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FELLA – the free electron laser atomic, molecular, and optical physics program package

Christian Buth, Robin Santra

Atomic, Molecular, and Optical Physics Group

Chemical Sciences and Engineering Division

Intellectual Property Decision Group (IPDG) Meeting, March 11, 2008

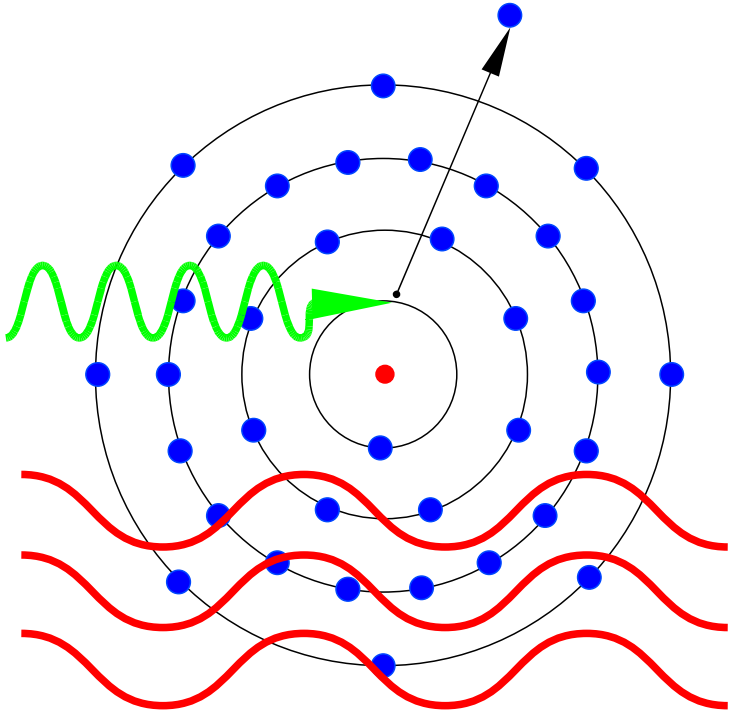
Contents

What means FELLA?

- FELLA stands for **free electron laser atomic, molecular, and optical physics program package**

- X-ray free electron laser: a novel light source
  - Stanford, California, USA
  - Hamburg, Germany
  - Harima Science Garden City, Hyogo, Japan

- Primary mission: laser-matter interaction



Modules of FELLA

- FELLA is a collection of programs and libraries

- Atomic physics
  - `hermsk, oneel, giant, mulph, twoph, dreyd`
- Molecular physics
  - `alignmol`
- Optical physics
  - `pulseprop`

- Libraries: `lanczos, anglib, ...`

Software engineering

- Written in **FORTRAN95**
- Latest release is version 1.2.0
- Runs under any operating system with the free `g95` compiler
- About **two man-years** of software development
- Code consists of 15,950 lines or 535,721 characters

Authors

- **Mostly** written by Robin Santra and Christian Buth
  - Contributed roughly the same amount
- `hermsk` by Herman, Skillman, and Pauli
- `oneel` by Greene, Baertschy and Christ
- `lanczos` from `CO-ADC` package by Meyer and Sommerfeld
  - Lesser GNU General Public License
- `anglib` by Stevenson
  - Lesser GNU General Public License

Internet platform for CO-ADC program package

CO-ADC - Trac - Opera

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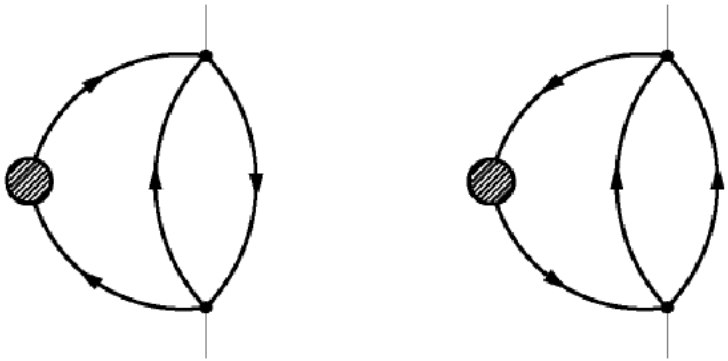
Crystal orbital algebraic diagrammatic construction



