Tutorial Introduction to Computational Physics SS2012

Lecturers: Ralf Klessen & Rainer Spurzem

Tutors: Jan Rybizki/Tobias Brandt & Mykola Malygin

Sheet 4 (May 10, 2012)

Return by noon of May 18, 2012)

1 Numerov algorithm for the Schrödinger equation

The Numerov algorithm is a high accuracy discretisation 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} only, with $k_i := k(x_i)$ and $y_i = y(x_i)$. The Numerov algorithm is an efficient algorithm to solve numerically the time independent Schrödinger equation. It reads:

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

For the harmonic oscillator problem one has $V(z) = mz^2/2$.

- The dimensionless form of this equation is obtained from $x = z/z_0$, with a suitable z_0, and looks as follows:
$$\psi"(x) + (2\varepsilon - x^2)\psi(x) = 0$$
- Write a computer program that uses the Numerov algorithm to solve this equation. Test it against the known analytic solution:
$$\psi(x) = \frac{H_n(x)}{(2^n n! \sqrt{\pi})^{1/2}} \exp\left(-\frac{x^2}{2}\right)$$
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] `http://mathworld.wolfram.com/HermitePolynomial.html`

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

to define the higher order polynomials. n which $H_n(x)$ are the Hermite polynomials.

- The functions $\psi(x)$ given above are the analytical solutions for the energy eigenvalues $\varepsilon = n+1/2$. The solutions for even n are symmetric around $x = 0$, while the ones for uneven 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 normalisation factor (if $\psi(x)$ is a solution, also $a\psi(x)$ is one, for any a).

2 Neutrons in a gravity field (homework)

Another possible application of the Numerov algorithm is the calculation of stationary states $\Psi(z)$ of neutrons in the gravity field of the Earth[2]. The gravity of the Earth is given by $V(z) = mgz$ for $z \geq 0$. At $z = 0$ a horizontal perfectly reflecting mirror reflects the neutrons so that one can take $V(z) = \infty$ for $z < 0$. We seek solutions for $z \geq 0$, since $\Psi(z) = 0$ for $z < 0$. After a proper choice of length and energy units (please specify!) the above equation can be rewritten as

$$\psi\text{"}(x) + (\varepsilon - x)\psi(x) = 0$$

1. (10 points) Use your Numerov program 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 behaviour 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 behaviour.

2. (10 points) The eigenvalues ε_n of Schrödinger's equation belong to normalisable eigenfunctions, for which it is $\psi(x) \to 0$ 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.

[2] See `http://www.uni-heidelberg.de/presse/news/2201abele.html`