Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

A tug-of-war between electronic excitation and confinement in a dynamical context

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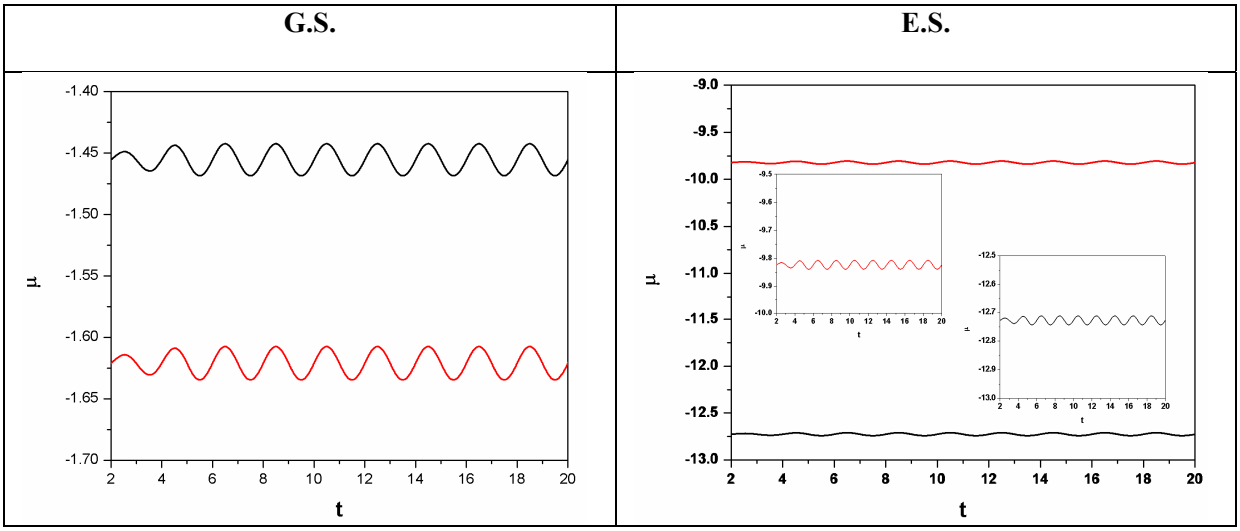

Fig. S1. Time evolution of chemical potential (μ, in a.u.) when helium atom in ground state (G.S.) and excited state (E.S.) is placed in intense laser field. (Amplitude = 0.01 a.u.). Black line represents unconfined system and red line represents confined system. Weizsäcker and Fermi-Amaldi functionals are used in these cases.

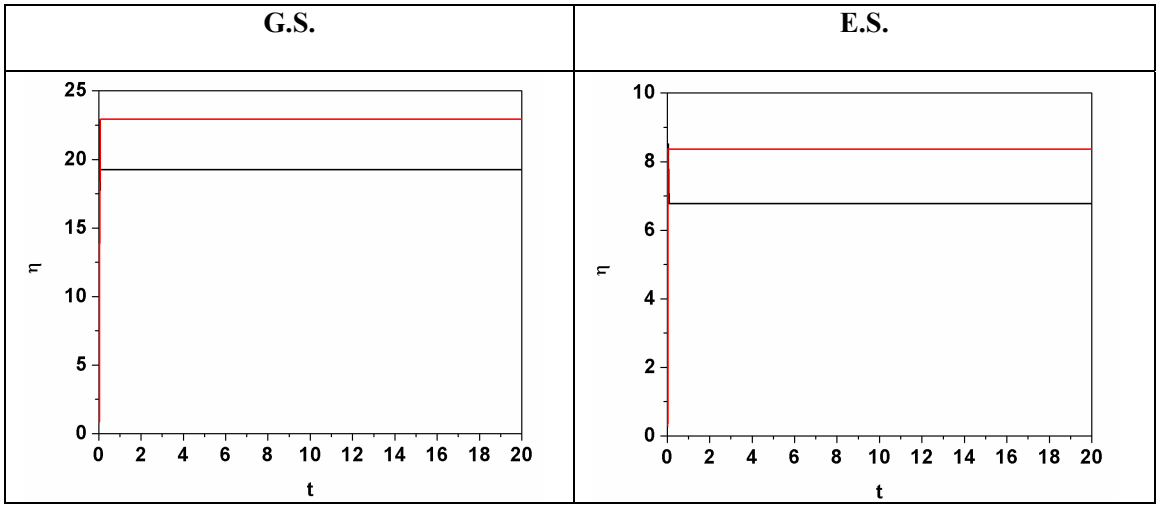

Fig. S2. Time evolution of chemical hardness (η, in a.u.) when helium atom in ground state (G.S.) and excited state (E.S.) is placed in intense laser field. (Amplitude = 0.01 a.u.). Black line represents unconfined system and red line represents confined system.