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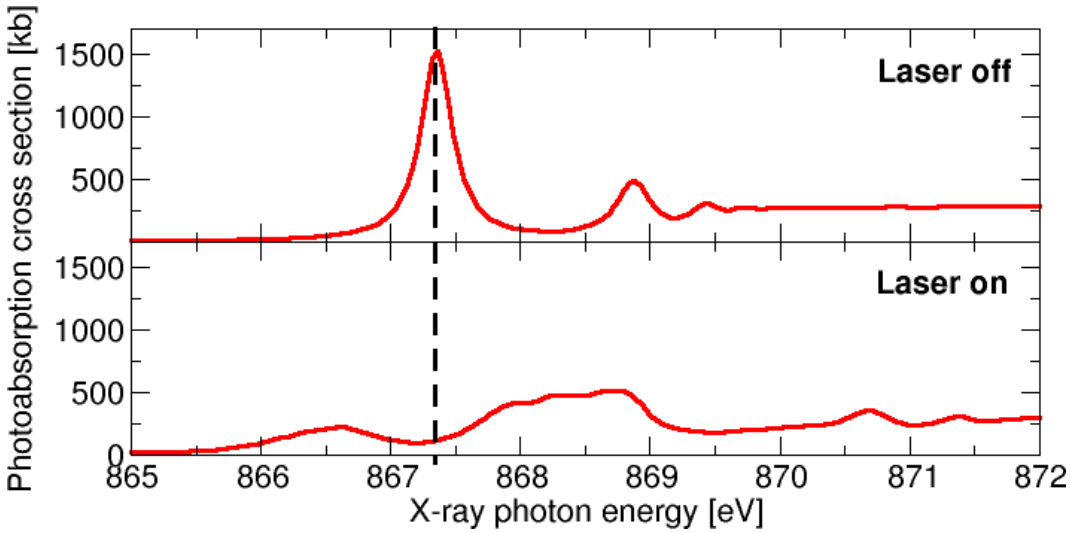
Effect: Electromagnetically induced transparency for x rays

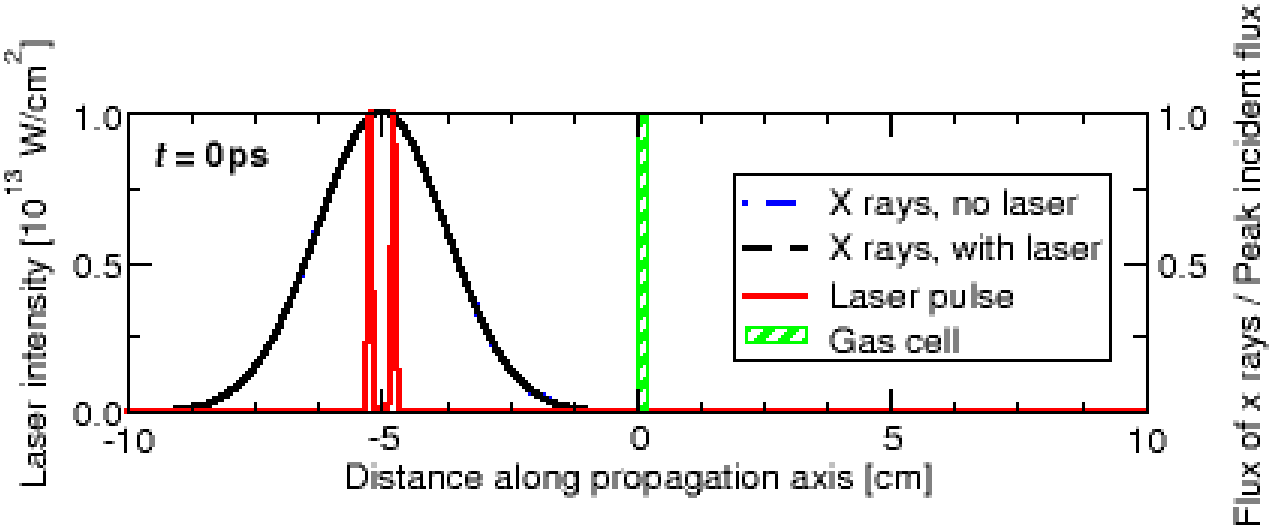
- Shine x rays on neon gas => **x rays are absorbed**
- Shine laser and x rays simultaneously on neon gas => **gas transparent for x rays**
- Electromagnetically induced transparency for x rays
- `dreyd` module of FELLA



