

DejaVu Serif DejaVu Sans DejaVu Sans Mono

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QmPy

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Contains numerical solvers for the schroedinger equation

`solvers.calculate_expval(xcoordsarray, wfuncsarray, xmin, xmax, npoints)`

Calculates the expected values for the x-coordinate

#### Parameters

- `xcoordsarray` (*1darray*) – Array containing the x-coordinates
- `wfuncsarray` (*ndarray*) – Array containing the wave functions that
- to the x-coordinates (*correspond*) –
- `xmin` (*float*) – Minimal value of the x-axis
- `xmax` (*float*) – Maximal value of the x-axis
- `npoints` (*int*) – Number of points in the interval [xmin, xmax]

**Returns** The expected values of the x-coordinate

**Return type** `expval` (1darray)

`solvers.calculate_uncertainty(xcoordsarray, wfuncsarray, xmin, xmax, npoints)`

Calculates the uncertainty (which is the square root of the expected value of  $x^2$  minus the square of the expected value of  $x$ ) for the x-coordinate

#### Parameters

- `xcoordsarray` (*1darray*) – Array containing the x-coordinates
- `wfuncsarray` (*ndarray*) – Array containing the wave functions that
- to the x-coordinates (*correspond*) –
- `xmin` (*float*) – Minimal value of the x-axis
- `xmax` (*float*) – Maximal value of the x-axis
- `npoints` (*int*) – Number of points in the interval [xmin, xmax]

**Returns** The expected values of the x-coordinate

**Return type** `uncertainty` (1darray)

`solvers.schroedinger(mass, xcords, potential)`

Solves the 1-dimensional schroedinger equation for given numerical values of a potential.

**Parameters**

- **mass** (*float*) – The mass of the system in atomic units.
- **xcords** (*1darray*) – X-coordinates corresponding to the potential values.
- **potential** (*1darray*) – Numerical values of the potential.

**Returns**

**energies, wfuncs**

- **energies** (*1darray*) - The energy levels of each wavefunctions. The entries correspond to the rows in wfuncs.
- **wfuncs** (*ndarray*) - Array where each row contains the numerical value of a computed wavefunction. Each column corresponds to one x-coordinate of the input array.

**Return type** tuple

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