INTENSE LASER-DRIVEN ATOMIC PROCESSES

Anthony F. Starace

The University of Nebraska-Lincoln,
Department of Physics and Astronomy,
116 Brace Laboratory,
Lincoln, NE 68588-0111
Research Focus: Realistic theoretical and computational description of energy transfer processes from the intense EM radiation to matter.

Illustrative Research Projects:

1. Laser acceleration of electrons to GeV energies (DOE)
2. Laser-induced double ionization of Li$^-$ (DOE)
3. Time-dependent effective range theory description of intense laser interactions with negative ions (NSF)
GeV Electrons from Ultra-Intense Laser Interaction with Highly Charged Ions

Suxing Hu and Anthony F. Starace

Department of Physics and Astronomy,
The University of Nebraska-Lincoln
Lincoln, NE 68588-0111
Geometry of Intense Laser Ionization of a Highly Charged Ion Target

J.D. Gillaspy, JPB 34, R93 (2001): “Any charge state of any ion can be produced.”
Three Dimensional (3D), Classical Relativistic Monte-Carlo Method
[Leopold and Percival, PRL 41, 944 (1978); Schmitz et al., PRA 57, 467 (1998)]

1. **Prepare a “micro-canonical ensemble”** to represent the initial ion target.

2. **Numerically integrate** the relativistic Newtonian equations:

   \[
   \frac{dr}{dt} = \frac{p}{\gamma}, \\
   \frac{dp}{dt} = - (E_L + E_C + p \times B_L / \gamma c), \tag{1}
   \]

   where \( \gamma \equiv \sqrt{1 + p^2 / c^2} \) is the relativistic factor in atomic units. Initial conditions are chosen randomly from the micro-canonical ensemble.

3. **Repeat step (2)** until a statistically unchanged result is obtained.
Illustration of Electron Energy Gain Prior to Ionization of Fe$^{25+}$

$I = 2 \times 10^{22} \text{ W/cm}^2$, $\lambda = 1054 \text{ nm}$, 15-cycle laser pulse, $w_0 = 10 \mu\text{m}$. 
Illustration of Electron Energy Gain Following Ionization of V^{22+}

\[ I = 8 \times 10^{21} \text{ W/cm}^2, \lambda = 1054 \text{ nm}, 15\text{-cycle laser pulse, } w_0 = 10 \mu\text{m}. \]
3D Classical, Relativistic Monte Carlo Results for $V^{22+}$

Note: 12,000 trajectories calculated; 4,000 were ionized.
GeV Electrons: Computational Challenge

Current: Classical relativistic calculations:
(a) 12,000 trajectories
(b) Time needed: 4-5 days with 32 processors

Desirable: Quantum relativistic (Dirac) calculations:
(a) Fine mesh in both space and time
(b) Four-component quantum wave function
(c) Spatial grid: $2000 \times 2000 \times 500 = 2 \times 10^9$ points
(d) Time needed: 10 weeks with 64 processors
Two Electron Detachment by Half-Cycle and Single-Cycle Pulses

Two Electron Detachment

Geometry

\[ \gamma(h\omega) + e_k \rightarrow p_1 + p_2 \]

Long-range Coulomb interactions
Angular Distributions Produced by (a) HCP, (b) DHCP, and (c) SCP
Two Electron Processes: Numerical Challenges

One must calculate a five-dimensional wavefunction in 3-dimensional coordinate space:

$$\Psi = C \sum_{l_1, l_2, L} R_{l_1, l_2, L}(r_1, r_2, t) |l_1, l_2, L >$$

(1) Typically 8 values of L are used and a sphere of 300 a.u. is employed.

(2) For each value of L, the radial functions are expanded in terms of 3,000 spatial eigenfunctions.

(3) One run involves solving 20,000 ODEs.

(4) For short laser pulses and weak laser intensities, 24 hour run times are typical with a fast workstation having 1 Gb RAM.

(5) For long laser pulses and strong laser intensities, 50 hours with 200 processors is required.
Strong Field Detachment Processes

Anthony F. Starace

Department of Physics and Astronomy, The University of Nebraska-Lincoln

Collaborators

Mikhail V. Frolov, University of Nebraska-Lincoln, USA
Nikolai L. Manakov, Voronezh State University, Russia
Geometry

$V(\mathbf{r}, t) = eF(t)\mathbf{r}$,

$F(t) = F \text{Re} \left\{ e^{-i\omega t} \right\}$,

$e = \hat{\varepsilon} + i\eta[\hat{k} \times \hat{\varepsilon}]$

$l = \frac{1 - \eta^2}{1 + \eta^2}, \quad \xi = \frac{2\eta}{1 + \eta^2}$. 

Laser Beam
Angular Distributions

Linear polarization ($\xi = 0$)

S-state

P-state

$\xi = 0$

$E_n/U_p \approx 1$

$E_n/U_p \approx 2$

$E_n/U_p \approx 4$

$E_n/U_p \approx 6.0$

$E_n/U_p \approx 7$

$E_n/U_p \approx 8$
Numerical Aspects for Intense Laser-Atom Interactions

(1) Effective range approach involves matrices having $200 \times 200 = 40,000$ elements.

(2) Calculation of the matrix elements takes about 1/2 hour on a single processor.

(3) During course of the calculation, the matrix must be calculated 10-15 times for a single laser intensity.

(4) To describe a laser pulse, typically 100 laser intensities are employed.

(5) Time required for calculation is 5,000 hours on a single processor, or about 1 week using 30 processors.
Conclusions

Intense laser interactions with atoms requires fast processors having large memory capability because:

(1) Events must be followed in time.
(2) Laser intensity varies throughout a laser pulse.
(3) Interactions are non-perturbative.
(4) High laser intensities require a relativistic treatment.
(5) Complexity increases the larger the number of particles that are simulated.