One- and two-electron processes in multi-center collisional systems
- codes development -

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J. Caillat

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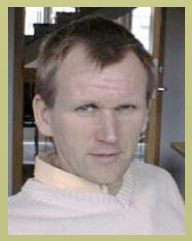


J.P. Hansen

T. Birrkeland

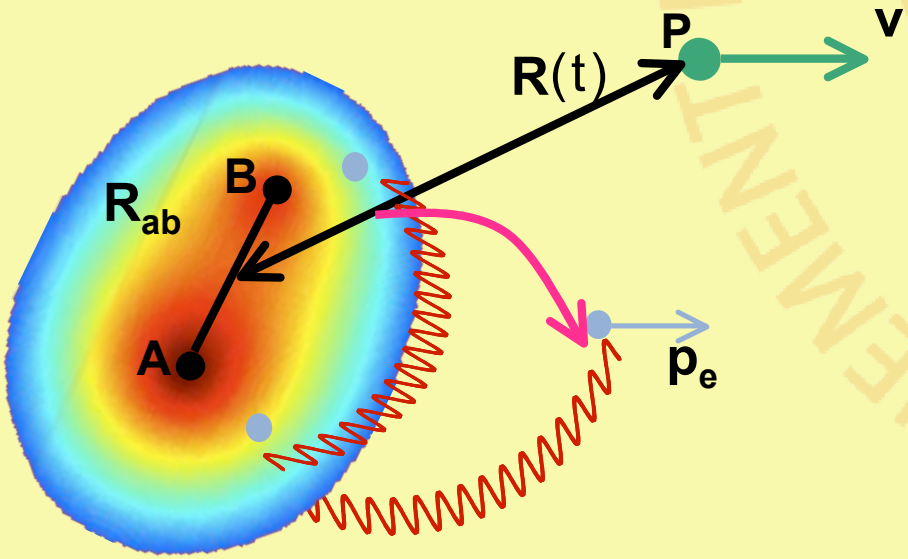
L. Sælen

I. Sundvor

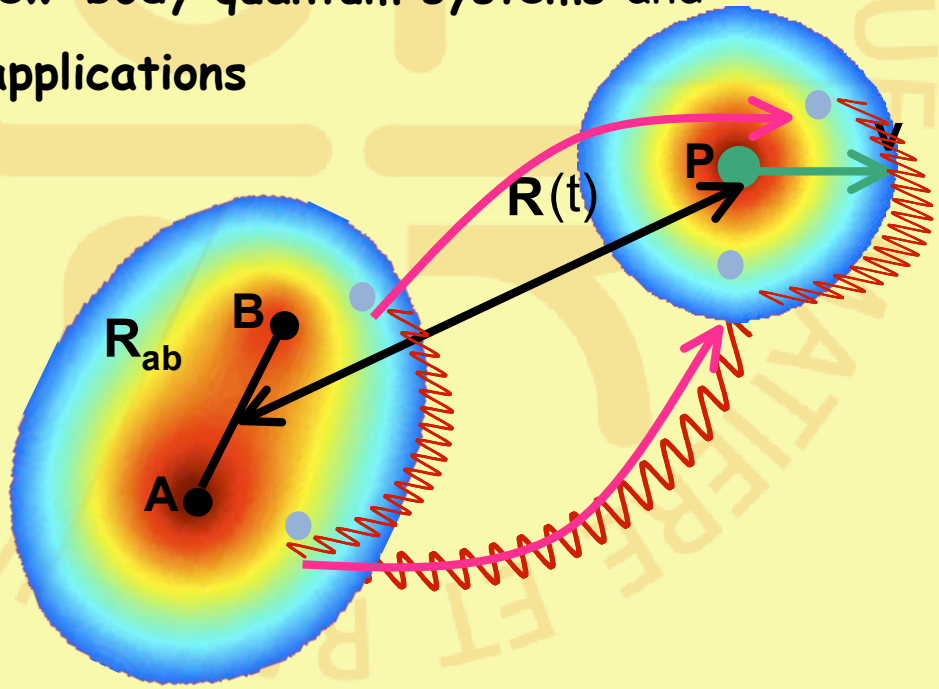
the Bergen team

MOTIVATIONS

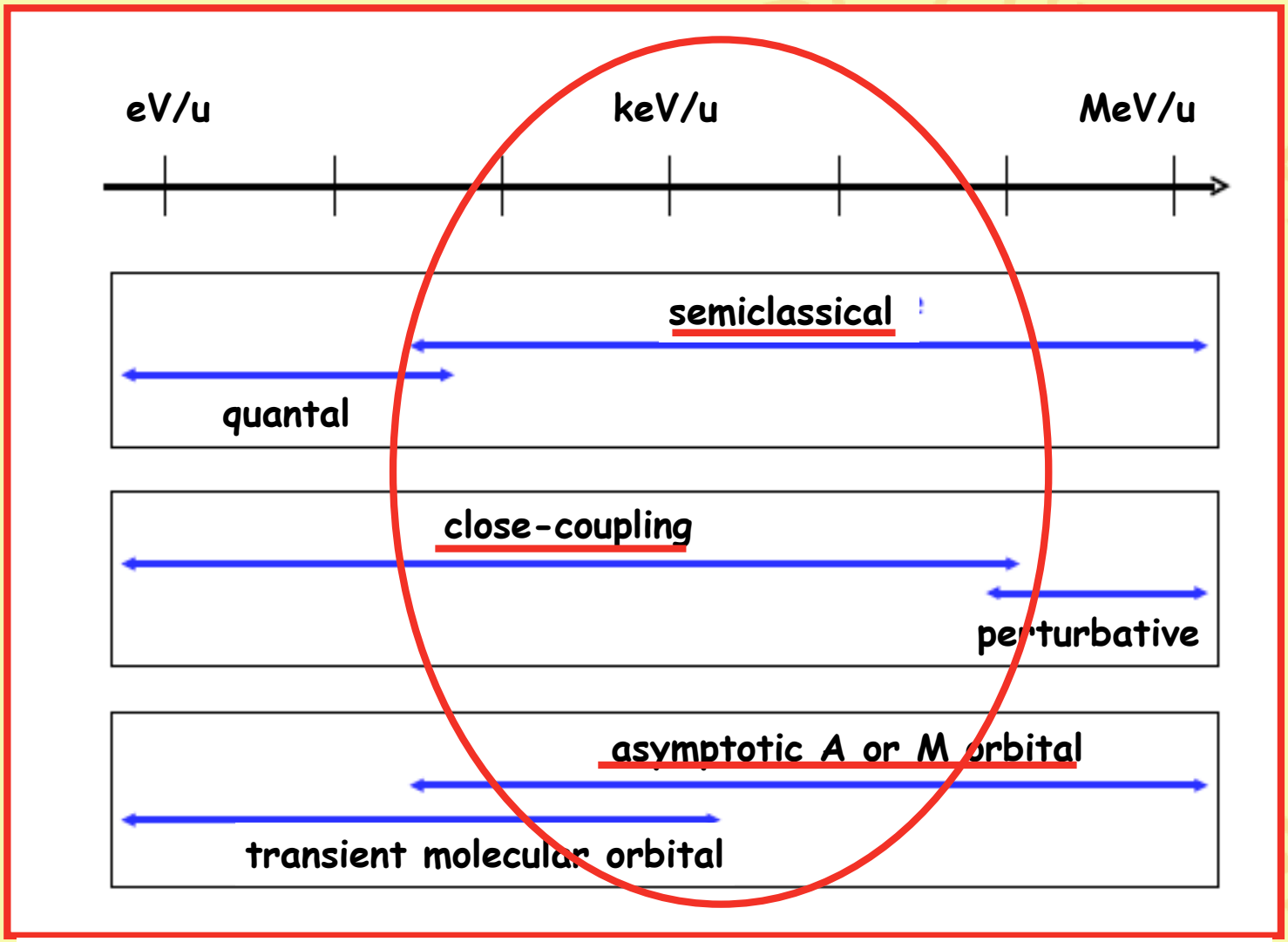
- the modelisation of
  - the **ultra-fast** dynamics of atomic and molecular systems
  - the interplay of the many open channels ⇒ non-perturbative treatments
  - Dynamical **electronic correlation** and the "complete" atomic/molecular electronic spectrum (including **continuum**)
