

I. Introduction

Atomic and molecular physics has witnessed a revolution due to attosecond pulses [1,2]. The true understanding of the phenomena in attosecond and strong-field physics often needs the quantum evolution of an involved atomic system driven by a strong laser pulse [3-5]. Since the solution of the corresponding Schrödinger equation in this non-perturbative range is beyond reach, approximations are unavoidable and very important. For linearly polarized laser pulses, the main dynamics happens along the electric field of the laser pulse which underlies the success of some one-dimensional (1D) approximations [6] that provide quantum features for a fraction of computational costs. However, the particular 1D model potential, chosen to account for the atomic system, heavily influences the results. Below we introduce and test novel 1D atomic model potentials to simulate such time-dependent processes physically as correctly as possible.

II. 1D modeling with atomic potentials

1D model equations

We work in the framework of a simple theoretical model with dipole approximation for the interaction of a single active atomic electron with the classical electromagnetic field in the length gauge. We aim to model the 3D reference results [7] that start from the ground state of the atomic or molecular system. We simulate the time evolution with the following time-dependent 1D Schrödinger-equation using atomic units:

$$i \frac{\partial}{\partial t} \Psi^{1D}(z, t) = \left[-\frac{1}{2\mu} \frac{\partial^2}{\partial z^2} + V_0^{1D}(z) + z \cdot \mathcal{E}_z(t) \right] \Psi^{1D}(z, t)$$

and we seek improved forms of the 1D atomic model potential that match the 3D results as good as possible. The external electric field is the same as in the 3D case. We solve this equation using a high-order finite difference Crank-Nicolson method.

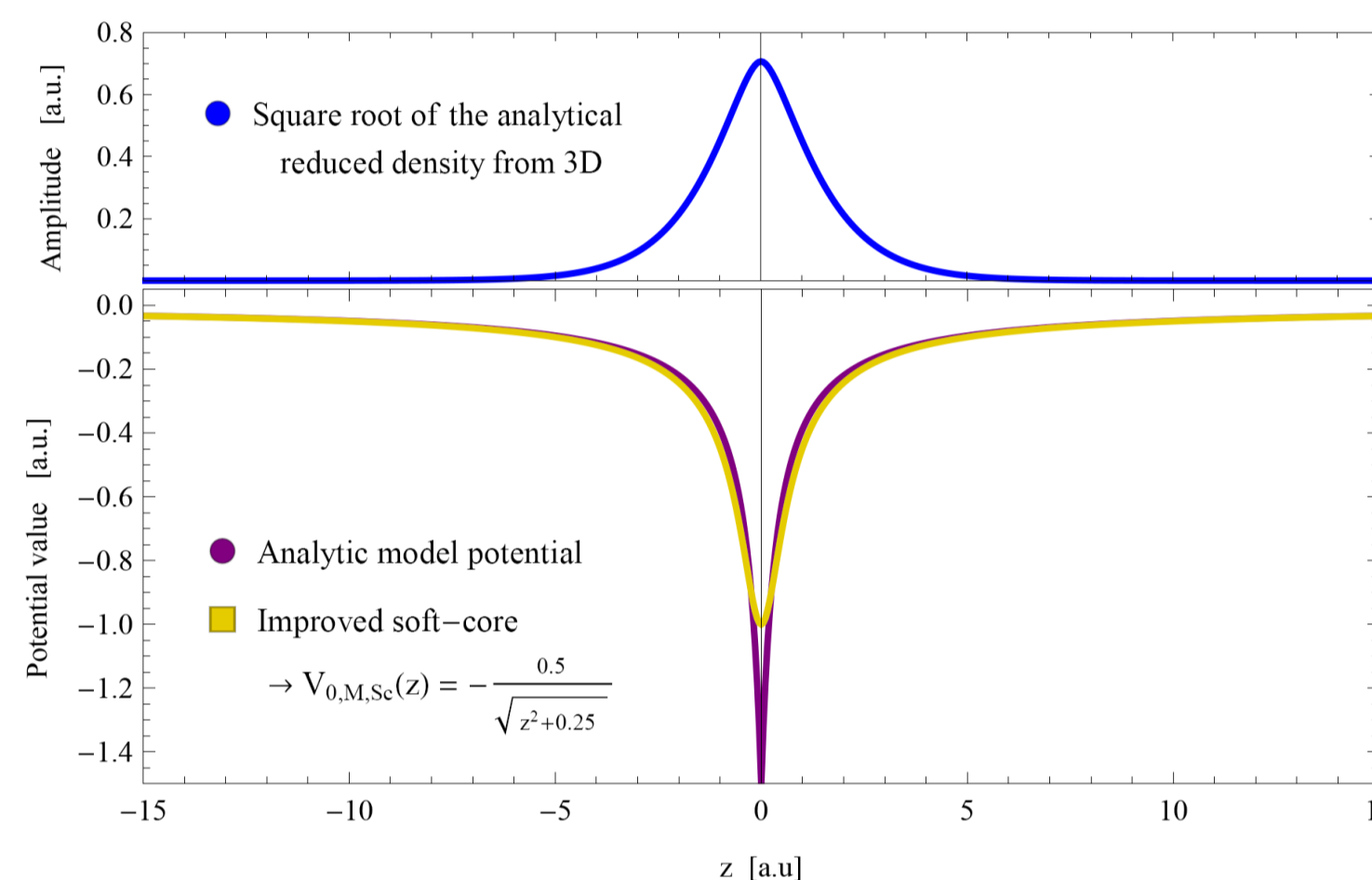
Derivation of the 1D model atomic potential