[Buth, Santra, Young, Phys. Rev. Lett. 98, 253001 (2007)]

Application: Ultrashort pulse shaping of x rays

- Neon gas cell
- Laser pulse shape is **imprinted** on x rays
- Invention: x-ray pulse shaper **ANL-IN-07-055**
- `pulseprop` module of FELLA



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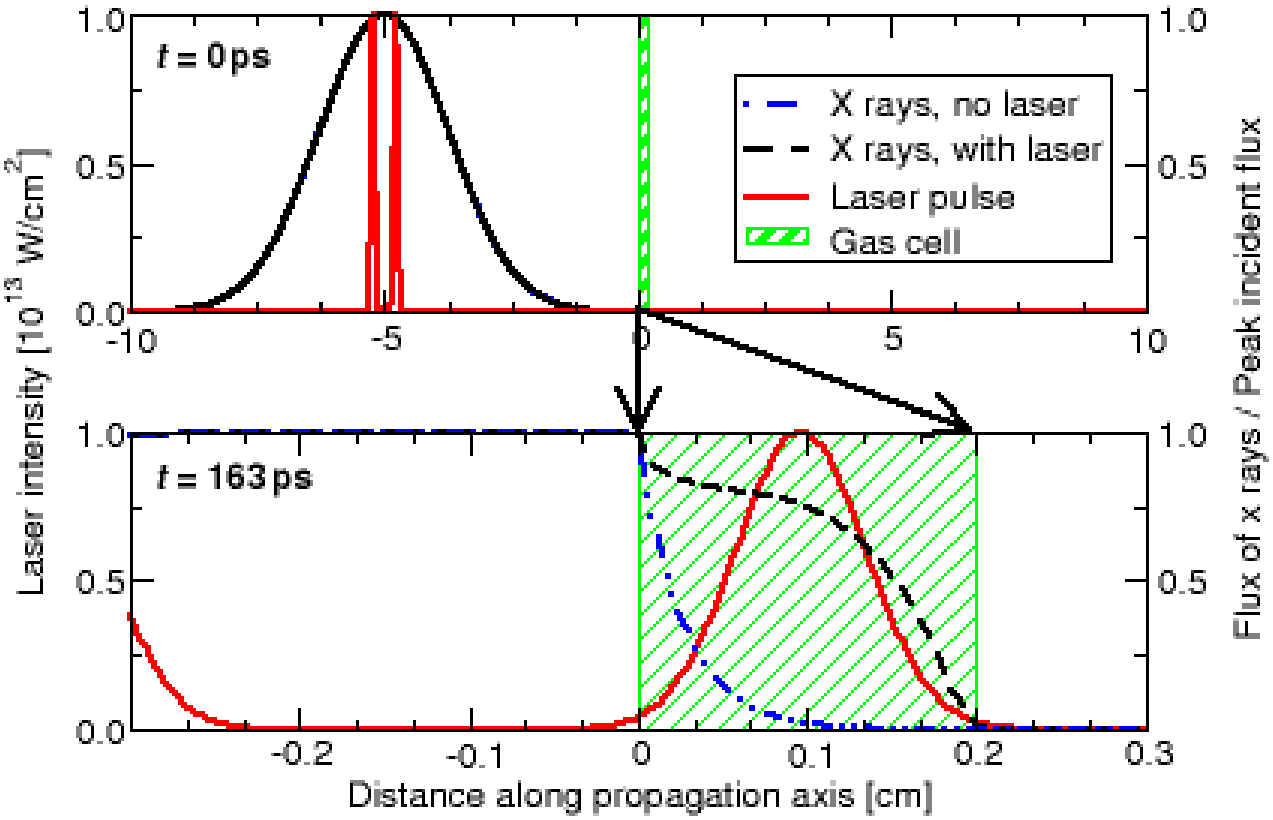