- Fundamental aspects of **dynamical few-body quantum systems** and **computations** of cross sections for **applications**



Single ionisation of molecules



Double electron transfer from molecules to ions



Approximate regions of validity of various theoretical approaches.

Theoretical models :

✓ Semi-classical approach

$$\vec{R} = \vec{b} + \vec{v}\,t$$

$$\left[\hat{H}_{\rm el} - i\frac{\partial}{\partial t}\right]\Psi(\vec{r},t) = 0$$

$$\hat{H}_{\rm el} = -\tfrac{1}{2}\nabla^2_{\rm r} + V_{\rm Te} + V_{\rm Pe}$$

✓ Sudden approximation (R_{AB} fixed)

✓ Non-perturbative

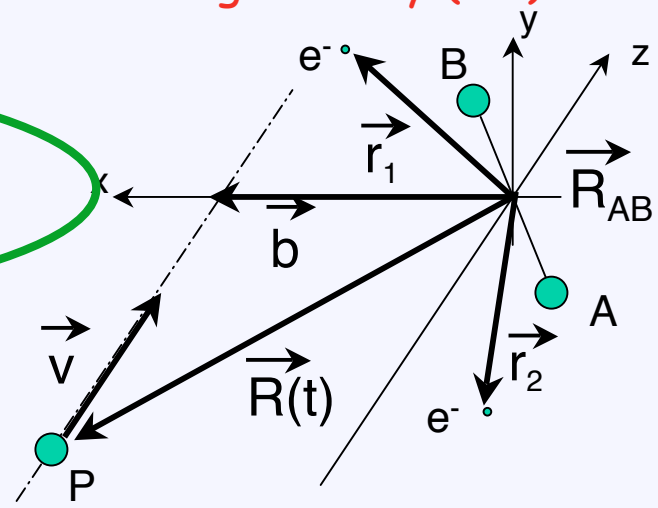
*** For high impact energies (> 1 Mev/u)**

