Classical Trajectory Monte Carlo method – „Watching quantum physics in real time”

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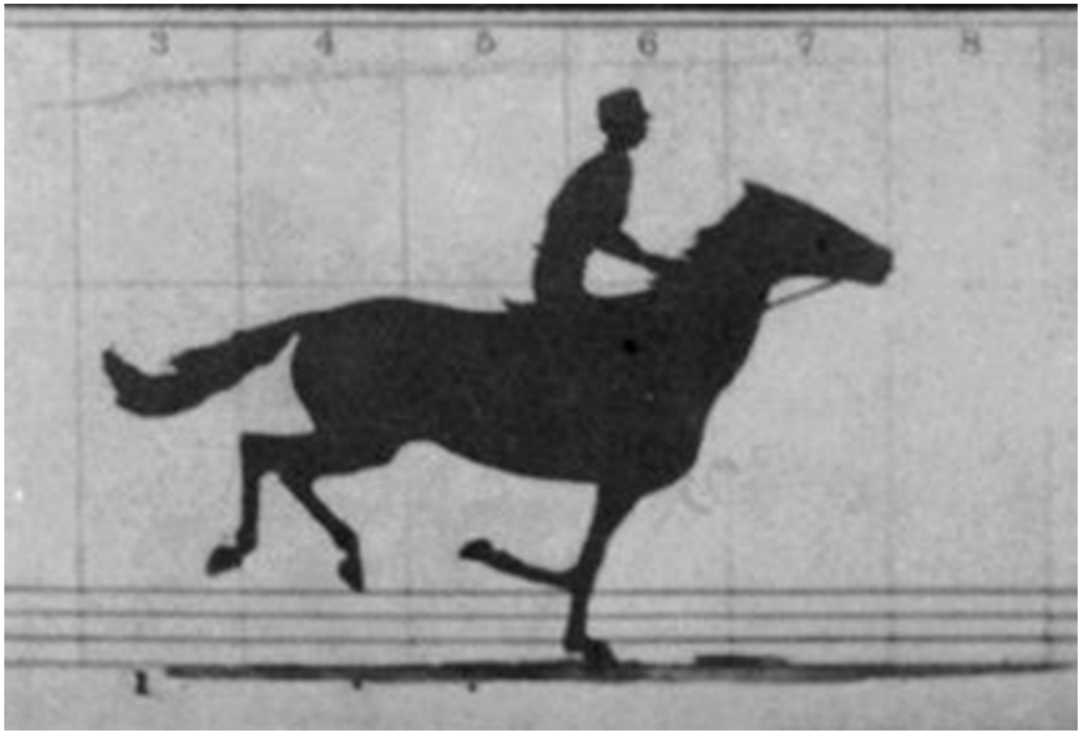
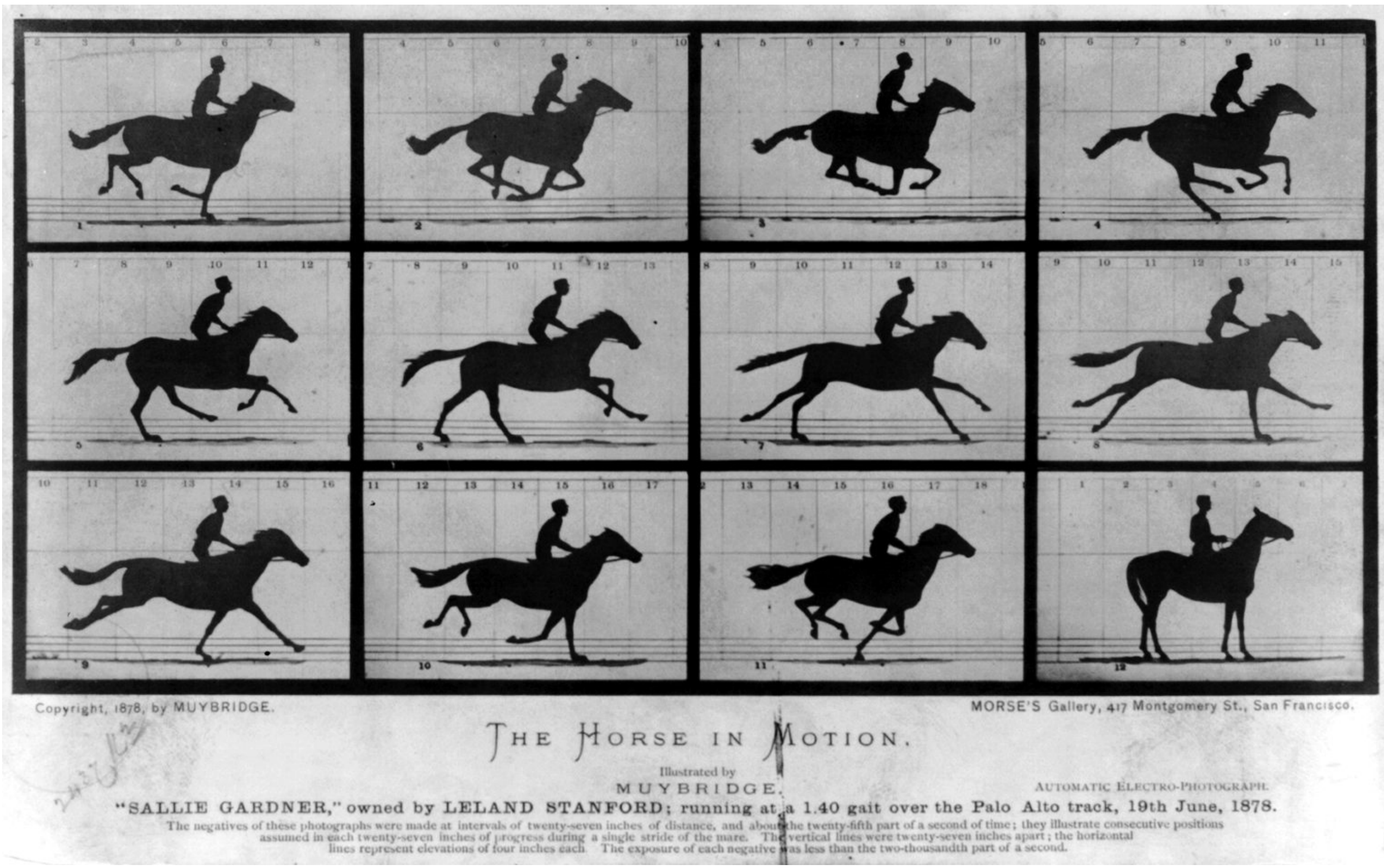
Horses: Time-resolved motion



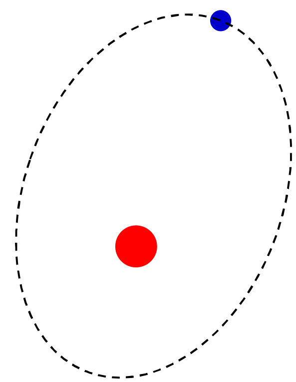
Eadweard Muybridge: The horse in motion (1878)

