCISE 2.3: **Stability of Root Finding (Fractals)**
Consider the function $f(z)$ of one complex variable z:

$$f(x) \;=\; z^3 - 1\,.$$

It should be clear that the roots of $f(z)$ are given by the three unit roots 1, $\exp(\pm 2\pi i/3)$.
The Newton-Raphson algorithm can be easily generalised to functions with one complex variable. With such an extension, investigate for which initial values in the complex plane with $-2 \leq \text{Re}z$, $\text{Im}z \leq 2$, the algorithm converges to the real root 1.

EXERCISE 2.4:* **Still more Root Finding**
Combine the bisection algorithm and the Newton-Raphson algorithm into one routine whose convergence properties are more stable.