We derive our model potential from first principles in analogy with the Kohn-Sham theory having a single Kohn-Sham orbital. We start from the 1D Schrödinger equation

$$E_0 \psi_0(z) = \left[-\frac{1}{2\mu} \frac{\partial^2}{\partial z^2} + V_{0,M}^{1D}(z) \right] \psi_0(z)$$

where $\psi_0(z) = \sqrt{\varrho_z^0(z)}$.

The reduced ground state density is $\varrho_z^0(z)$.



However, instead of reducing the density from multiple electron coordinates to the spatial coordinates x, y, z , we reduce the density from x, y, z coordinates to the z coordinate. We define the source 1D density from the ground state of the 3D Coulomb problem:

$$\varrho_z^0(z) = N^2 2\pi \int_0^\infty e^{-2\mu Z \sqrt{z^2 + \rho^2}} \rho d\rho \Rightarrow \psi_0(z) = \sqrt{\frac{\mu Z}{2} \sqrt{2\mu Z |z| + 1} e^{-\mu Z |z|}}$$

Then we solve for the model potential in 1D using:

$$V_{0,M}^{1D}(z) = E_{0,M} + \frac{1}{\psi_0(z)} \frac{1}{2\mu} \frac{\partial^2}{\partial z^2} \psi_0(z), \quad \lim_{|z| \rightarrow \infty} V_{0,M}^{1D}(z) = 0$$

This determines the form of the potential and also its ground state energy:

$$V_{0,M}^{1D}(z) = -\frac{1}{2\mu} \frac{1}{2^2 \left(|z| + \frac{1}{2\mu Z} \right)^2} - \frac{\frac{1}{2} Z}{|z| + \frac{1}{2\mu Z}}, \quad E_{0,M} = E_0 = -\frac{\mu Z^2}{2}$$

Note that this is a nontrivial result. The reduced density of the 3D Coulomb problem selected a potential that has a leading (nonsingular) Coulomb term with half of the original charge, and it preserves the true eigenenergy and the Coulomb form of 3D case through asymptotes.

Alternatively, we introduce the simpler form of what we call as **improved soft-core Coulomb potential**:

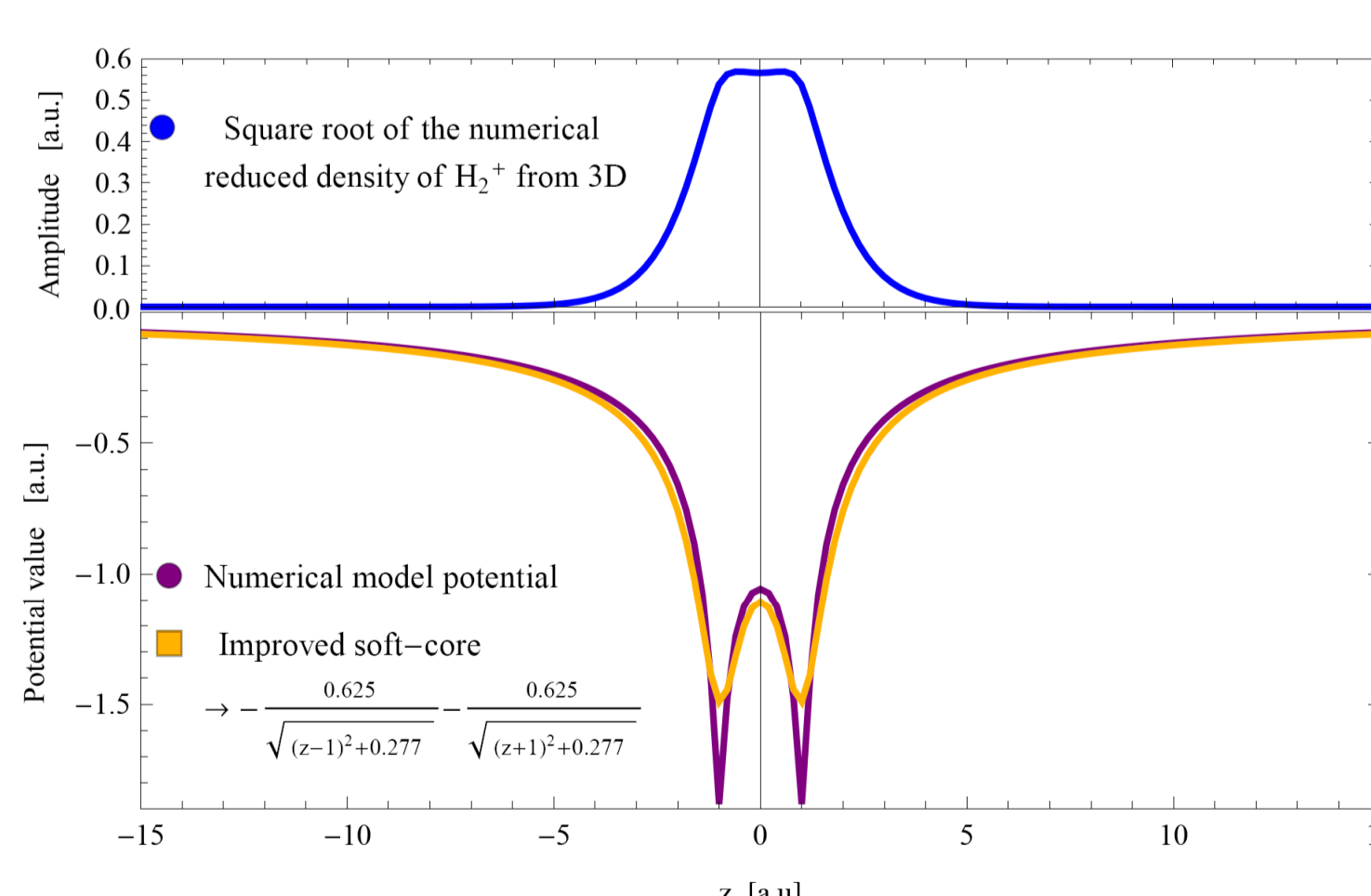
$$V_{0,M,Sc}^{1D}(z) = -\frac{bZ}{\sqrt{z^2 + \alpha^2}}$$

where α is determined by the target energy. Hydrogen atom: $Z = 1$, $\mu = 1$, $b = 0.5$, $\alpha^2 = 0.25$.

III. Advanced applications in 1D

1D hydrogen molecular ion model

Fixed cores at a distance $d = 2$ [a.u.]. We calculated our 1D model potential numerically, the ground state of which has the same reduced density as the 3D case. It has again a 1D asymptotic Coulomb form, and the same eigenenergy as the true 3D case. The asymptote changes with the core-to-core distance, for $d = 2$ it is about $-1.25/|z|$ and for $d = 1.4$ about $-1.194/|z|$. The sum of the improved soft-Coulomb forms match this asymptote.



1D hydrogen molecule model

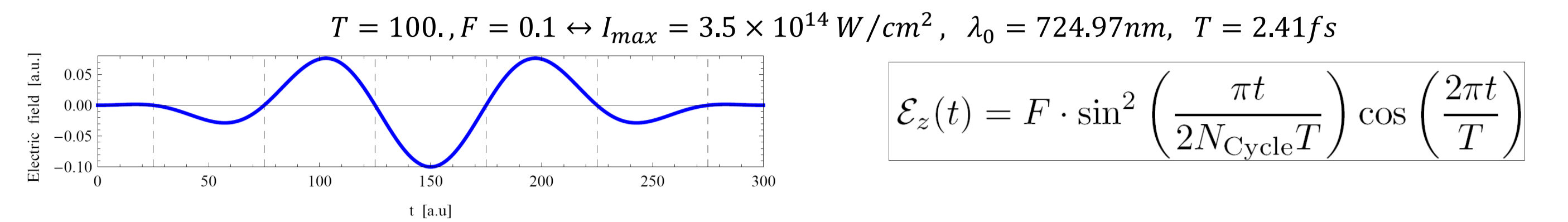
Fixed cores at a distance $d = 1.4$ [a.u.]. We use different improved soft Coulomb forms from H_2^+ ion as the core potentials, and also as the electron-electron interaction. We solve the corresponding 2D Schrödinger equations using the Hamiltonian

