

## Schrödinger equation (1.5 LP)

We consider one-dimensional Schrödinger equation in dimensionless form

$$i\frac{\partial\psi}{\partial t} = \hat{H}\psi = \left(-\frac{\partial^2}{\partial x^2} + V(x, t)\right)\psi$$

**Problem 1:** Consider the eigenvalue problem for this equation and find first four eigenvalues and eigenfunctions for the double-well potential  $V(x) = \frac{A}{2}(1 - x^2)^2$ .

**Problem 2:** Simulate time-dependent Schrödinger equation using the Crank-Nicholson discretization scheme.

**Problem 2a:** Check accuracy of the total probability  $\int_{-\infty}^{\infty} |\psi|^2 dx$  conservation in dependence on the space step.

**Problem 2b:** Use eigenfunctions found as initial conditions and check stationarity in the time-dependent runs

**Problem 2c:** Use combinations of two eigenfunctions as initial conditions and check if time evolution of the observable  $p_{left} = \int_{-\infty}^0 |\psi|^2 dx$  shows the expected periodicity in time.

Literature:

Scherer, Computational Physics, sec. 17.3.4 (Crank-Nicholson method), Ch. 19 (Schrödinger eq.)

Koonin, Computational Physics, sec. 3.5 (stationary eq.), Ch. 7 (nonstationary eq.)

Landau, Paez, Bordeianu, A Survey of Computational Physics, sec. 9.10-9.11 (stationary eq.); sec. 18.5-18.7 (nonstationary eq.)