

Low dimensional modeling of atomic and molecular systems

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In this contribution, we present our recent results on novel atomic 1D and 2D model potentials derived according to an unusual application of the Hohenberg-Kohn theorems [1]. We outline the construction of such low dimensional model potentials, which have the important property that their ground state densities equal the reduced exact ground state densities of the 3D hydrogen atom. We present some results of the analytical properties of the respective quantum system in 1D, and compare the resulting nontrivial atomic potential to the familiar low dimensional atomic Coulomb potentials [2].

Our motivation for these advanced model potentials is their potential use in simulations of atomic or simple molecular systems driven by strong fs laser pulses, since quantum features play a fundamental role in attosecond physics [3]. Currently, these experimental techniques enable to measure the electrons' dynamics in atoms and molecules with attosecond time resolution [4, 5]. However, this new quantum metrology demands more theoretical knowledge about the fundamental quantum properties of these processes.

We test the physical correctness of our low dimensional model potential based on our 3D simulation results of a hydrogen atom interacting with a strong, linearly polarized few-cycle laser pulse, computed with a numerical solution of the Schrödinger equation [6]: we compare its results to those of our DFT based and of other commonly used low dimensional atomic model potentials [2] using various quantities derived from the respective wave functions. Our results show that it is possible to achieve quantitatively acceptable results even in these situations by using our model system instead of the 3D simulations.

We also intend to present some advanced applications of this DFT based model potential: we construct a low dimensional hydrogen molecular ion and a 1D hydrogen molecule and investigate how our model potential can be used to construct low dimensional molecules. We also present how the electron clouds of these systems interact with the above mentioned few-cycle strong field laser pulse, which is linearly polarized parallel to the molecular axis.

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