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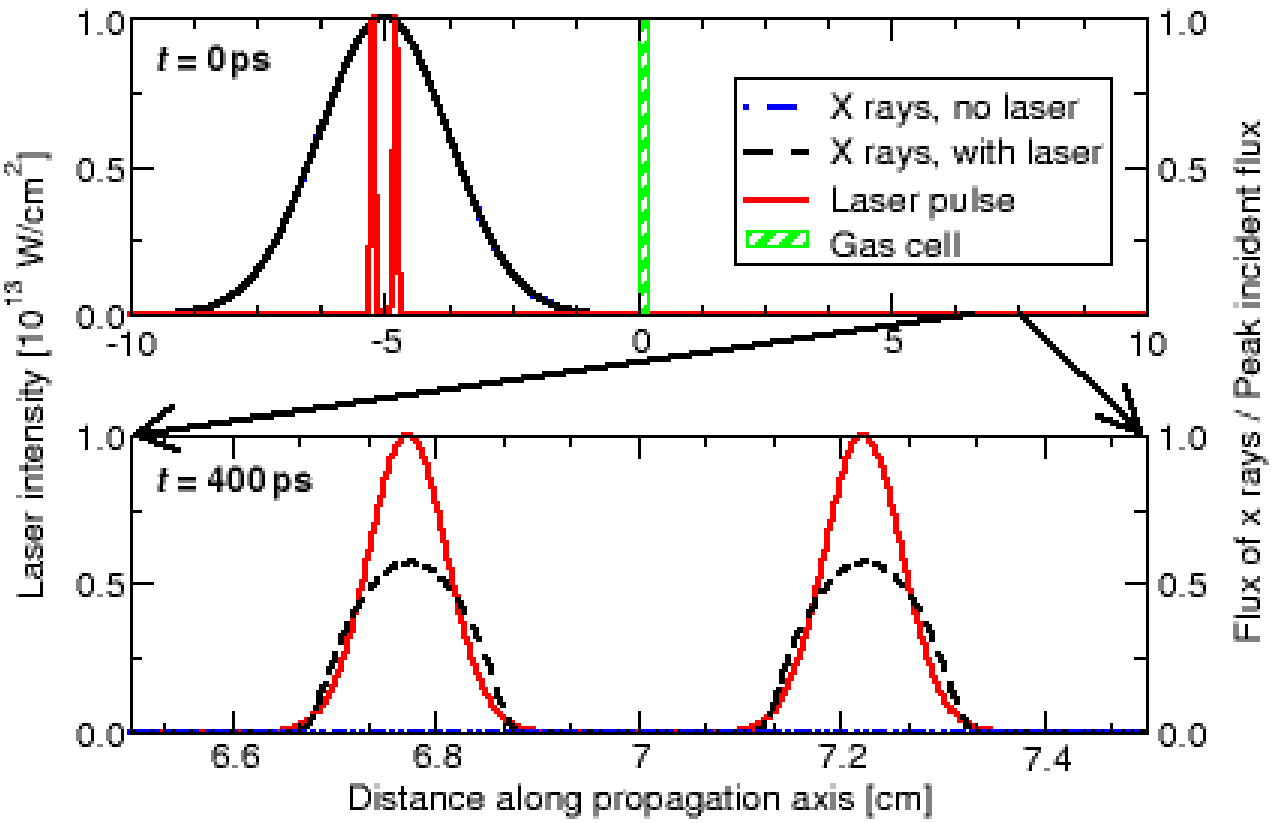
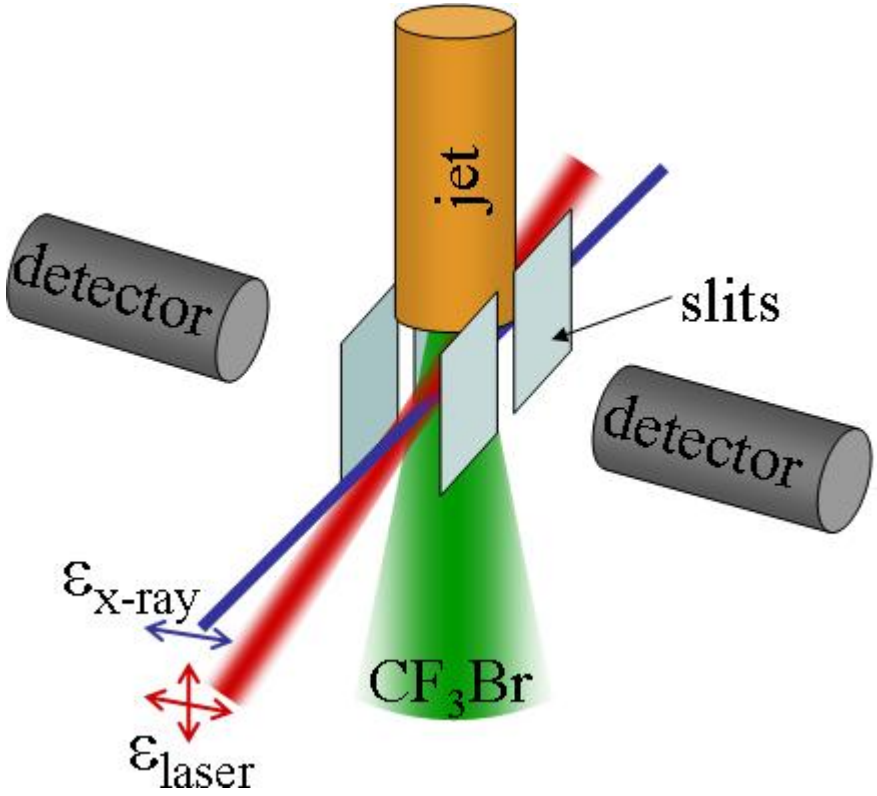


