Statistical mechanics

Emanuele Coccia

Dipartimento di Scienze Chimiche e Farmaceutiche

Practical info

- ecoccia@units.it
- C11 building, fourth floor, room 453/454
- Wednesday 15h-17h (or whenever you want, just send an email to me)
- Register on Moodle
- Teams group:
  - "597SM - STATISTICAL MECHANICS - COCCIA EMANUELE (2020)"
  - Search it on https://corsi.units.it/didattica-a-distanza (insert "Coccia")

Programme

- Definition of statistical mechanics and concepts of thermodynamics

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- Quantum ideal gas: Fermi-Dirac and Bose-Einstein statistics

Where studying

- Lesson notes
- *Statistical mechanics: A concise introduction for chemists*, Benjamin Widom, Cambridge
- Notes on Moodle
- "Extra": *An Introduction to Statistical Thermodynamics*, Terrell L. Hill, Dover Publications

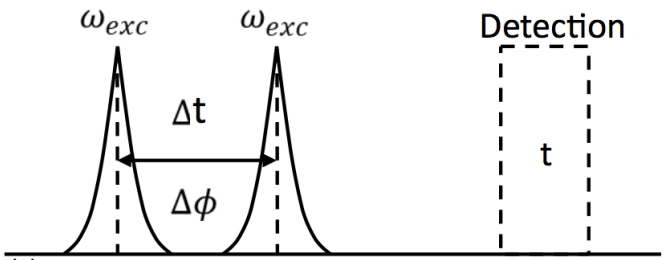
Exam

- Oral exam: (at least) three questions, possible simple numerical problems to solve
- Exam done in a lecture room (two rounds in winter session, two rounds in summer session, one round in september)

My research lines (for the master thesis)

Simulating time-resolved ultrafast spectroscopies: role of quantum coherence in molecules, metallic clusters and nanostructures

Collaboration with the University of Padova

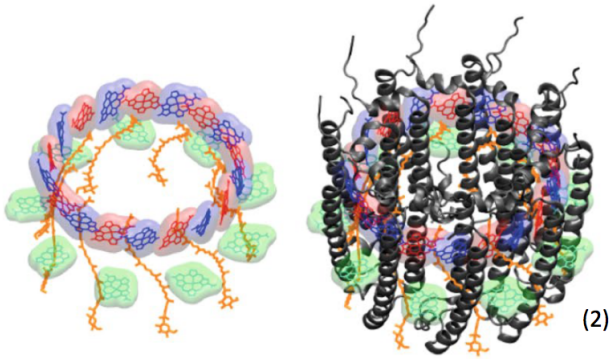


(1)

Ultrafast Spectroscopy →

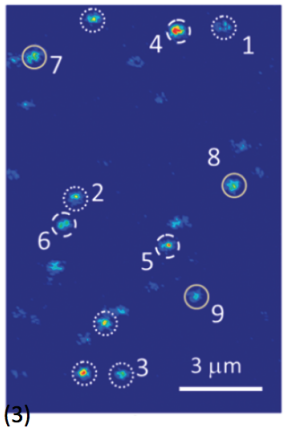
Ultrashort pulses to interrogate system dynamics

Femtosecond timescale processes


(2)

Coherence →

Superposition of quantum states



(3)

Single Molecules →

High spatial resolution

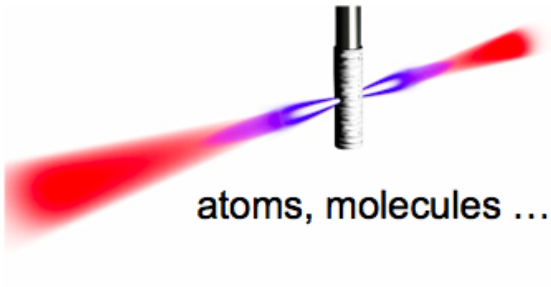
Prevent intrinsic inhomogeneity of molecules

Simulating nonlinear optical responses in strong electric fields: high-harmonic generation spectroscopy of molecules (H_2, CO_2, thymine, uracil, benzene etc.)