Horses: Time-resolved motion



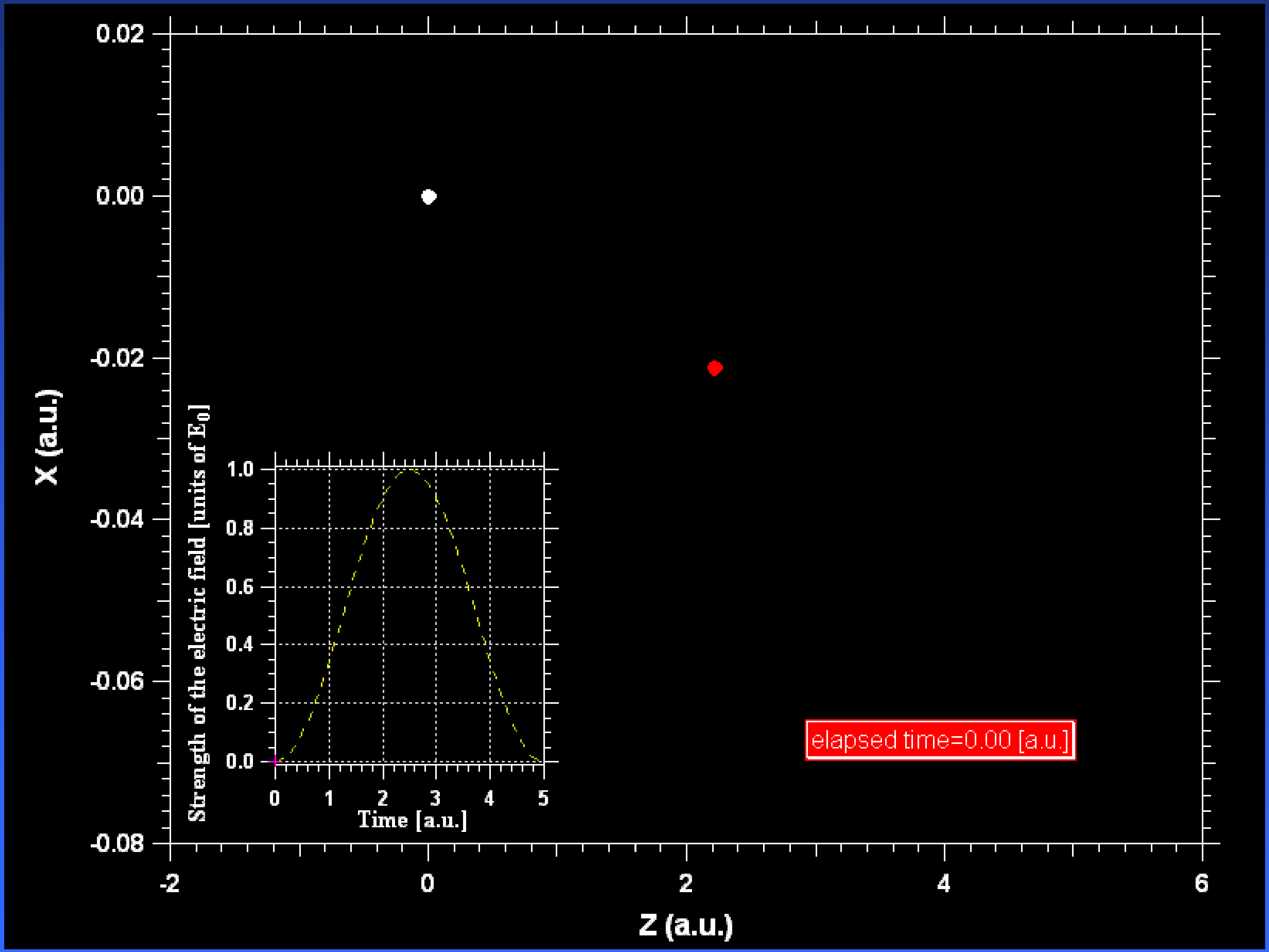
Time scales: ultrashort

t	
10^{0} s	second
10^{-3} s	millisecond
10^{-6} s	microsecond
10^{-9} s	nanosecond
10^{-12} s	picosecond
10^{-15} s	femtosecond
10^{-18} s	attosecond



← Time scale of quantum dynamics of electrons

Visualization of the classical trajectories



CTMC simulations

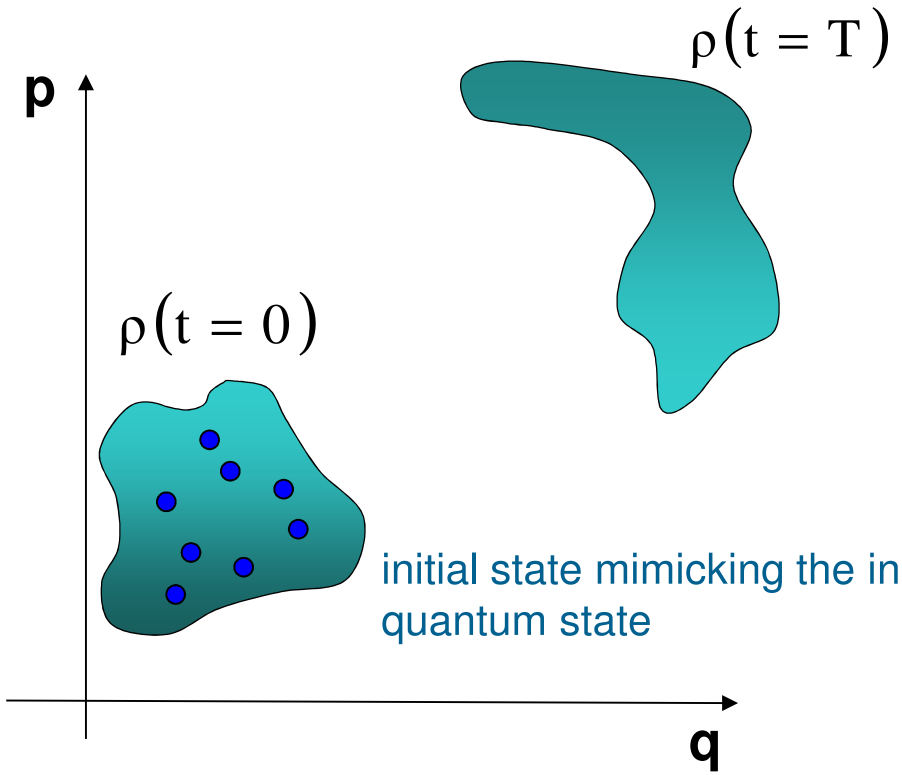
State of the classical electron: $\rho(\boldsymbol{q},\boldsymbol{p},t)$

Dynamics for probability density:
Liouville equation $\frac{\partial}{\partial t}\rho(\mathbf{q},\mathbf{p};t) = -\{\rho, H\}$

individual classical particles follow: $\dot{p}_i = \vec{F}_i(t)$

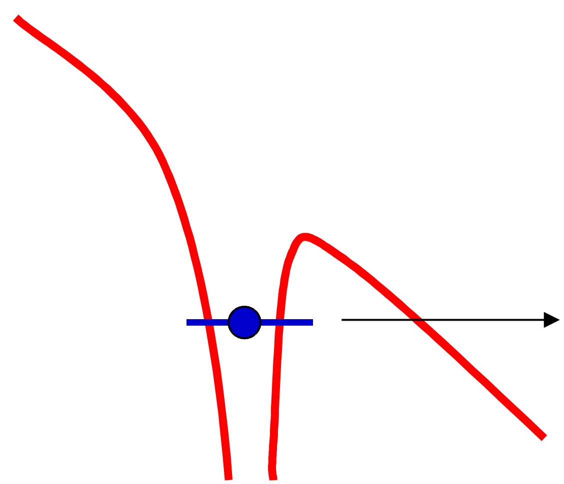
B. Sulik, Cs. Koncz, **K Tőkési,** A. Orbán, D. Berényi, Physical Review Letters **88** (2002) 073201.

