Introduction to Computational Physics SS2023

Lecturers: Rainer Spurzem, Stefan Reißl, Ralf Klessen
Tutors (group number in brackets): Jeong Yun Choi (1), Patricio Alister (2), Vahid Amiri (3), Matheus Bernini Peron (4), Bastián Reinoso (5), León-Alexander Hühn (6), Florian Schulze (7), Marcelo Vergara (8)

Exercise 4 from May 10, 2023
Return before noon of May 19, 2023

1 Numerov algorithm for the Schrödinger equation

The Numerov algorithm is a highly accurate discretization method used for special variants of Sturm-Liouville differential equations of the type

$$y''(x) + k(x)y(x) = 0 \; .$$

It is given by

$$\left(1 + \frac{1}{12}h^2 k_{n+1}\right) y_{n+1} = 2 \; \left(1 - \frac{5}{12}h^2 k_n\right) y_n - \left(1 + \frac{1}{12}h^2 k_{n-1}\right) y_{n-1} + \mathcal{O}(h^6)$$

and provides 6th order accuracy by using the three values y_n, y_{n-1}, y_{n+1} with $k_n = k(x_n)$ and $y_n = y(x_n)$. The Numerov algorithm is an efficient approach to numerically solve the time-independent Schrödinger equation. It reads

$$\Psi''(z) + \frac{2m}{\hbar^2}(E - V(z))\Psi(z) = 0 \; .$$

The potential of the harmonic oscillator is $V(z) = \frac{1}{2}m\omega^2 z^2$, where ω is the oscillator frequency and where the quantum mechanical energy eigenvalues result as $E_n = (n + \frac{1}{2})\hbar\omega$.

- The dimensionless form of this equation is obtained from $x = z/z_0$, with a suitable z_0, and looks like

$$\psi''(x) + (2\varepsilon - x^2)\psi(x) = 0 \; .$$

- Write a computer program that uses the Numerov algorithm to solve this equation. Test it against the known analytic solution,

$$\psi(x) = \frac{H_n(x)}{(2^n n! \sqrt{\pi})^{1/2}} \exp\left(-\frac{x^2}{2}\right) \; ,$$

  where $H_n(x)$ is the Hermite polynomial of order n. A definition of $H_n(x)$ can be found in the web.[1] For practical computational purposes the most efficient way to compute $H_n(x)$ is to start with $H_0(x) = 1$, $H_1(x) = 2x$ and then use the recurrence relation,

[1] For example at http://mathworld.wolfram.com/HermitePolynomial.html

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \ ,$$

to define the higher order polynomials.

- The functions $\psi(x)$ given above are the analytic solutions for the energy eigenvalues $\varepsilon = n + 1/2$. The solutions for even n are symmetric around $x = 0$, while the ones for odd n are antisymmetric. In order to start your Numerov algorithm you have to choose $\psi(0) = a$ and $\psi(h) = \psi(0) - h^2 k_0 \psi(0)/2$ for symmetric solutions, and $\psi(0) = 0$ and $\psi(h) = a$ for the antisymmetric ones. The value of a is a free parameter of order unity. Since Schrödinger's equation is linear in ψ there is a free normalization factor, which means if $\psi(x)$ is a solution, the also $a\psi(x)$ is one, for any a.

2 Neutrons in the gravitional field (HOMEWORK)

Another interesting application of the Numerov algorithm is the calculation of stationary states $\Psi(z)$ of neutrons in the gravitational field of the Earth[2]. For small changes in the vertical amplitude z the potential can be expressed as $V(z) = mgz$ for $z \geq 0$. Place a perfectly reflecting horizontal mirror at $z = 0$ so that $V(z) = \infty$ for $z < 0$. Neutrons that fall onto the mirror are reflected upwards, and so we only seek solutions for $z \geq 0$. After a proper choice of length and energy units (please specify!) the above equation can be rewritten as

$$\psi''(x) + (\varepsilon - x)\psi(x) = 0 \ .$$

1. Use the Numerov method to solve this differential equation. Choose some values of ε and plot the solution from $x = 0$ to $x \gg \varepsilon$ (i.e. well into the classically forbidden zone). We are interested in the asymptotic behavior of the solution for large x, i.e. whether it goes to positive infinity or negative. Show (plot) two solutions obtained from your program (for two values of ε), one with positive and one with negative asymptotic behavior. (10 points)

2. The eigenvalues ε_n of Schrödinger's equation belong to normalizable eigenfunctions with $\psi(x) \to 0$ for $x \to \infty$. It means that while varying ε_n from smaller to larger values, the function $\psi(x)$ for $x \to \infty$ changes sign. Use this property to determine the eigenvalues ε_n of the first three bound states to 2 decimals behind the comma.
(10 points)

[2] See `http://www.uni-heidelberg.de/presse/ruca/ruca03-2/schwer.html` (in German) original publication, see `http://www.nature.com/nature/journal/v415/n6869/full/415297a.html`