$$H = \sum_{k=1}^2 \left(-\frac{1}{2} \frac{\partial^2}{\partial z_k^2} - \frac{b}{\sqrt{(z_k - 0.7)^2 + \alpha^2}} - \frac{b}{\sqrt{(z_k + 0.7)^2 + \alpha^2}} + z_k \cdot \mathcal{E}_z(t) \right) + \frac{b}{\sqrt{(z_1 - z_2)^2 + \alpha^2}}$$

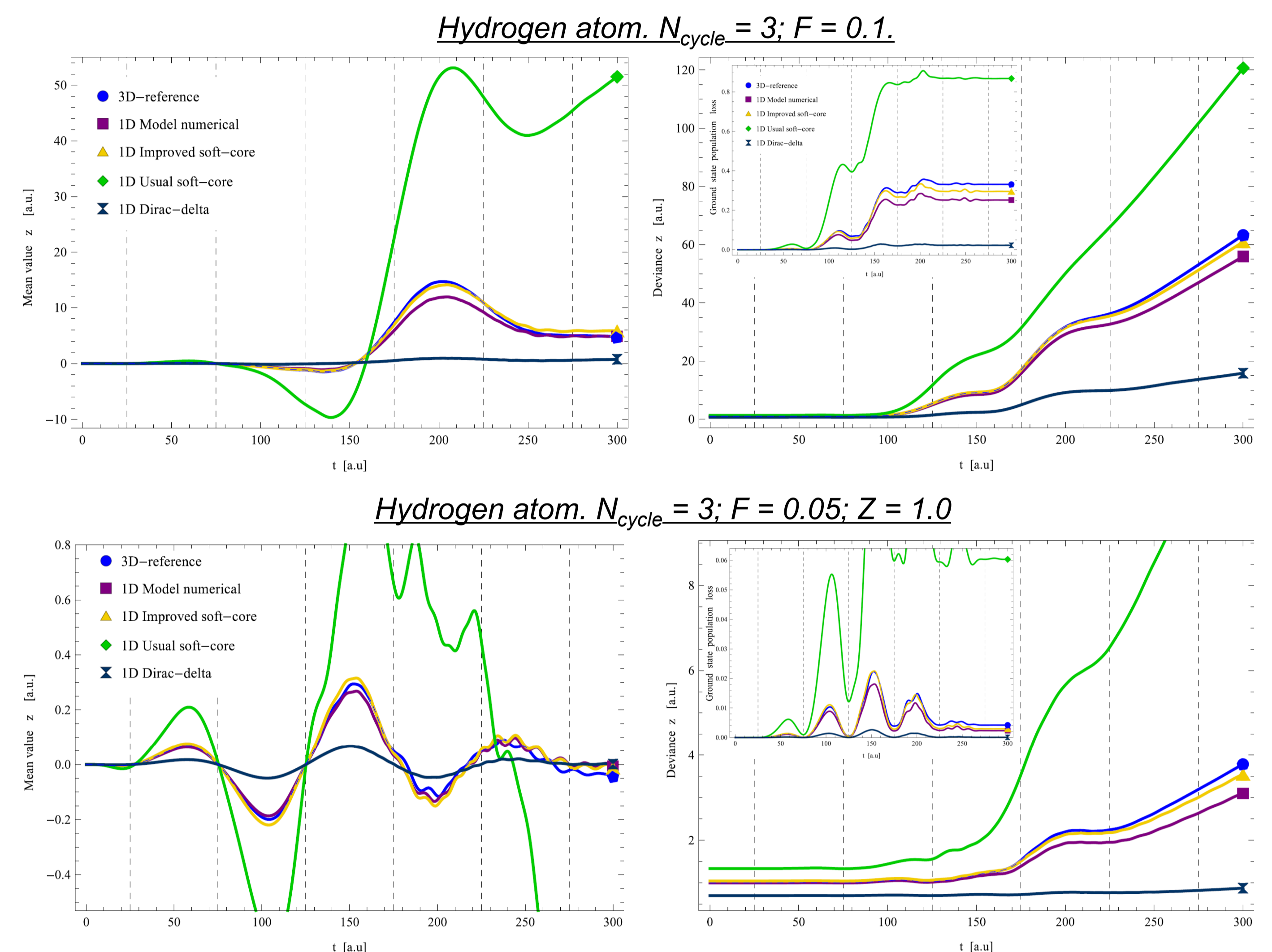
This 1D model system's ground state energy was without parameter fitting -1.93 [a.u.]. The 3D reference solution uses a Hartree-Fock or mean field method, its ground state energy was -1.84 [a.u.], yielding about 5% error in the ab initio 1D model. For consistency of the time-dependent simulations with external electric field, the 1D ground state energy was modified to match this energy by changing α .