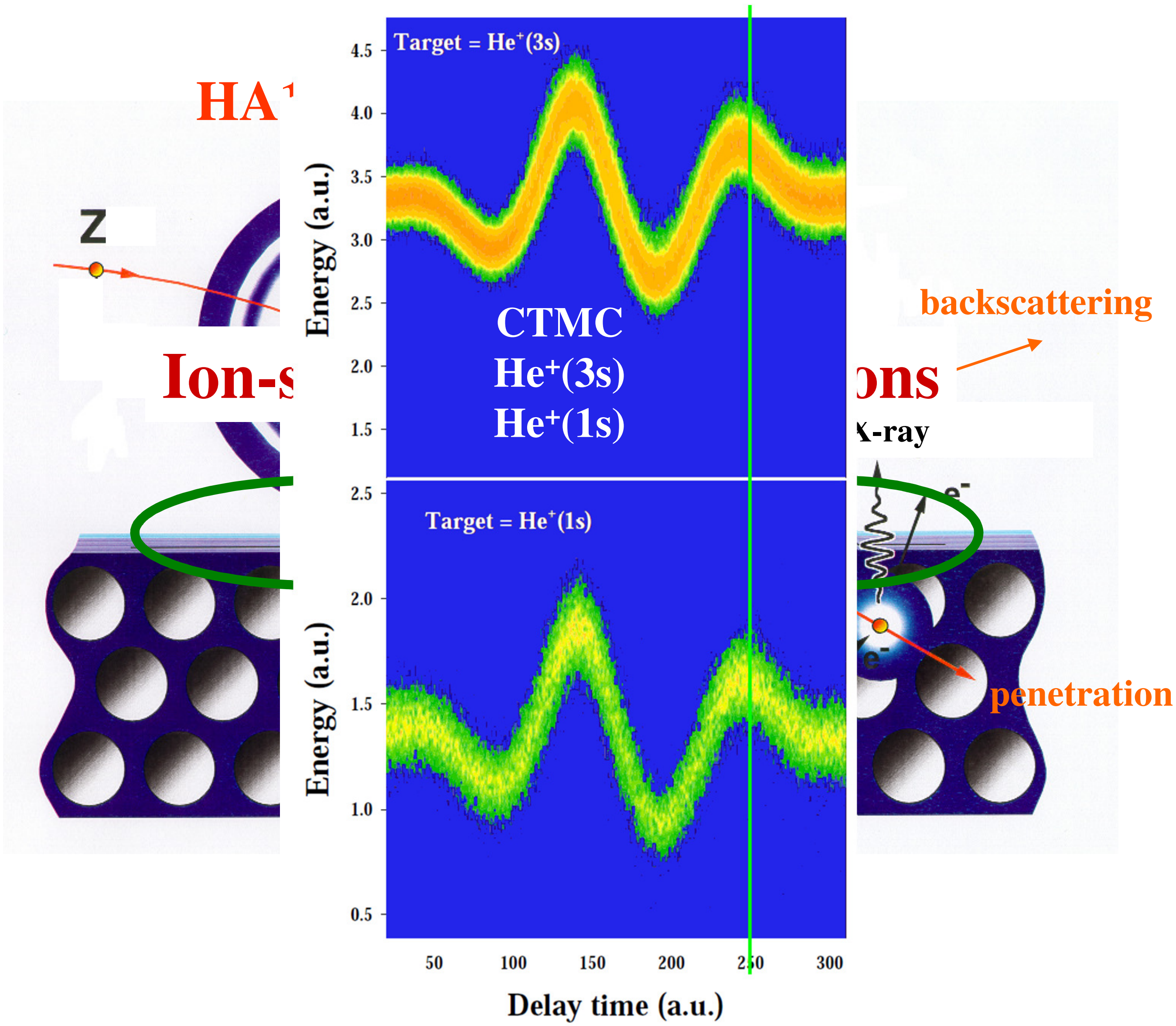
Monte Carlo solution



initial state mimicking the initial quantum state

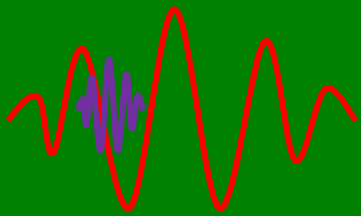
ad-hoc QM corrections:
e.g. CTMC + tunneling





Target = He+(3s)
CTMC
He+(3s)
He+(1s)
Target = He+(1s)
Energy (a.u.)
Delay time (a.u.)
4.5
4.0
3.5
3.0
2.5
2.0
1.5
0.5
1.0
50
100
150
200
250
300
Z
backscattering
penetration
e-

Application to laser-matter interaction
Previous works



2005: *Laser induced electron emission from surfaces*

C. Lemell, X. -M. Tong, **K. Tőkési,** L. Wirtz, J. Burgdörfer, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms **235** (2005) 425.

2008-2010: *Ionization by intense ultrashort laser pulses*

S. Borbély, **K. Tőkési**, L. Nagy, Rev. A**77** (2008) 033412-1-033412-12.

2009: Simulation of attosecond streaking of electrons emitted from a tungsten surface

C. Lemell, B. Solleder, K. Tőkési**, and J. Burgdörfer, Phys. Rev. A 79 (2009) 06290-1 - . 06290-8.**

2011: Time-resolved photoemission by attosecond streaking

S. Nagele, R. Pazourek, J. Feist, K. Doblhoff-Dier, C. Lemell, **K. Tőkési**, J. Burgdörfer, J. Phys. B: At. Mol. Opt. Phys. Fast Track Communication **44** (2011) 081001 (6pp)

2014 *Spatial and temporal interference during the ionization by few-cycle XUV laser pulses*