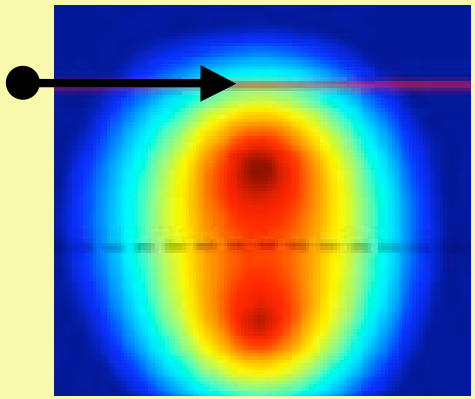
lattice representation : **1e**-(1-3)D, **2e**-1D

*** For intermediate energies (≈ 1 keV/u)**

travelling AO/MO basis sets expansion **2e**

Collision geometry (3D)





High (MeV) energy processes :

$$A^{q+} + H_2 \longrightarrow A^{q+} + H_2^+ + e^-$$

ionisation

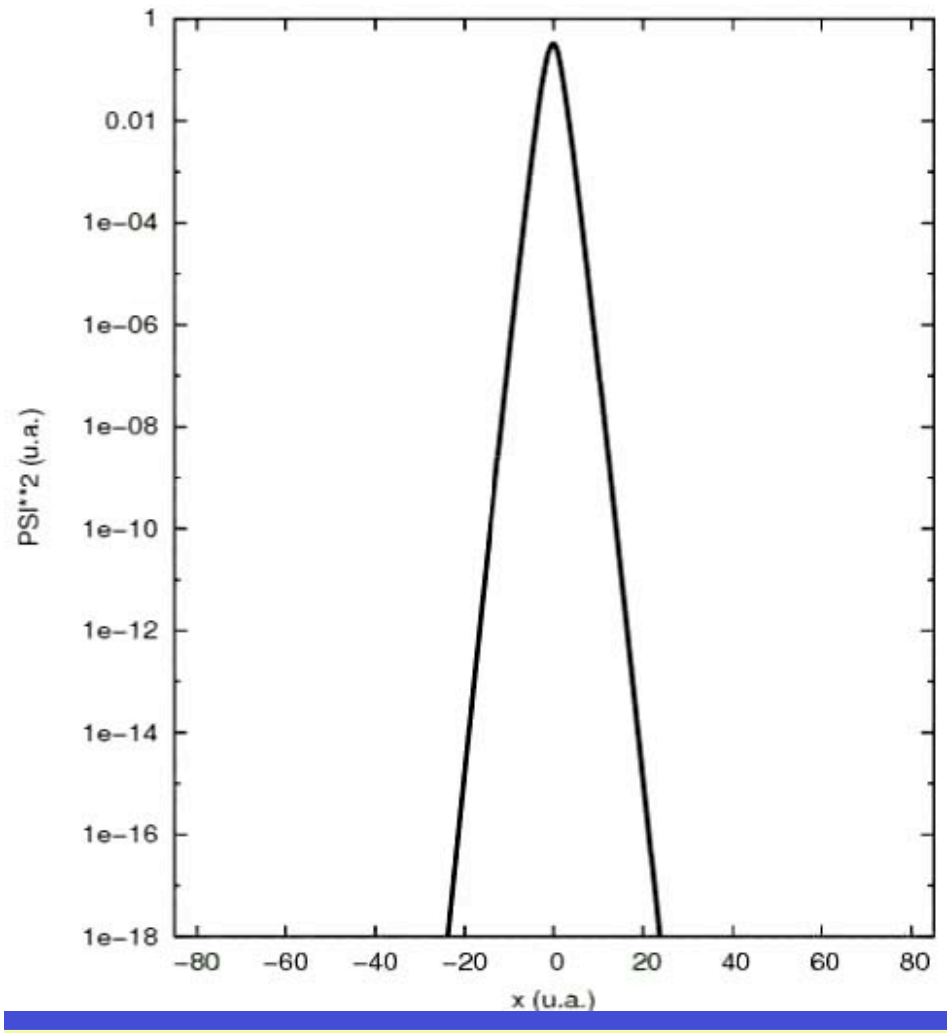
Lattice representation

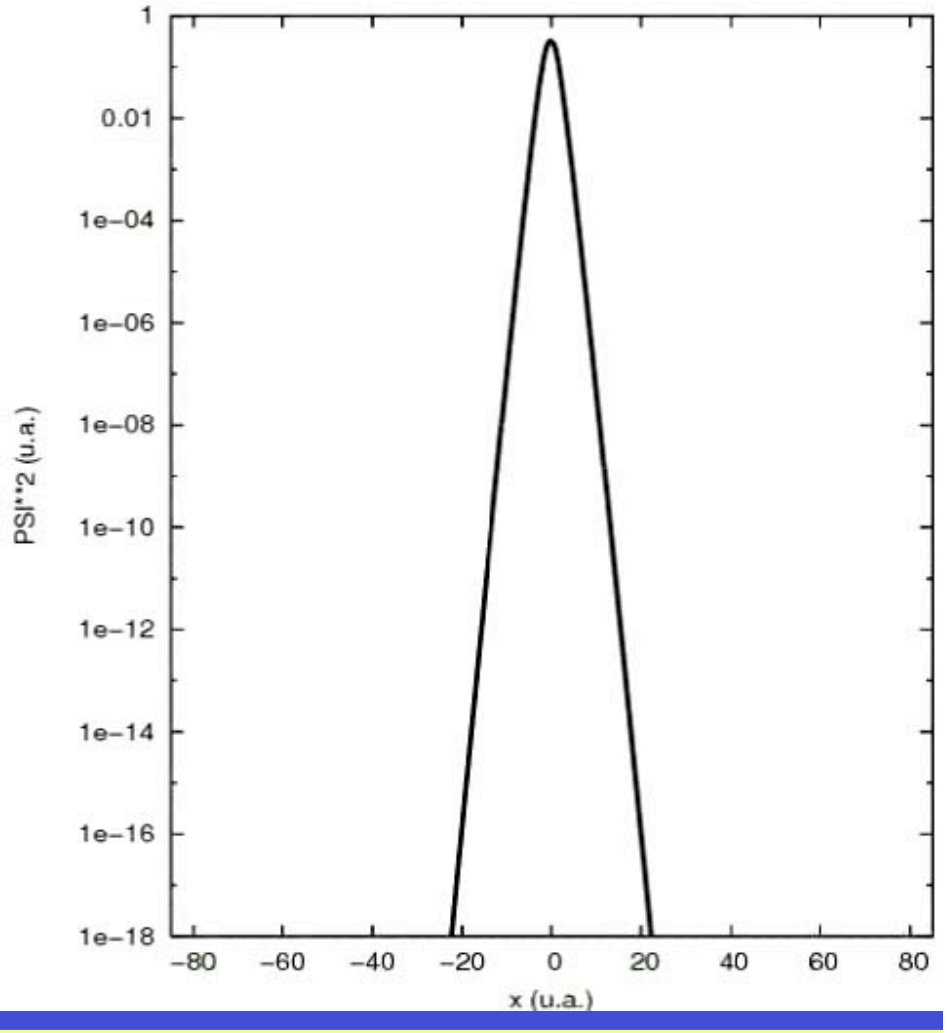
63 MeV/u

Kr^{34+} - H

1e - 1D

Kr^{34+} - H_2

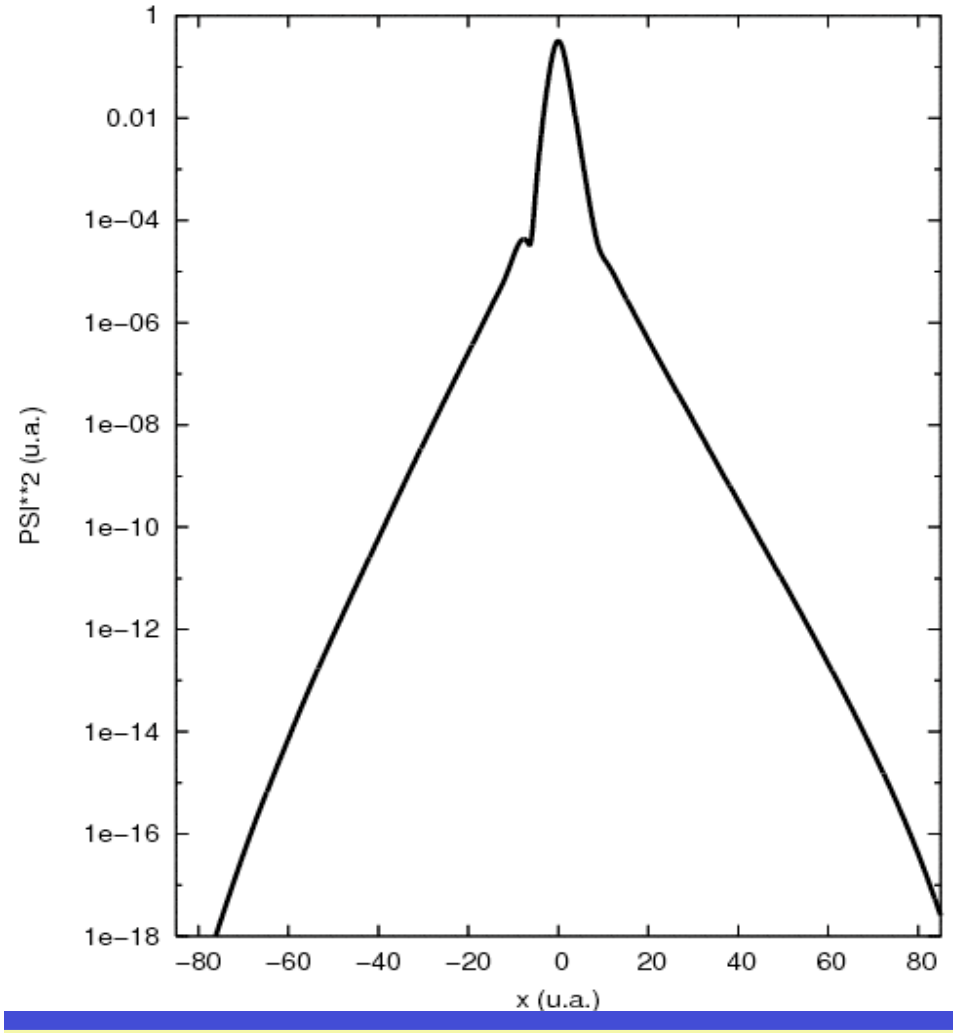


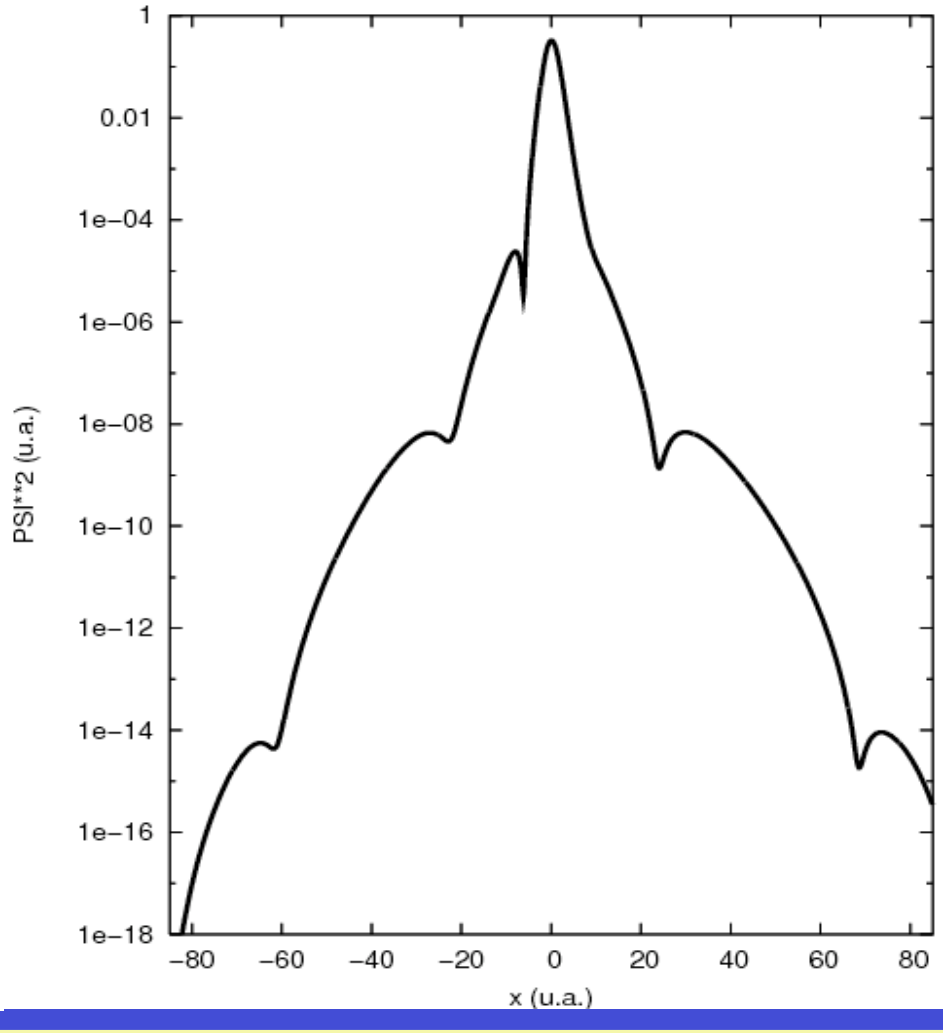