IV. Simulation results

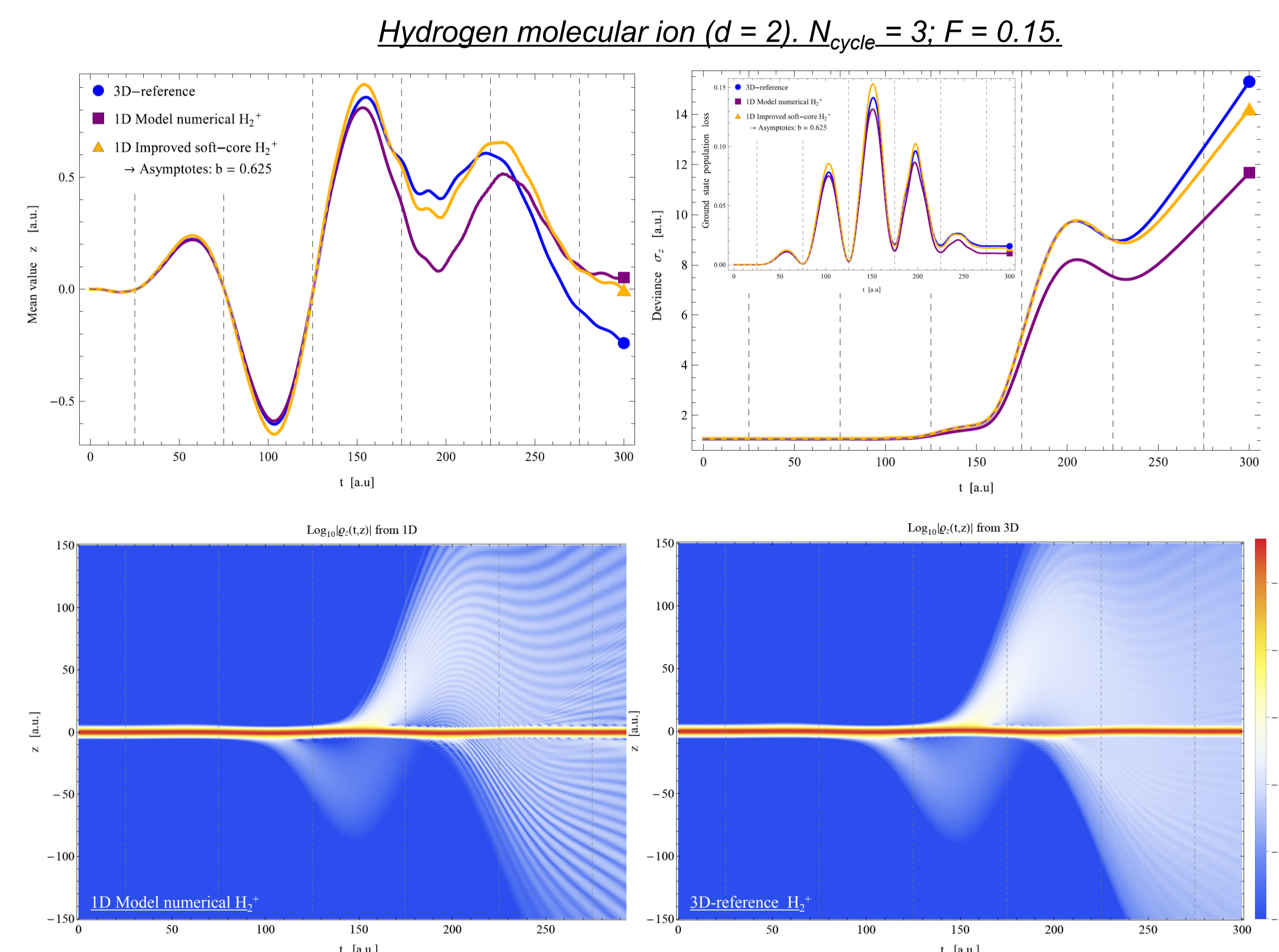
External electric field function form during the simulations



Comparison of dynamics of various 1D model potentials vs. time



Results from hydrogen molecular ion and hydrogen molecule in 1D



References

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