S. Borbély, A. Tóth, **K. Tőkési**, and L. Nagy, PHYSICAL REVIEW A **87**, (2013) 013405-1 - 013405-9.

2015 *Real-time observation of collective excitations in photoemission*

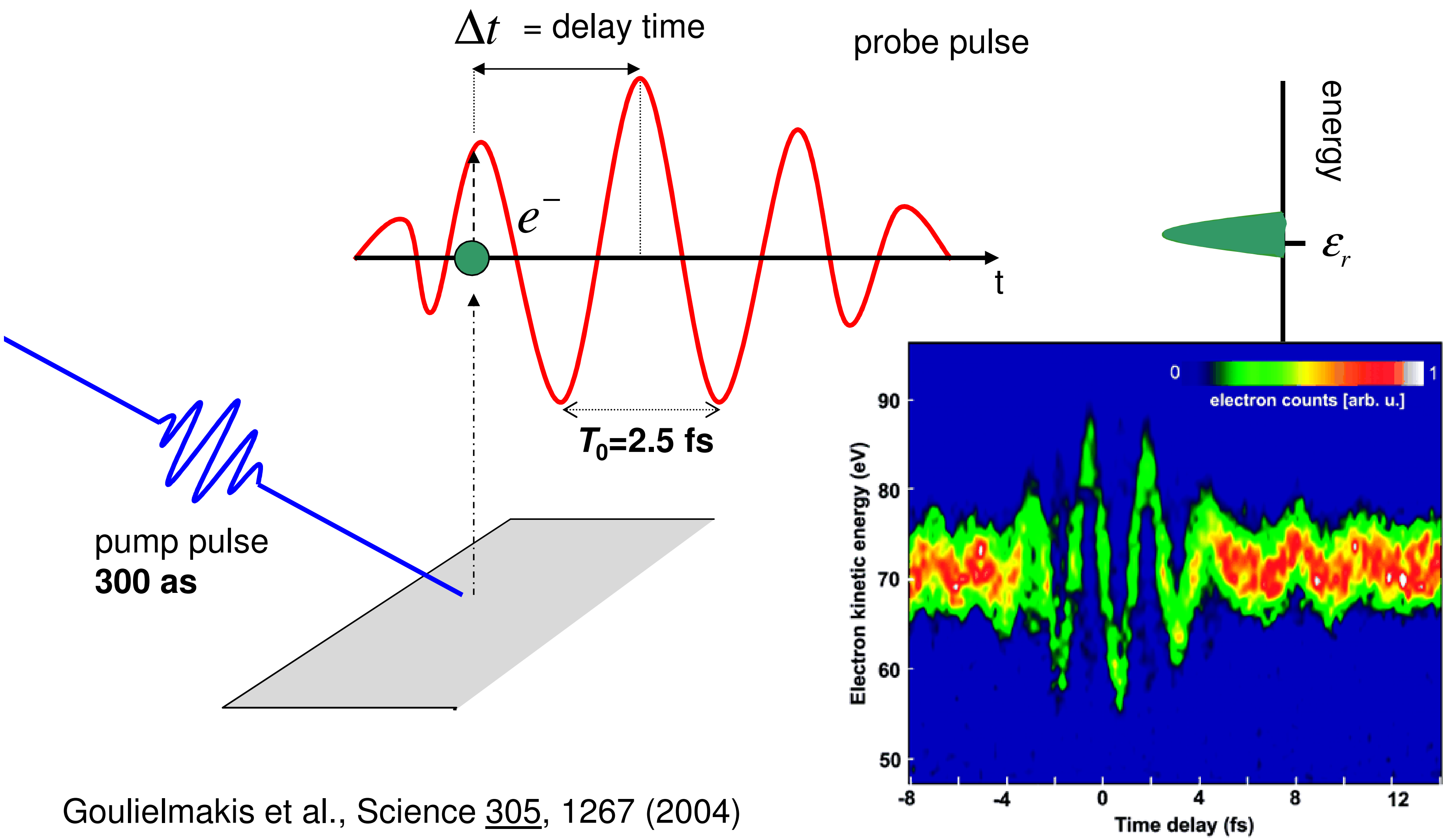
C. Lemell, S. Neppl, G. Wachter, **K. Tőkési**, R. Ernstorfer, P. Feulner, R. Kienberger, and J. Burgdörfer, Phys. Rev. B: Rapid Communication, in press.

Attosecond physics ...

- **... is a new, rapidly developing field of research**
- **... is at the edge of of current technology and relies on the progress in laser development and nonlinear optics**
- **... deals with atomic , molecular, condensed matter and nanosystems**

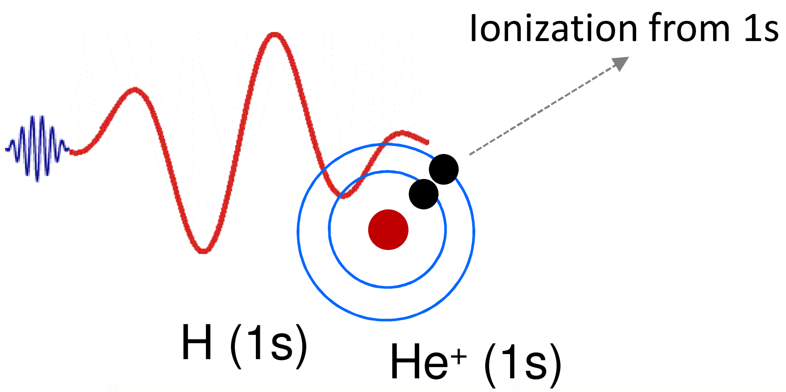
- - attosecond streaking

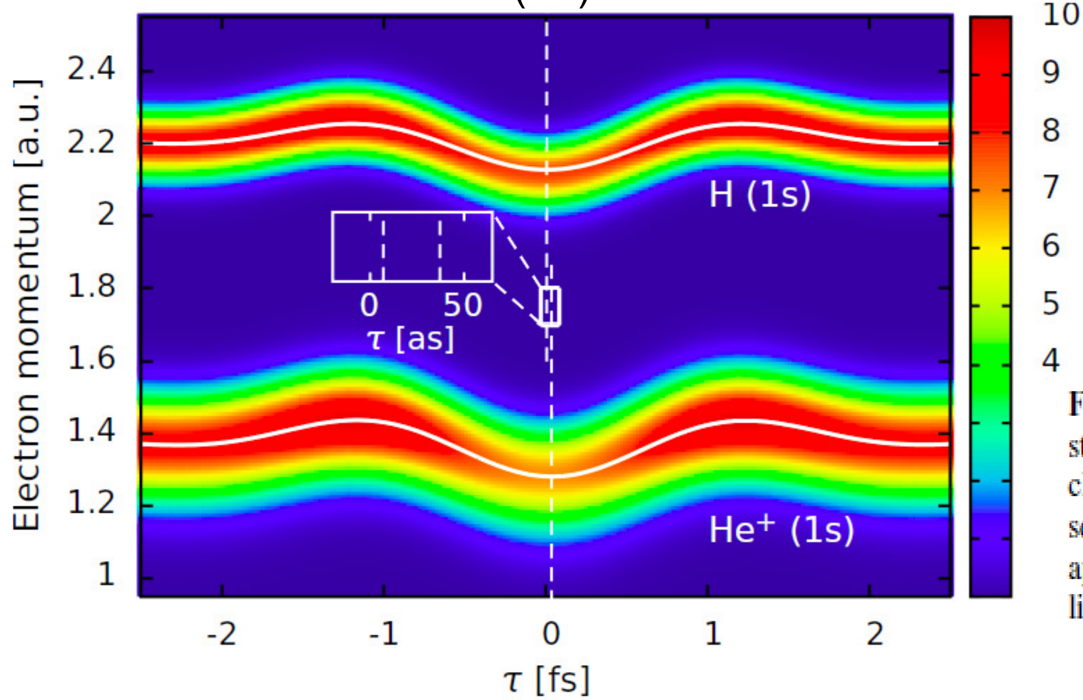
(Classical) time to energy mapping: attosecond streaking



Goulielmakis et al., Science 305, 1267 (2004)

