Worksheet 12: Schrödinger-equation

July 9, 2013

General Remarks

- Deadline is **Tuesday, 16th July 2013, 10:00**
- On this worksheet, you can achieve a maximum of 10 points.
- To hand in your solutions, send an email to
  - Olaf (`olenz@icp.uni-stuttgart.de`; Wednesday, 14:00–15:30)
  - Elena (`minina@icp.uni-stuttgart.de`; Wednesday, 15:45–17:15)
  - Tobias (`richter@icp.uni-stuttgart.de`; Friday, 15:45–17:15)
- Attach all required files to the mailing. If asked to write a program, attach the *source code* of the program. If asked for a text, send it as PDF or in the text format. We will *not* accept MS Word files!
- The worksheets are to be solved in groups of two or three people. We will not accept hand-in-exercises that only have a single name on it.
- The tutorials take place in the CIP-Pool of the Institute for Computational Physics (ICP) in Allmandring 3.

This worksheet is about solving the (stationary, one-dimensional) Schrödinger-equation numerically. The equation reads[1].

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + V(x)\psi(x) = E\psi(x).$$

Contrary to Poisson's equation the Schrödinger equation is an eigenvalue problem, hence a different algorithm is needed to solve it.

Aufgabe 12.1 (5 points): Infinite square well

The infinite square well can be described by the following potential:

$$V(x) = \begin{cases} 0 & \text{, if } 0 < x < L \\ \infty & \text{, otherwise} \end{cases}$$

The energy-eigenvalues and the corresponding wave-functions can be calculated analytically.

[1] with no loss of generality, we will use a reduced unit system with $\frac{\hbar^2}{2m} = 1$

- 12.1.1 (1 point) Discretize the 1-dimensional, stationary Schrödinger-equation using the finite differences method of linear order. Implement a python function `schroedinger_matrix(V, h)`, which generates and returns the $N \times N$-matrix that is needed to solve the eigenvalue problem. Here `V` is a 1-dimensional numpy-array, which contains N values of the potential at $x \in [0, Nh]$; `h` is the distance between two values x.

- 12.1.2 (1 point) Implement a python-function `solve_schroedinger_scipy(V, h, n)`, which solves the discretized Schrödinger equation and returns the `n` smallest energy eigenvalues together with numerical approximation of the eigenfunctions. Use `scipy.linalg.eigh` and `schroedinger_matrix(V, h)`.

  Hint Take care of the parameter `eigvals` of the `scipy.linalg.eigh()` function.

- 12.1.3 (1 point) What has to be done in order to get the actual solution for the infinite square well?

  Hint If you don't find the solution, change the first and last entry of the potential array to a large number (*e.g.* 1000)

- 12.1.4 (2 points) Solve the Schrödinger-equation for a single particle in the infinite square well potential ($L = 10$). Use $N = 50$ points. Make a plot of the differnt solutions ψ and label them with their energy eigenvalue E. Compare the results to the analytical solution of the infinite square well $E = \frac{n\pi}{L}, n = 1, 2, 3, \ldots$.

  Hint To make the plot more optically appealing shift the eigenfunctions ψ by their corresponding energy eigenvalue E on the y-axis.

Task 12.2 (2 points): QR-decomposition

- 12.2.1 (1 point) Implement a python function `solve_schroedinger_qr(V, h, n, tolerance)`, that calculates and returns the energy eigenvalues and the eigenvectors by QR-decomposition as described in the lecture script.

- 12.2.2 (1 point) Solve the Schrödinger equation for the infinite square well with the function of the previous task and plot the solution as before. As tolerance use 10^{-1}.

  Hint This technique converges badly if the potential is infinitely high. It is better to set the values at the borders to 1000.

Task 12.3 (3 points): More potentials

Solve the Schrödinger equation numerically for the following potentials with $N = 50$, $L = 10$ and generate plots of results similar as in task 12.1.4

- 12.3.1 (1 point) Finite square well:

$$V(x) = \begin{cases} \infty & \text{, if } x < 0 \vee x > L \\ 2 & \text{, if } 0 < x < \frac{1}{5}L \\ 2 & \text{, if } \frac{4}{5}L < x < L \\ 0 & \text{, otherwise} \end{cases}$$

- 12.3.2 (1 point) Double well:

$$V(x) = \begin{cases} \infty & \text{, if } x < 0 \vee x > L \\ 2 & \text{, if } \frac{2}{5}L < x < \frac{3}{5}L \\ 0 & \text{, otherwise} \end{cases}$$

- 12.3.3 (1 point) Harmonic potential:

$$V(x) = \begin{cases} \infty & \text{, if } x < 0 \vee x > L \\ \frac{1}{10}(x - \frac{L}{2})^2 & \text{, otherwise} \end{cases}$$