N. Sisourat, J. Caillat, A. Dubois and P. D. Fainstein, Phys. Rev. A **76**, 012718 (2007)

63 MeV/u

Kr^{34+} - H | **1e - 1D** | **Kr^{34+} - H_2**





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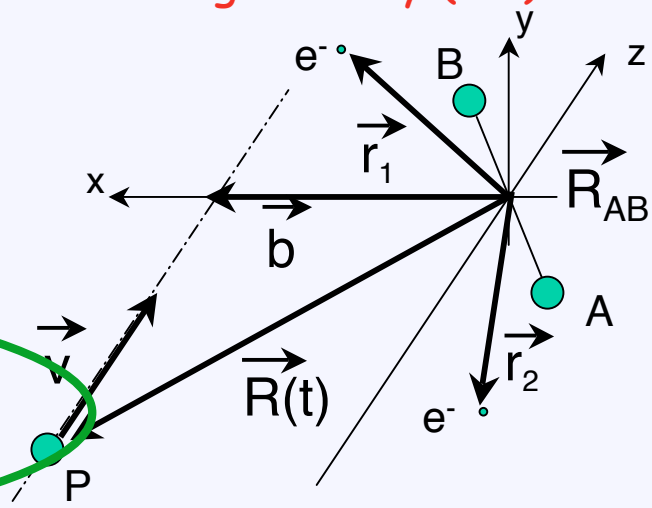
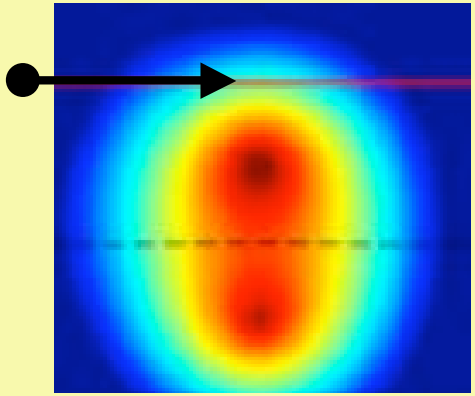


