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Summary of Short Term Scientific Mission

The objective of this STSM was to device a code that would retrieve the ultra fast dynamical information after ionisation of molecules subject to ultrafast laser fields. The process of inonisation can result in attosecond resolved spectroscopy such as High Harmonic Generation. Here the electron of the ion recombines with itself after ionization thus releasing a XUV photon. Recreating harmonic spectra will be the main application of the code.

The theoretical framework of the code is based on a one dimensional model. This essentially is the solution of the time-dependant Schrödinger equation (TDSE) in one dimension along a coordinate x in which the laser field is linearly polarised.

$$i\frac{\partial}{\partial t}\psi(x,t)=H(t)\psi(x,t).$$

We use the finite difference approach to represent x and t in terms of discretised steps on a grid, which leads to the Crank Nicholson Propagation Scheme. The time discretisation is represented by a grid of t values, separated by the time step Δt . The final wave function at $t+\Delta t$ is then deduced from the initial wave function at t .

To achieve the discretization of the Schrödinger equation, we can express the wave function in terms of the time-evolution operator.

$$\psi(x,t+\Delta t)=e^{-iH(t+\frac{\Delta t}{2})\Delta t}\psi(x,t)$$

A second approximation is made to find the finite-difference representation on the wave function that is unitary. By taking the first order of the Taylor expansion of the exponential function we get.

$$\psi(t+\Delta t)\simeq\frac{1-iH(t+\frac{\Delta t}{2})\frac{\Delta t}{2}}{1+iH(t+\frac{\Delta t}{2})\frac{\Delta t}{2}}\psi(x,t).$$

This turns out to be the Crank-Nicholson propagation scheme,

$$1+iH(t+\frac{\Delta t}{2})\frac{\Delta t}{2}\psi(t+\Delta t)\simeq 1-iH(t+\frac{\Delta t}{2})\frac{\Delta t}{2}\psi(x,t),$$

The computation of the right hand side is a straightforward matrix multiplication, and the inversion of the left-hand side matrix A is done with a Gaussian elimination method adapted to tridiagonal systems. The ground state)and any bound state needed for the analysis of the propagated wave function was computed in a preliminary stage, using standard diagonalisation methods.