**1. Starting point**

Electronic wavefunctions:

Nuclear wavefunctions:

**2. Overlap, potential energy, discretization**

Here, denotes the grid discretization

Analogously:

**3. Reciprocal space representation of the nuclear wavefunctions**

Direct-space wavefunction

Reciprocal-space wavefunction

Indeed:

**4. Kinetic energy**

Assuming:

Discretization:

**5. Power of nuclear wavefunction momentum**

**6. TD-SE**

Project on (assuming orthonormal!)

Here,

**7. Direct solution of the TD-SE by the discretization**

Simple discretization:

So, the equation:

becomes:

**Second-order scheme:**

Introduce:

**First-order in time:**