Strong-Field Ionization in Hydrogen and Small Molecules

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Abstract

Ionization is the process in which an electron is removed from an atom or molecule. Since an electron is negatively charged and a nucleus is positively charged, they experience an attractive force. To ionize the electron, we need a source of energy that is strong enough to overcome the attractive force. In this research we use lasers to create an electric field.

The particle now feels an external force from the field, as well as the internal force from the attraction to the nucleus. This is called the potential energy of the atom. The potential forms a barrier that the particle must have enough energy to overcome. However, in quantum mechanics, there is a phenomenon called tunneling. When this occurs, a particle will go through a barrier that it could not overcome classically.

The strength of the electric field will alter the potential. The stronger the electric field, the more the potential is distorted, thus the shorter distance the particle would have to tunnel through. As the distance becomes shorter, the chances of tunneling rapidly increase.

Adding an electric field to the system also alters the ground-state energy of the particle. I wanted to find how the strength of the electric field affected the energy level, tunnel length, and therefore the ionization rate.

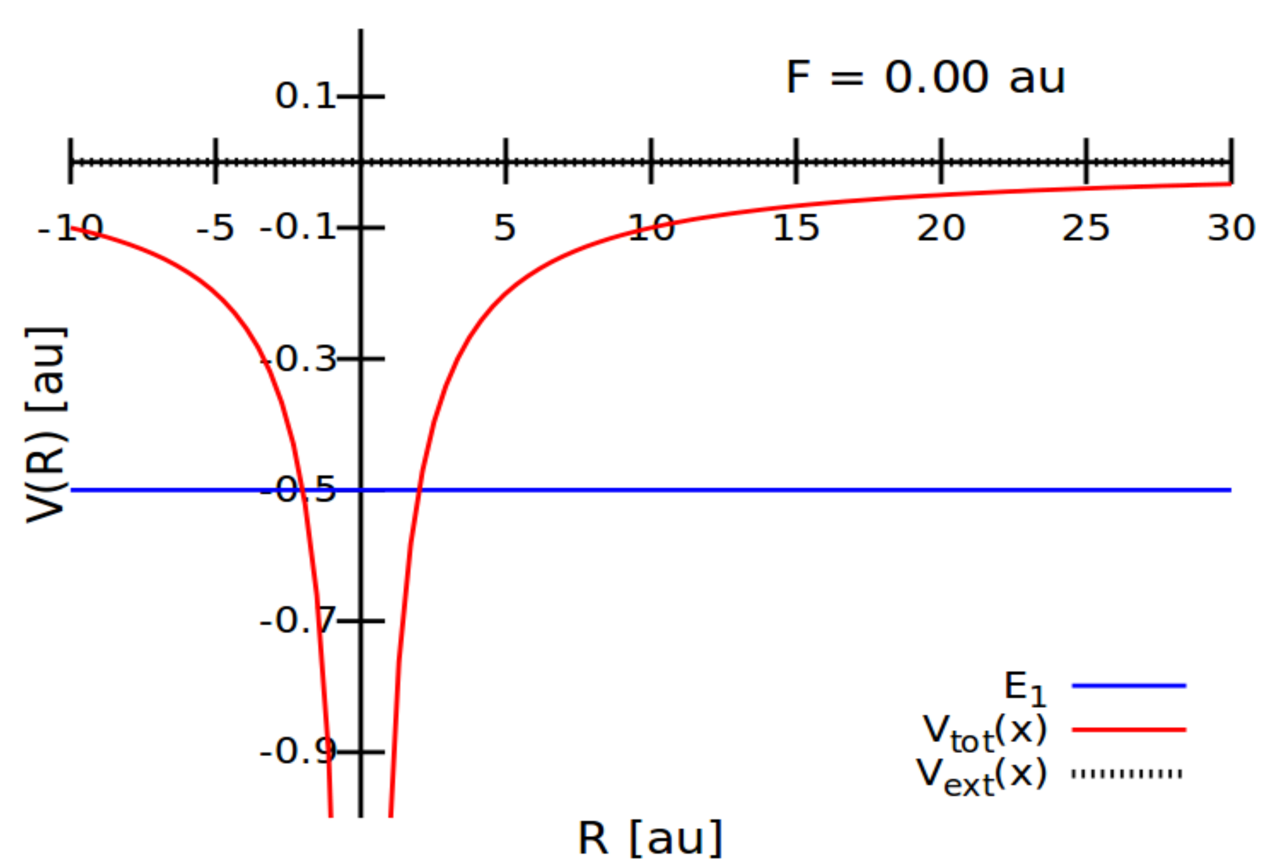
Purpose

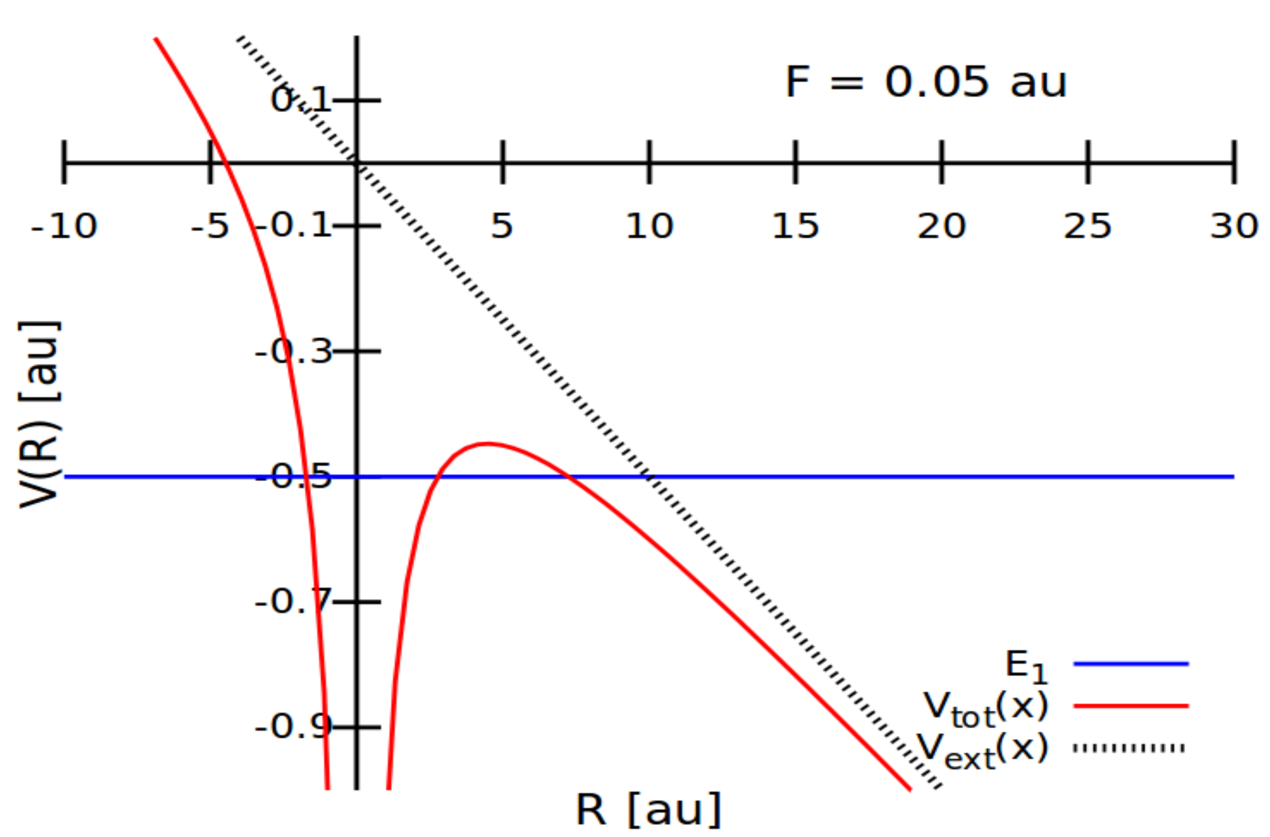