[Buth, Santra, Young, Phys. Rev. Lett. 98, 253001 (2007)]

Contents

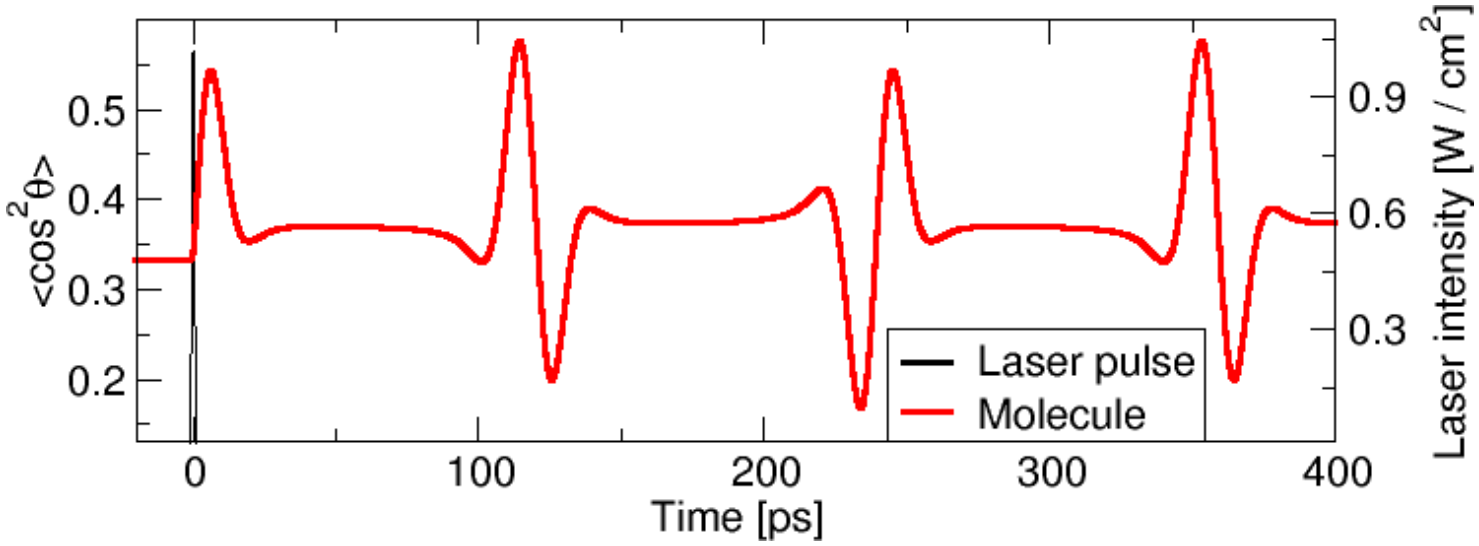
X-ray absorption by laser-aligned molecules