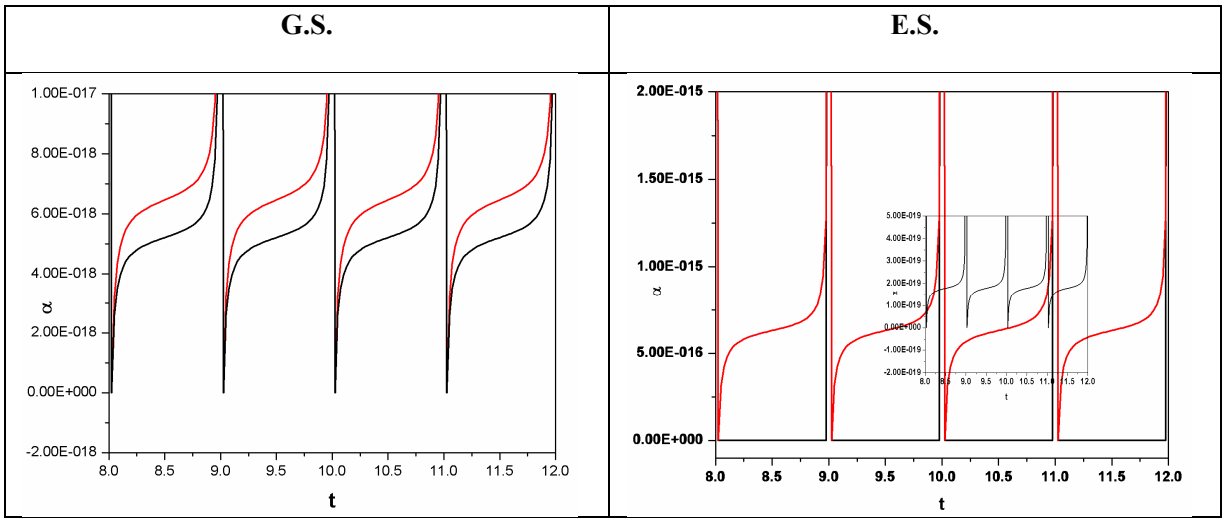

Fig.S3. Time evolution of polarizability (α, in a.u.) when helium atom in ground state (G.S.) and excited state (E.S.) is placed in intense laser field. (Amplitude = 0.01 a.u.). Black line represents unconfined system and red line represents confined system.

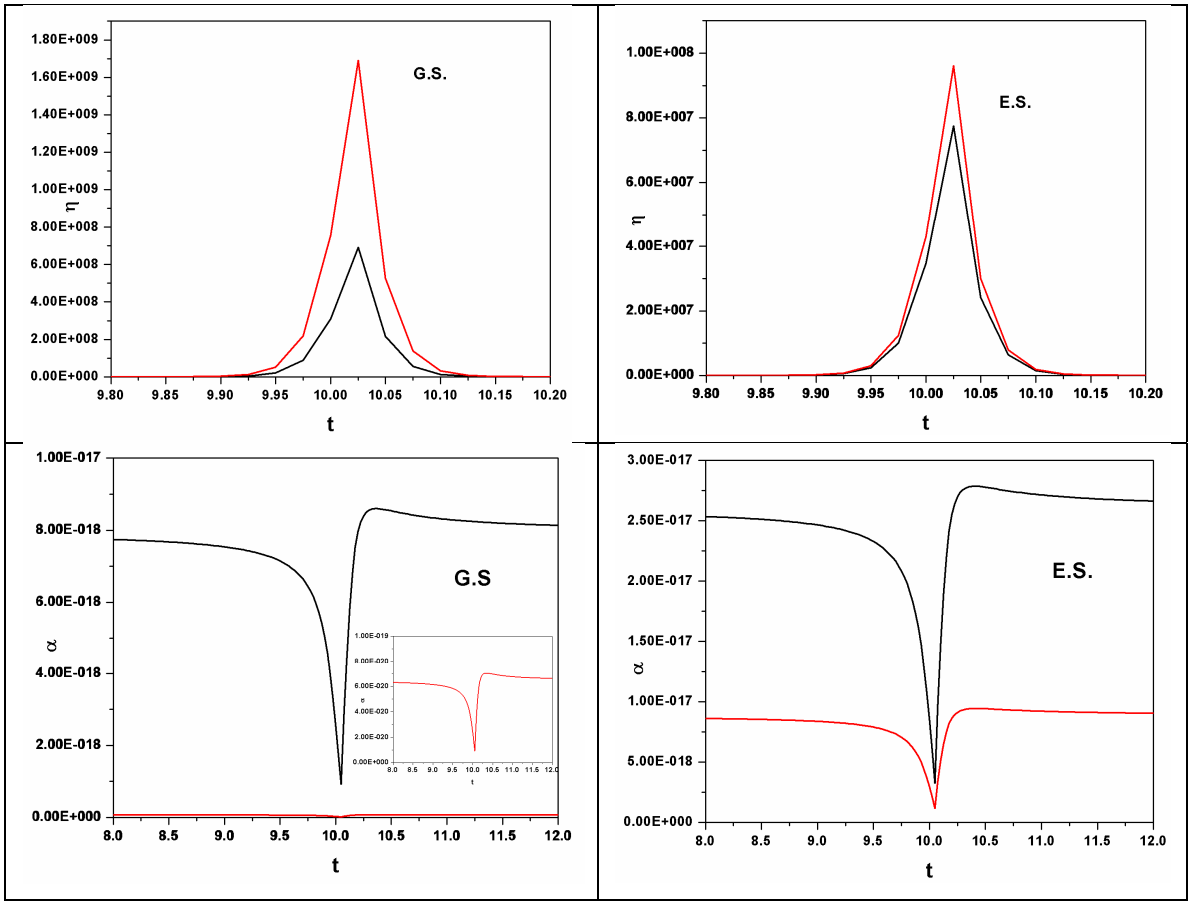

Fig. S4. Time evolution of hardness (η, in a.u.) and polarizability (α, in a.u.) during a collision process between a proton and helium atom in ground state and excited state. Black line represents unconfined system and red line represents confined system.