This research can allow us to study the dynamics of molecules and atoms. By measuring the tunnel distance and the amount of time it takes to ionize the electron, we can find the ionization rate of an atom or molecule.

Contributions

- My role in this research was to learn and understand the basic concepts of strong-field ionization.
- Studied the particle in a one-dimensional box (PIB) problem in order to understand wavefunctions.
- Wrote a python program to calculate the energy level of a particle in one-dimensional box
- Modified this program to include multiple wavefunctions as the basis set in order to receive a more accurate estimate of the ground state energy.
- Modified the program to include an electric field and potential energy inside the box.
- Adjusted this code to calculate the estimated ground state energy for a hydrogen atom, rather than a one- dimensional particle.

Electric Field's (F) Effect on Potential

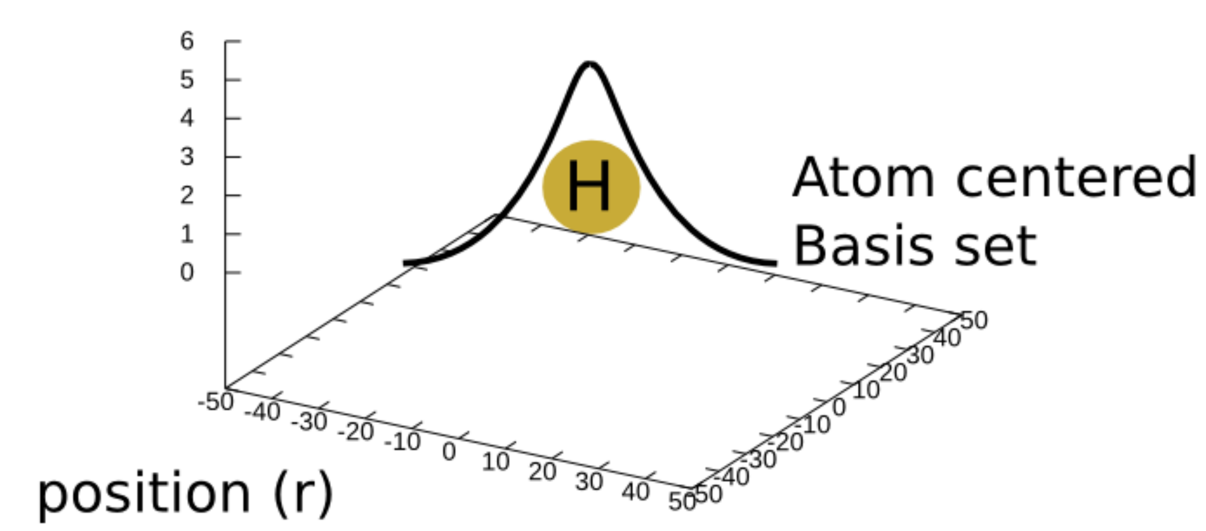




Basis Set

Molecular wavefunctions are extremely complex, so we need to use other functions to approximate them. In our research, we combine multiple Gaussian functions because they are easy to use for calculations.

The wave equations for PIB problem, however, are easy to work with. I used multiple of these equations to form a basis for the one dimensional box.



Results

- As the strength of the electric field increases, the ground-state energy level decreases.
- Using more functions in a basis set leads to a more accurate estimate of the energy level.

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