Classical vs Quantum Streaking





CTMC-TDSE

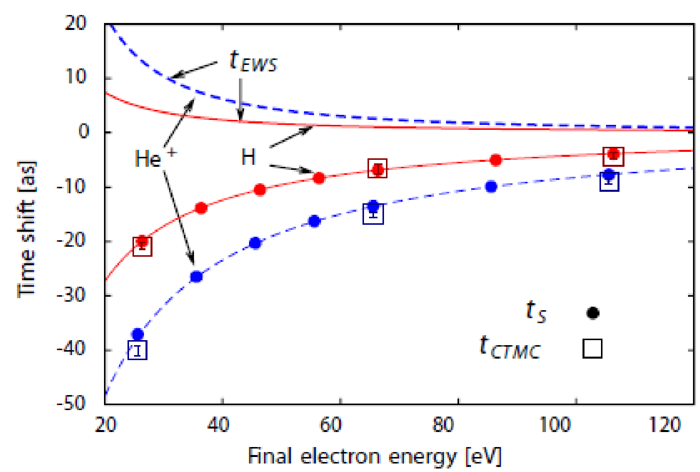
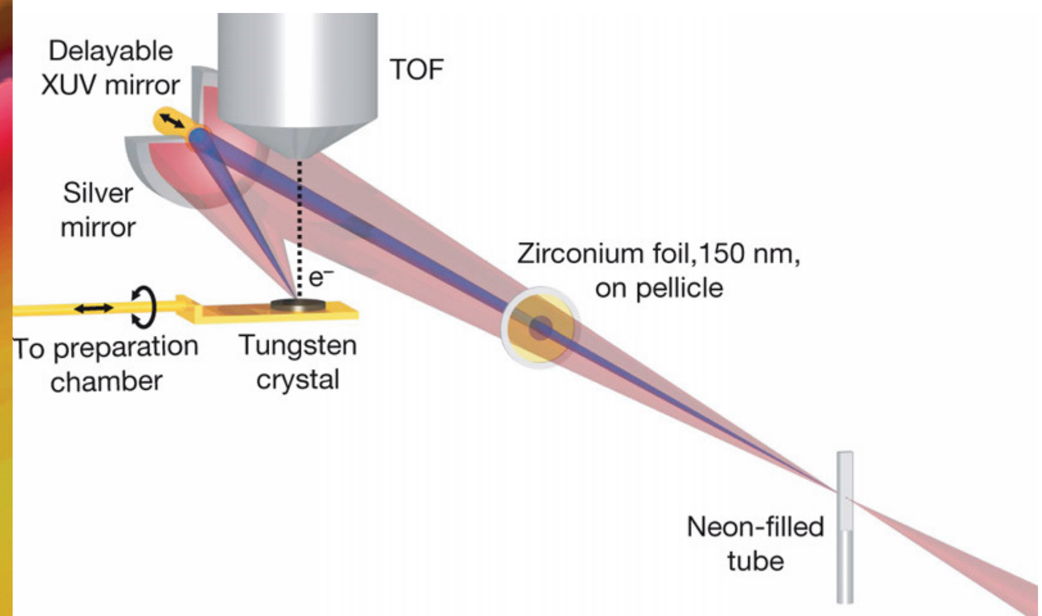


Figure 2. Temporal shifts t_S extracted from quantum mechanical streaking simulations (H(1s): red circles, He^+(1s): blue circles), classical streaking simulations (H(1s): red squares, He^+(1s): blue squares) and for comparison, the EWS time shift $t_{EWS} = d\varphi/dE$ applied to the Coulomb phase (H: red solid line, He^+: blue dashed line).

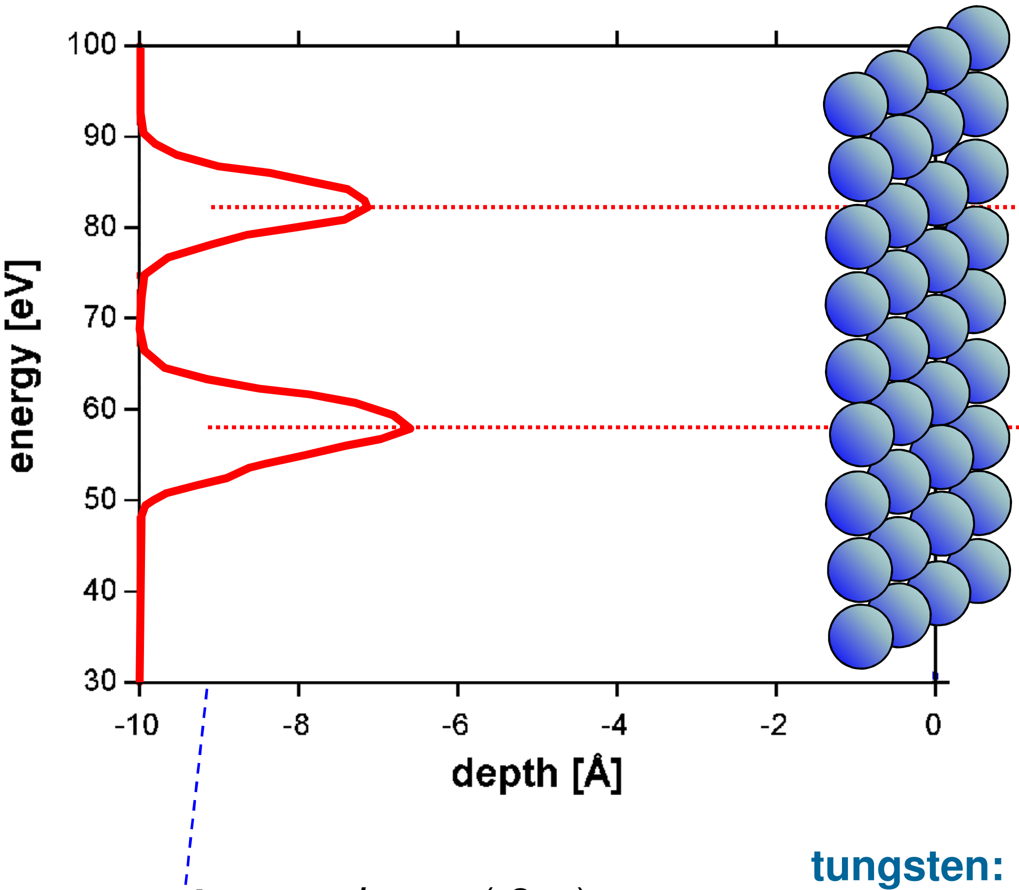
S. Nagele, R. Pazourek, J. Feist, K. Doblhoff-Dier, C. Lemell, **K. Tőkési**, J. Burgdörfer, J. Phys. B: At. Mol. Opt. Phys. Fast Track Communication **44** (2011) 081001 (6pp))