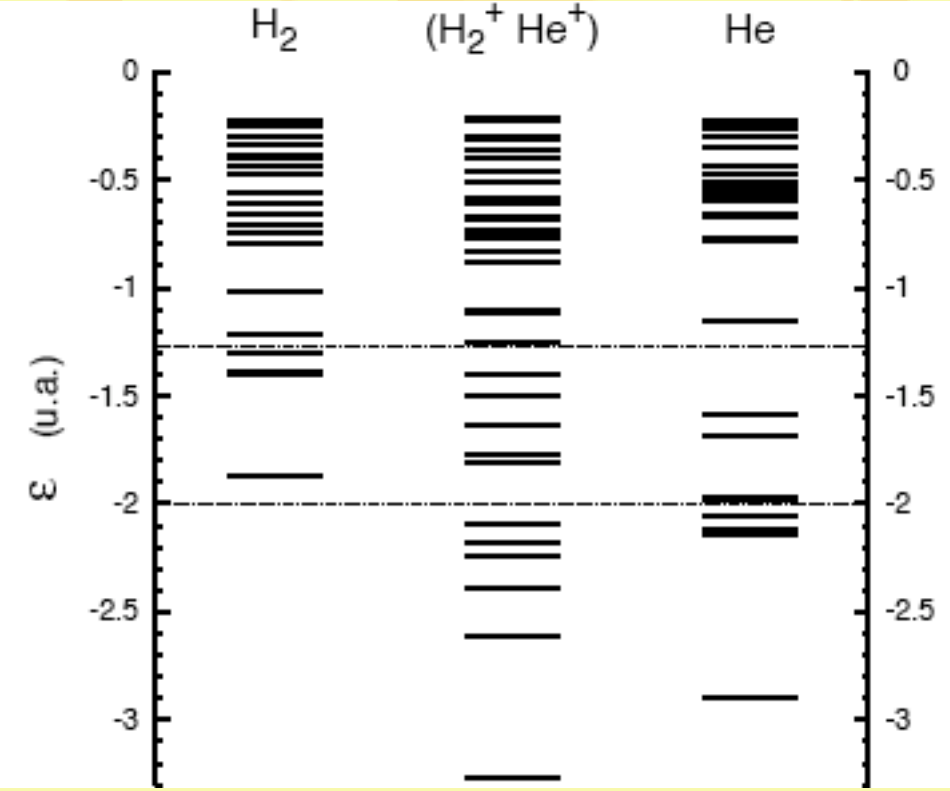


Intermediate (keV) energy processes :

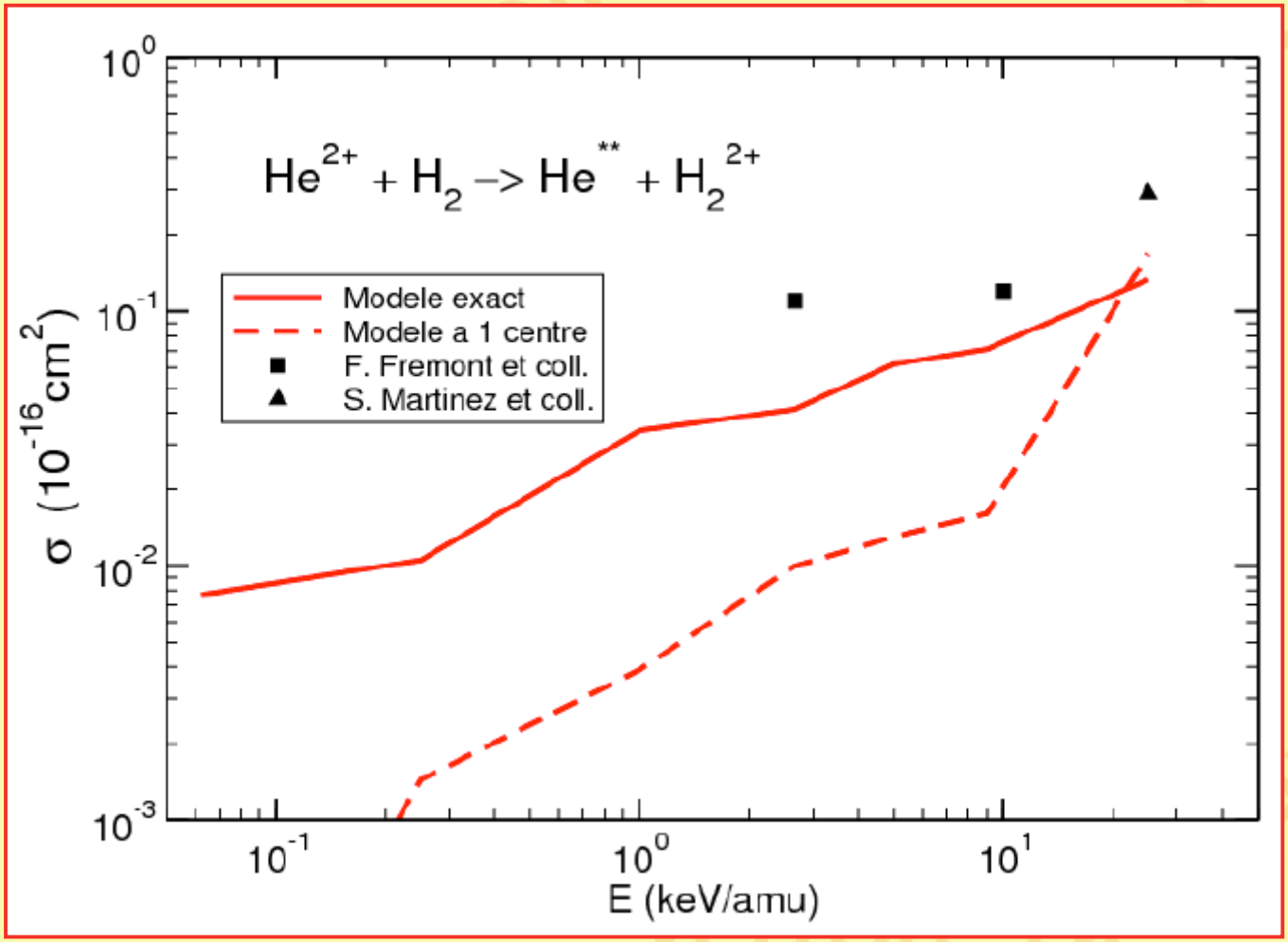
$$He^{2+} + H_2 \longrightarrow He^{**} + H_2^{2+}$$