- Bromotrifluoromethane (CF_3Br) gas jet
- Laser and x-ray beam overlap
- Measure x-ray absorption
- `alignmol` module of FELLA



[Buth, Santra, Phys. Rev. A 77, 013413 (2008)
Peterson *et al.*, Appl. Phys. Lett. 92, 094106 (2008)]

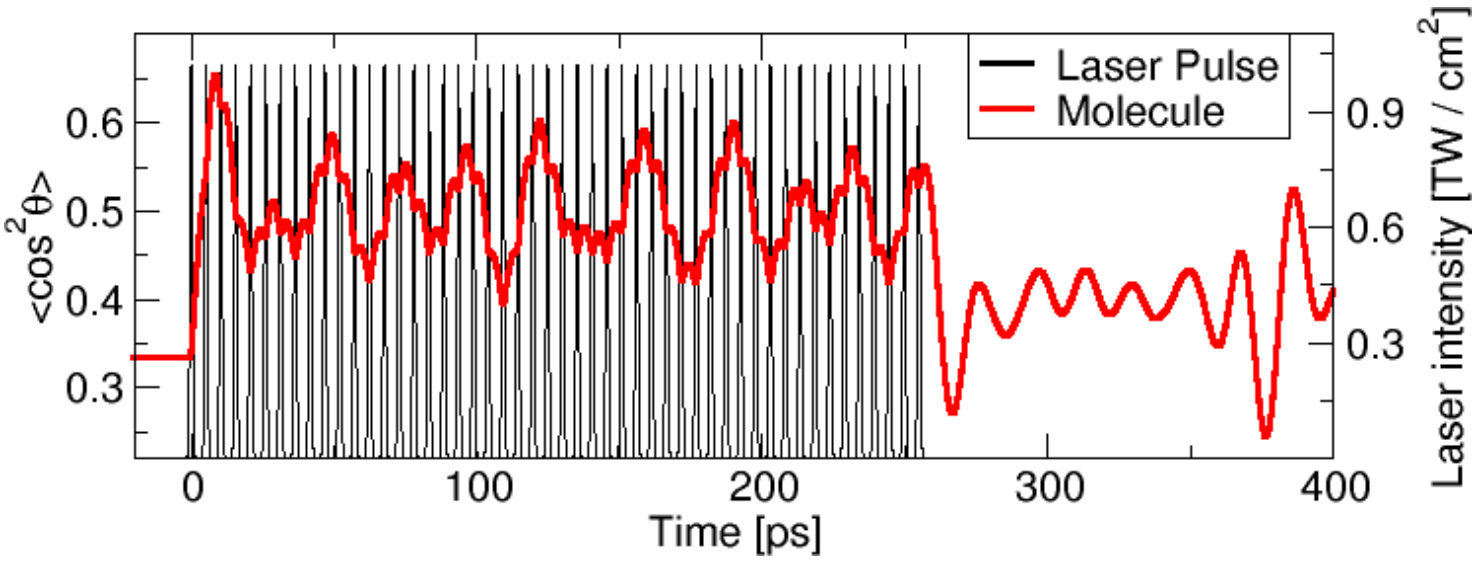
Picosecond clock



- Laser controls molecular rotation
- Rotation **imprinted** on x rays
- Picosecond clock

[Buth, Santra, J. Chem. Phys. 129, 134312 (2008)]

Optimal control of rotational motion



- Apply control theory
- Use sophisticated **laser pulse shaping** technology
- Obtain flexible x-ray pulse shapes

[Buth, Santra, J. Chem. Phys. 129, 134312 (2008)]

Conclusion

- FELLA is a versatile program package for atomic, molecular, and optical physics
- Interaction of light with atoms and molecules
- Used to **predict novel effect** electromagnetically induced transparency for x rays
- Used to study **control of x-ray absorption** by laser-aligned molecules