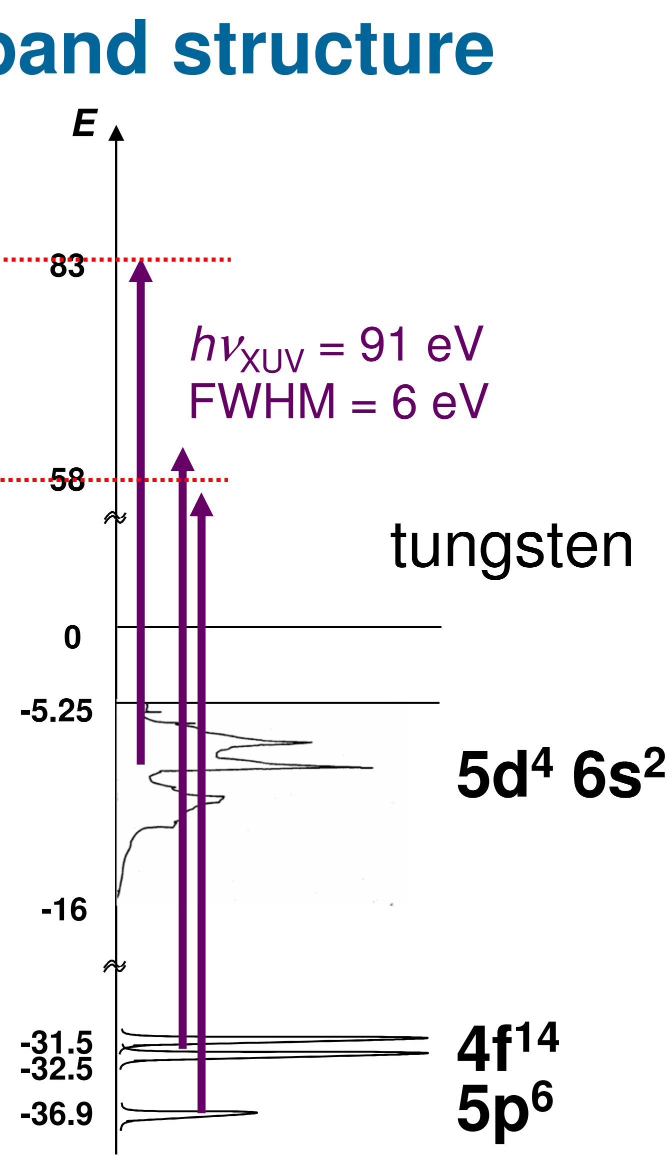
- \- attosecond streaking
  in solid (W)– the case of core and
  valence electrons

Attosecond streaking of photoemission from surfaces



Depth profile of excitation spectrum



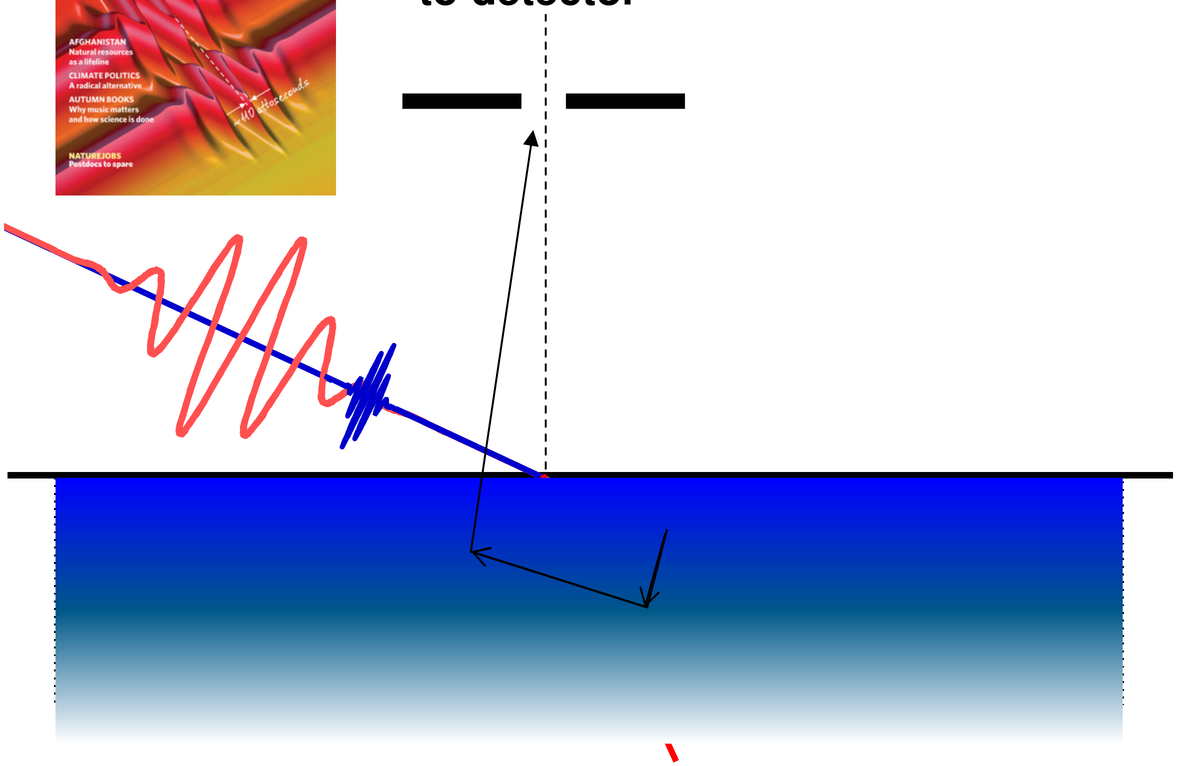


evanescent wave: $I \sim \exp(-2\kappa z)$
$\kappa \sim 0.013$/Å ~**17 atomic layers**

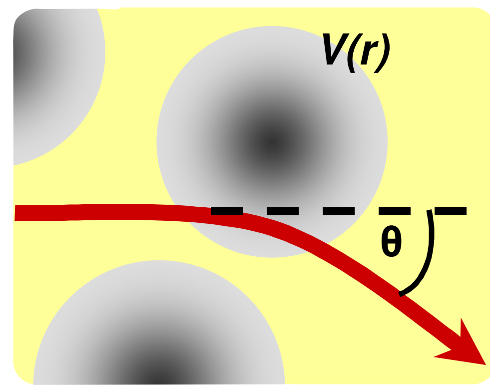
tungsten:
a **= 3.16 Å**
$d_{(110)}$ **= 2.24 Å**