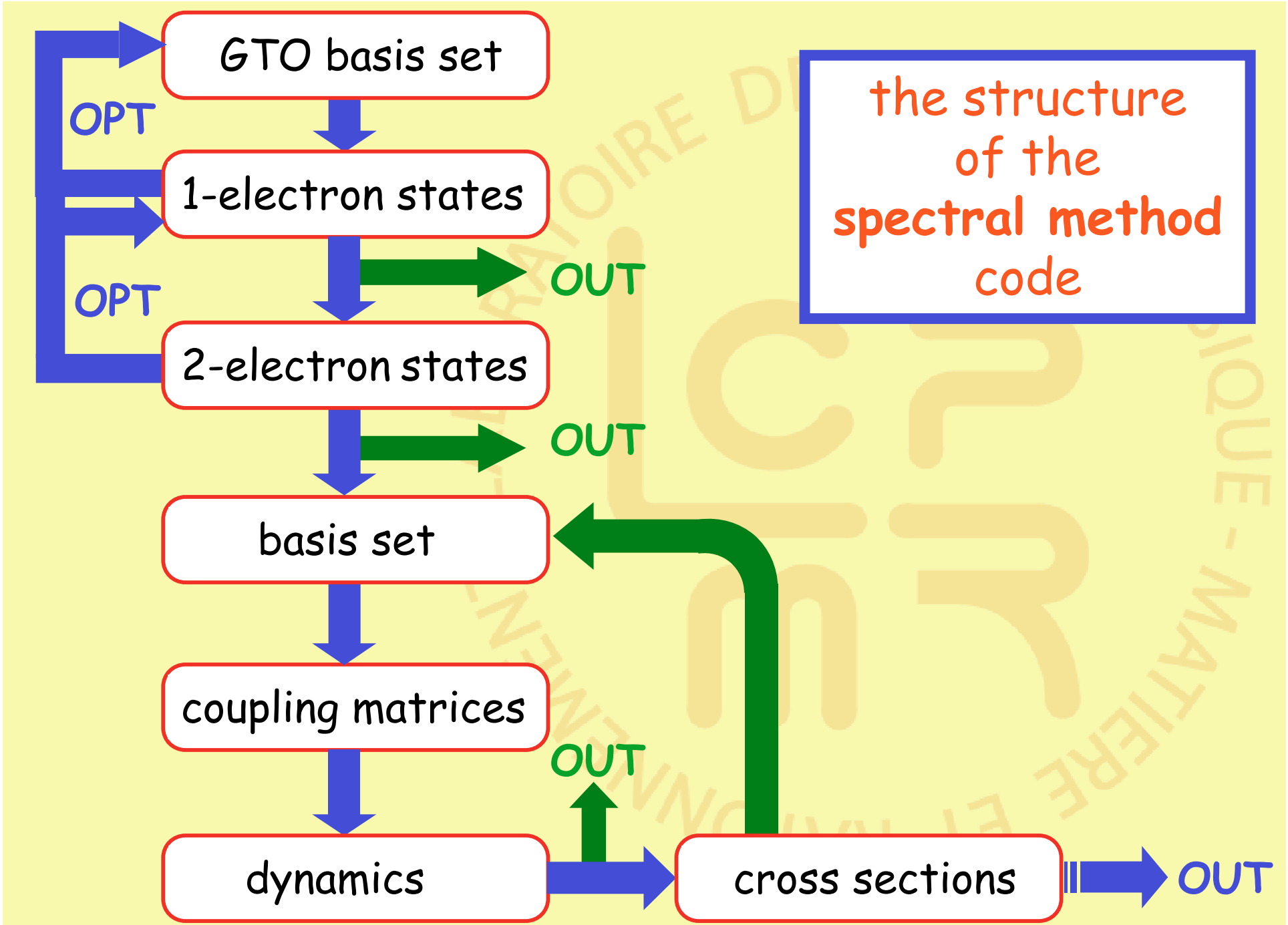
double electron transfer

Spectral method



double capture to autoionizing states




GTO basis set
OPT
1-electron states
OUT
OPT
2-electron states
OUT
basis set
coupling matrices
OUT
dynamics
cross sections
OUT
the structure
of the
spectral method
code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500 km
Bergen, J.P. Hansen
Copenhagen, S.E. Nielsen
Paris
A. Dubois
Vienna F. Aumayr
Garching
J. Schweinzer
Ísland
Norge
Sverige
Eesti
Ireland
Éire
United Kingdom
Danmark
Polska
Belarus
Deutschland
Luxembourg
France
Liechtenstein
Österreich
România
Srbija
България
Bulgaria
Portugal
España
Lisboa
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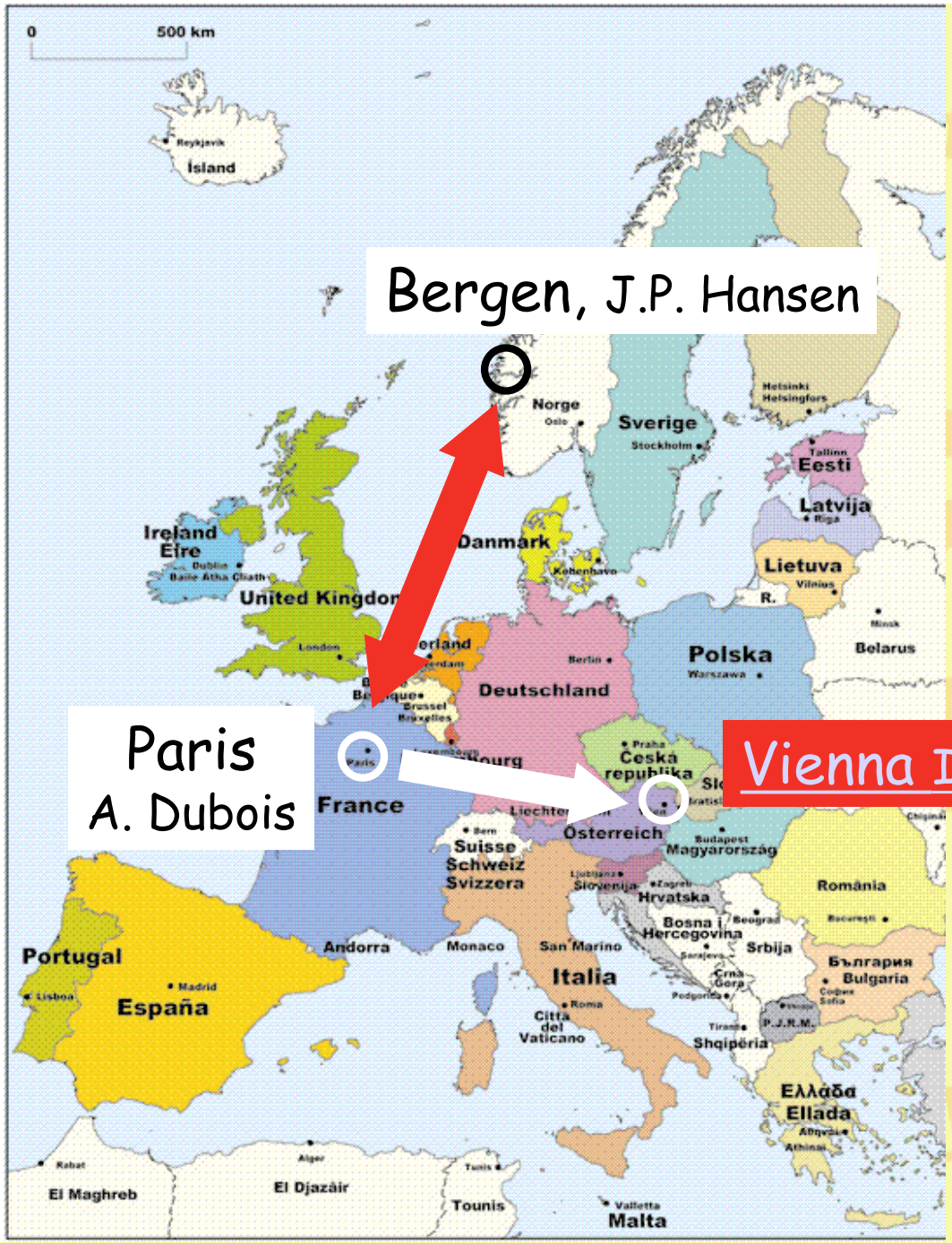
Shqipëria
Ελλάδα
Ellada
El Maghreb
El Djazáir
Tounis
Malta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Ελλάδα
Ellada
El Maghreb
El Djazáir
Tounis
Malta

IAEA A+M Unit action

- to transform a huge research code to a *safe* (but limited in use) **open code**,
- **implementation** @ IAEA with a web friendly (controled) interface (through individual invitations),
- provide the capacities to run the code @ IAEA,
- 2-4 customers per year, but not well informed,

FUTUR

- implementation on local computers at I.C.S. **Institut de Calcul et de la Simulation** @ UPMC
- extension to multi-electron collision systems, …
- keep the CCN meetings running with …
- organisation of specific meetings for code users.