Computational Physics — SuSe 2023
5. Exercise Sheet

Handing out: 19.5.2023 — Prof. H. Jelger Risselada
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Exercise 1: Schrödinger equation — 10 Points

Simulate a quantum mechanical particle in one dimension with wave function $\psi(x,t)$ in a harmonic potential. The accompanying Schrödinger equation is:

$$\mathrm{i}\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\partial_x^2\psi + \frac{1}{2}m\omega^2x^2\psi = \hat{H}\psi \tag{1}$$

The initial configuration shall be a normalized Gaussian packet (see (5)).
Note: You can use matrix libraries like Eigen for this exercise, i.e. for inversion and other matrix operations.

a) Non-dimensionalize the Schrödinger equation (1) by choosing a characteristic time scale of $\tau = \omega/2$. Calculate the characteristic length scale $1/\alpha$ needed to bring the Schrödinger equation into the shape:

$$\mathrm{i}\partial_\tau\psi = -\partial_\xi^2\psi + \xi^2\psi = \hat{\tilde{H}}\psi\,. \tag{2}$$

What is the characteristic energy scale $1/\beta$?

b) Use the Crank-Nicholson-Algorithm to solve the dimensionless Schrödinger equation (2) on a grid $\xi_j = j\Delta\xi$. The discretized Hamilton operator is now given as a matrix $\boldsymbol{H}$, with entries:

$$H_{nm} = -\frac{1}{\Delta\xi^2}\left(\delta_{n,m-1} + \delta_{n,m+1} - 2\delta_{nm}\right) + \Delta\xi^2 n^2\delta_{n,m}\,. \tag{3}$$

The discretized time evolution operator for a time step of length Δt is given in the Crank-Nicholson formulation:

$$\boldsymbol{S_H} = \left(\mathbb{1} + \frac{\mathrm{i}}{2}\boldsymbol{H}\Delta\tau\right)^{-1}\left(\mathbb{1} - \frac{\mathrm{i}}{2}\boldsymbol{H}\Delta\tau\right)\,. \tag{4}$$

Calculate this matrix with $\Delta\tau = 0.02$ for a system of size $\xi \in [-10, 10]$, discretized by $\Delta\xi = 0.1$.

c) The inital state shall be a normalized Gaussian packet

$$\psi(\xi,0) = \left(\frac{1}{2\pi\sigma}\right)^{1/4}\exp\left(\frac{-\left(\xi-\xi_0\right)^2}{4\sigma}\right) \tag{5}$$

with

$$\langle\xi\rangle = \int d\xi\,\xi|\psi(\xi,0)|^2 = \xi_0\,, \tag{6}$$

$$\langle(\xi-\xi_0)^2\rangle = \sigma\,. \tag{7}$$

What is the discretized inital state vector $\psi_j(0) \equiv \psi(\xi_j, 0)$? What is the dimension of this vector? Use $\xi_0 = \sigma = 1$.

d) Calculate the state at a time $t = 10$ for the inital state (5), by continued matrix multiplication with the time propagation operator (4). Check if the state stays normalized during the time propagation.

e) Visualize the temporal evolution of the wave function by animating/plotting the evolution of the probability distribution during the oscillation.

Exercise 2: Oscillating rectangular membrane — 10 Points

Consider an oscillating rectangular membrane of negligible bending stiffness in a fixed frame of lengths $a \times b$. Without damping or any external load, the deflection field of the membrane $u(x, y, t)$ is a solution to the wave equation

$$\frac{\partial^2 u(x,y,t)}{\partial t^2} = c^2 \left(\frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2} \right) , \tag{8}$$

where c denotes a constant phase velocity. You are supposed to implement an iteration procedure for solving the two-dimensional wave equation.

a) Discretize the x, y and t coordinate to reformulate the wave equation as a finite difference equation and derive

$$u_{i,j}^{n+1} - 2u_{i,j}^{n} + u_{i,j}^{n-1} = c^2 \Delta t^2 \left[\frac{u_{i+1,j}^{n} - 2u_{i,j}^{n} + u_{i-1,j}^{n}}{\Delta x^2} + \frac{u_{i,j+1}^{n} - 2u_{i,j}^{n} + u_{i,j-1}^{n}}{\Delta y^2} \right] .$$

b) Any perturbation of the solution $\delta u(x, y, t)$ can be expanded in its Fourier modes

$$\tilde{c}_{\omega,k_x,k_y} \exp(\mathrm{i}(k_x x + k_y y - \omega t)) .$$

Analyse the stability of the above iteration with respect to the Fourier modes. *Hint: The iteration becomes unstable if ω is complex. Why?*

c) The computation of the next time step $u^{(n+1)}$ involves the current $u^{(n)}$ and the previous $u^{(n-1)}$. However, initial conditions are typically given for the function values $u(x, y, 0)$ and ${}^{\partial u}/_{\partial t}|_{t=0}$. Given $u_{i,j}^0$, derive the first iteration step for $u_{i,j}^1$ using ${}^{\partial u}/_{\partial t}|_{t=0} = 0$.

d) Non-dimensionalise the wave equation (8) by an appropriate choice of length- and timescale.

e) Implement the iteration scheme and solve the wave equation for a fixed membrane in a frame with $a = 1$, $b = 1.5$ and for convenience $\Delta x = \Delta y$. Use the initial conditions

$$u(x,y,0) = \sin\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{b}y\right) \qquad \left.\frac{\partial u(x,y,t)}{\partial t}\right|_{t=0} = 0 .$$

Visualize the calculated solution for a few different time steps (e.g. $t = 0$ and $t = 10$) to check the plausibility and stability of the implementation.