Project Title:

Atoms and molecules driven by relativistic laser fields

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Background and purpose

In atomic and molecular strong-field physics, the process of electron rescattering is a central concept [1]: an electron ejected from an atom (or molecule) by field ionization is accelerated in the laser field and returns to the atomic core at high kinetic energy. Upon this return, several interesting processes can take place: emission of a high-energy photon (high harmonic generation), scattering, or ejection of a bound electron by impact ionization.

With a number of planned laser facilities such as the ELI [2], it is expected that laser intensities of the order of $10^{22}$ W/cm$^2$ or above will become routinely available in the near future. Since high laser intensity implies a strong electric field, it is of interest to consider the possibility of inducing recollision with particles heavier than electrons, for example protons. A proton accelerated to kinetic energies high enough to induce a nuclear reaction would enable the temporal control of nuclear processes on the sub-fs level, if we could make the proton recollide with another nucleus. For a proton, an impact energy (in the rest frame of the target nucleus) of about 1 MeV or greater is required for non-negligible. To accelerate protons directly to MeV energies, laser intensities of ~$10^{22}$ W/cm² are needed for 800 nm laser fields.

The aim of the project that has been undertaken during the present fiscal year is to demonstrate theoretically that it is feasible to induce nuclear reactions by proton recollison [3]. We propose to irradiate a neutral molecule, composed of a heavy nuclear isotope and one (or a few) protons, with a short, intense laser pulse. At the rising edge of the pulse, all electrons are instantaneously ejected by field ionization. This leaves a bare molecule stripped of all electrons, which would dissociate by the repulsive Coulomb force in absence of the laser field. In the presence of the intense laser field, however, the proton(s) are accelerated so as to overcome the Coulomb repulsion, and may (with some probability) collide with the nearby heavy nucleus. If the kinetic energy of the proton is high enough, this collision may induce a nuclear reaction. With the current proposal, we overcome limitations of previous realizations of proton recollison: In [4], exotic muonic molecules were required, and the setup suggested in [5] relied on the recolliding (alpha) particle being produced from alpha decay, which reduces the overall reaction rate. Furthermore, we extend the initial ideas in [6] by showing that the proton recollison process can be controlled by changing the carrier-envelope phase (CEP) of the laser pulse, and also by aligning the molecule with a weaker prepulse.

Theoretical Method

To theoretically calculate the probability of a nuclear reaction induced by proton recollison within a laser-driven molecule, we focus on the concrete example of a $^{15}$NH molecule (imidogen with the nitrogen-15 isotope), and the nuclear reaction $^{15}$N($p,\alpha$)$^{12}$C (alpha particle emission by proton impact on nitrogen). The probability for a $^{15}$N($p,\alpha$)$^{12}$C reaction to occur when $^{15}$NH is subjected to an intense laser pulse is calculated by the classical trajectory Monte-Carlo method, in the following way: The proton and the nitrogen-15 nucleus are given initial positions according to a distribution derived from the ground state wave function for the internuclear distance in NH (the bond length is approximately 1 Å) and the degree of alignment of the molecule. Zero initial velocity is assumed. Then, we solve numerically the classical equations of motion

$$M_{N,p} \frac{d^2 \mathbf{r}_{N,p}}{dt^2} = e^2 Z_N Z_p a_{N,p} \left( \frac{\mathbf{r}_{p} - \mathbf{r}_{N}}{r_{p} - r_{N}} \right)^3 + e Z_{N,p} \left[ \mathbf{E}(t) + \frac{\mathbf{v}_{N,p}}{c} \times \mathbf{B}(t) \right],$$

where $M_{N,p}$, $Z_{N,p}$, $r_{N,p}$, and $v_{N,p}$ are the mass, charge number, position and velocity, respectively, of the nitrogen nucleus and the proton, $c$ is the speed of light, $a_{p}=1$, $a_{N}=-1$, and $\mathbf{E}(t)$, $\mathbf{B}(t)$ is the electromagnetic field of the laser pulse. The explicit form adopted for the linearly polarized electric field is $\mathbf{E}(t)=\hat{\mathbf{e}}(t)\sin(\omega t+\phi)$, where $\hat{\mathbf{e}}$ is the polarization vector, $f(t)$ is an envelope function, $\omega$ is the angular frequency, and $\phi$ is
the CEP. After obtaining many different trajectories starting from slightly different initial conditions, we estimate the total reaction probability per laser pulse and molecule by counting the number of trajectories where the proton recollides with the nitrogen nucleus at small impact parameter at sufficient high kinetic energy, as measured by the total cross section for the $^{15}$N($p,\alpha$)$^{12}$C reaction.

**Simulation results**

The results of a simulation running $10^6$ trajectories, at laser parameters $I=2.5\times10^{22}$ W/cm$^2$, pulse width 3 fs, wavelength 800 nm, assuming a $^{15}$NH molecule aligned in the propagation direction of the laser pulse, with an orientation parameter $<\cos\theta>=0.98$ show that the recollision probability is strongly dependent on the CEP. The most favorable value of the CEP yields a total probability (per pulse and per molecule) of $P=1.5\times10^{-9}$ for alpha particle emission. The probability of recollision is small, but should be measurable at future laser facilities [3]. Employing an unaligned molecular ensemble reduces the total recollision probability with more than one order of magnitude. Further analysis of the recollision trajectories [3] reveals the importance of including also the magnetic part ($\nu/c\times B$) of the Lorentz force in the equations of motion. This force is responsible for the acceleration of the proton (and the nitrogen nucleus) in the laser propagation direction.

**Conclusions**

We have shown, by means of classical trajectory simulations, that alpha particle emission induced by proton recollision with the nitrogen nucleus in the $^{15}$NH molecule is possible, and that the recollision process can be controlled by varying the CEP of the laser pulse. Although the effect is largest for short pulses and strongly aligned molecules, non-negligible reaction probabilities are obtained also for slightly longer pulses and unaligned molecules. This process may provide an opportunity for an interesting experiment that can be performed at upcoming, ultra-intense laser facilities.

**References**

[Publication]

[Oral presentation at an international symposium]

[Others]
E. Lötstedt and K. Midorikawa, “Relativistic effects in strong-field double ionization” (poster), 11th European conference on atoms, molecules and photons (ECAMP 11), June 24-28, 2013, Aarhus, Denmark.