Collaboration with Sorbonne University in Paris (TCCM)

HHG is a nonlinear optical process

Laser source:
ω_L = 800 nm
10^{14}-10^{15} W/cm^2
linear polarization

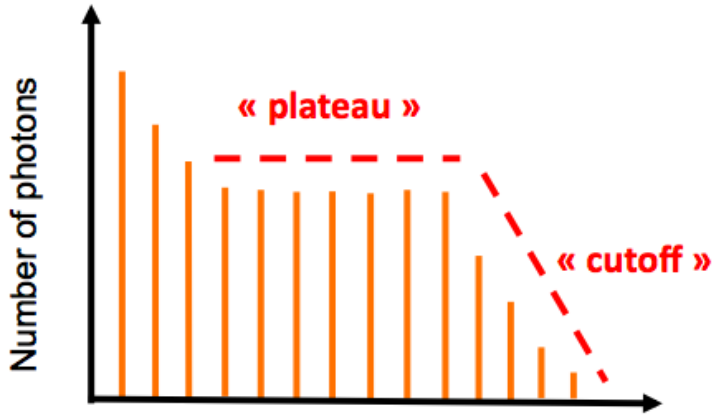


- **Energy: *XUV/Soft-X rays***
- **Temporal resolution: *attosecond pulses***

P. M. Paul et al. Nature **414**, 509 (2001)

Harmonic spectrum

LASER output



McPherson et al.
JOSA B **4**, 595 (1987)

$\omega_H=(2n+1)\ \omega_L$

Development and application of quantum Monte Carlo methods to the computation of electronic ground- and excited-state properties of molecules

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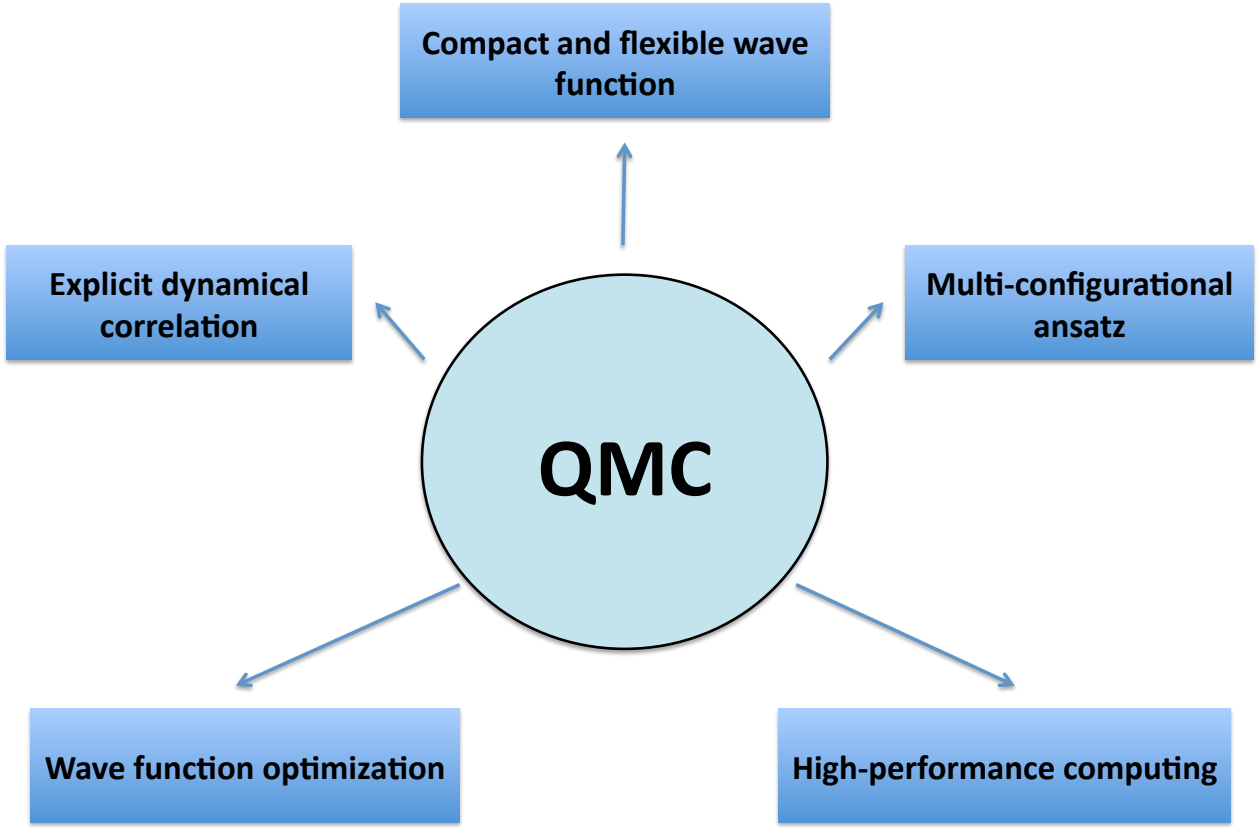

- Pros: Accurate, parallel, N_{el}^3 - N_{el}^4
- Cons: prefactor, error, no "black-box"