Time resolved photoemission from solid

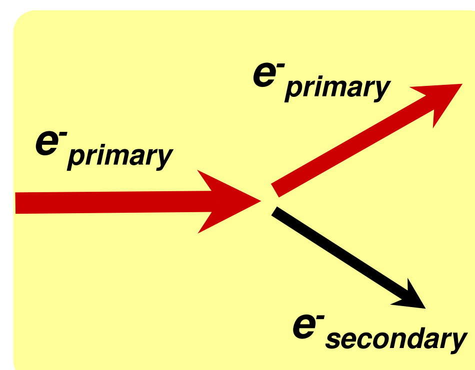
CTMC transport simulation



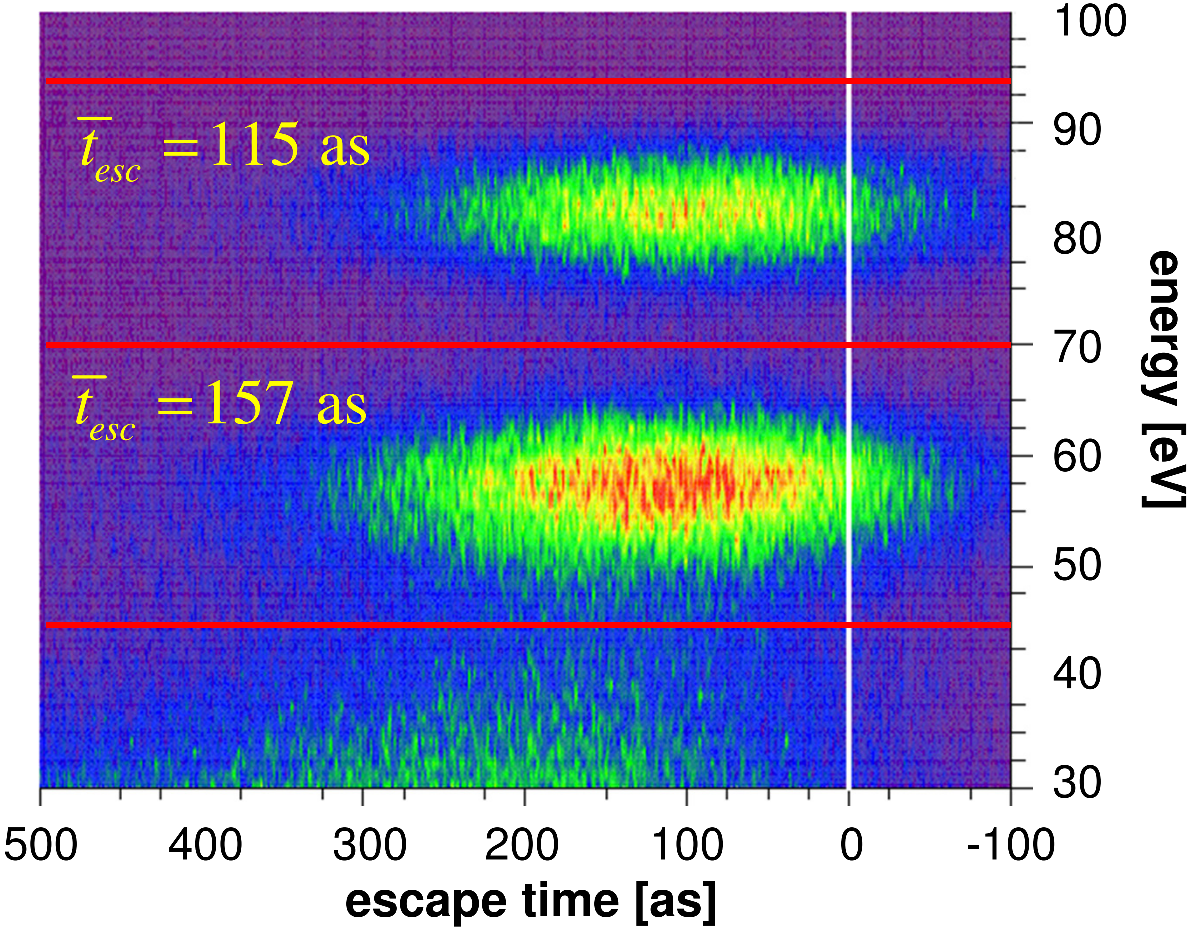
elastic scattering:



inelastic scattering:



Escape time of electrons

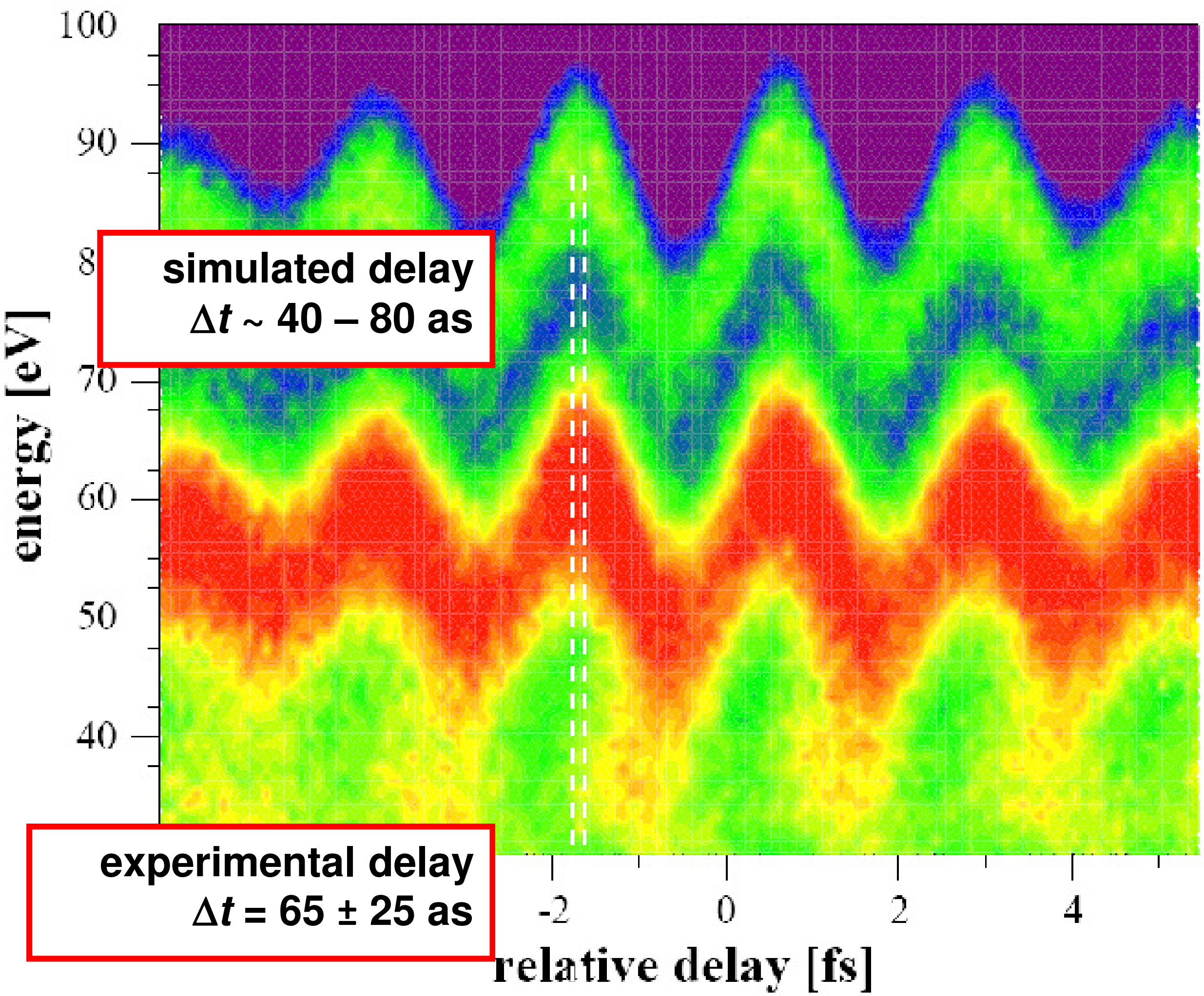


maximum of XUV pulse at *t* = 0

time difference:
Δt = 42 as

C. Lemell, B. Solleder, **K. Tőkési**, and J. BurgdörferPhys. Rev. A 79 (2009) 06290-1 - . 06290-8.

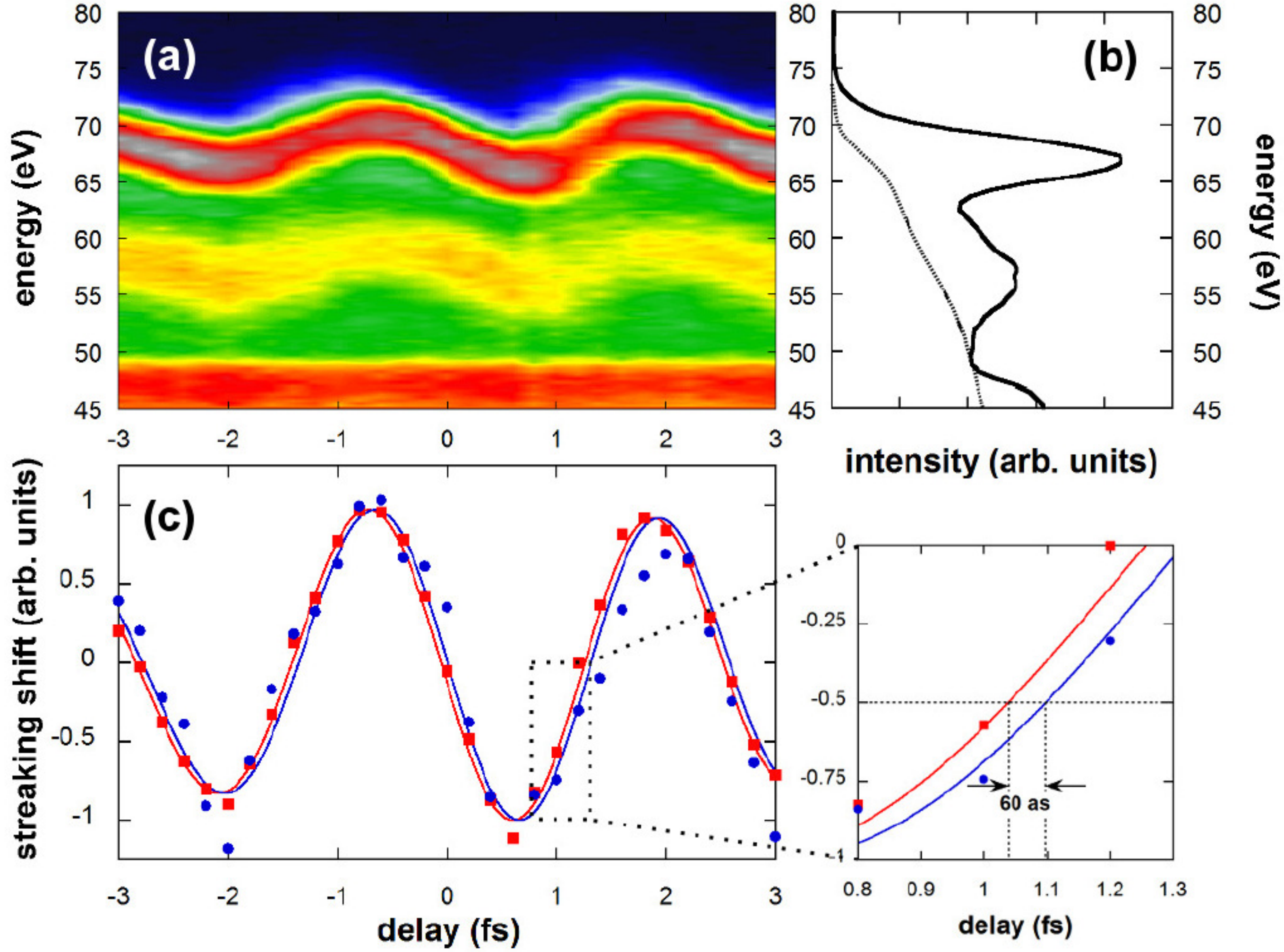
Simulated streaking spectrum for W



C. Lemell, B. Solleder, **K. Tőkési**, and J. BurgdörferPhys. Rev. A 79 (2009) 06290-1 - . 06290-8.

- - attosecond streaking
  in solid (Mg)– the case of intrinsic
  and extrinsic plasmon excittion

Time-resolved observation of collective excitations in photoemission Streaking traces of the Mg2p and plasmon-satellite lines



C. Lemell, S. Neppl, G. Wachter, **K. Tőkési**, R. Ernstorfer, P. Feulner, R. Kienberger, and J. Burgdörfer, Phys. Rev. B: Rapid Communication **91**, 241101(R) (2015).

- Classical --- semi-Classical
- Phase in the classical treatment

Two-step semiclassical model with interference

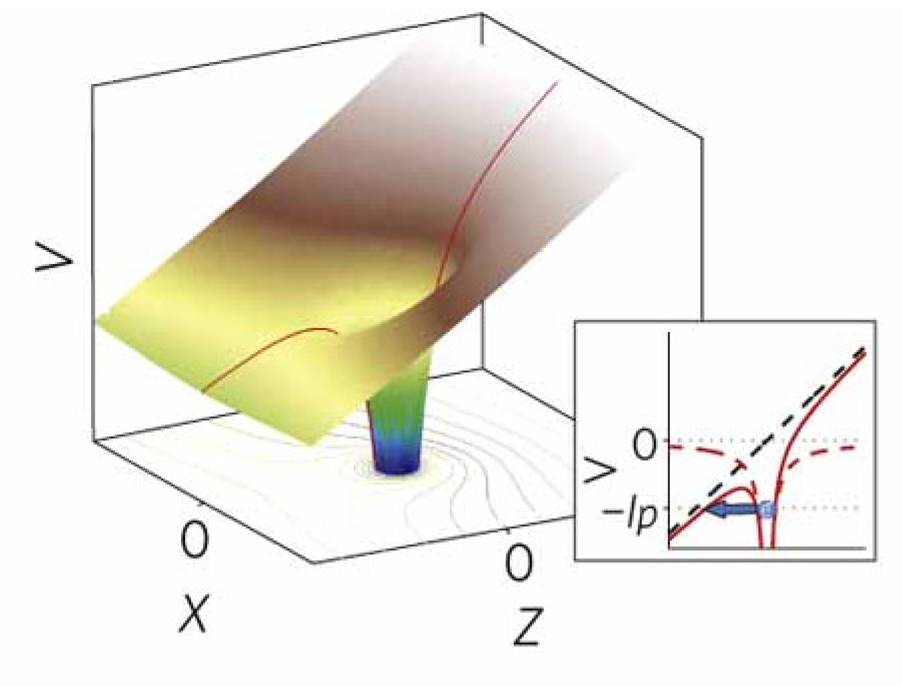
Each classical trajectory is associated with a certain phase, and the contributions of the trajectories ending up in a given bin are added **coherently**.

$$W(bin) = \left| \sum_j \sqrt{w(t_0^j, p_\perp^j)} \exp\left[-iS\left(t_0^j, p_\perp^j\right)\right] \right|^2$$

$$S\left(t_0^j, p_\perp^j\right) = \int_{t_0}^{\infty} \left[\frac{v^2}{2} + I_p - \frac{Z}{\left|\vec{r}(t)\right|} \right] dt$$

Initial conditions

Potential barrier formed by the atomic potential and the electric field of the laser in 1D cut **along the direction of the field**

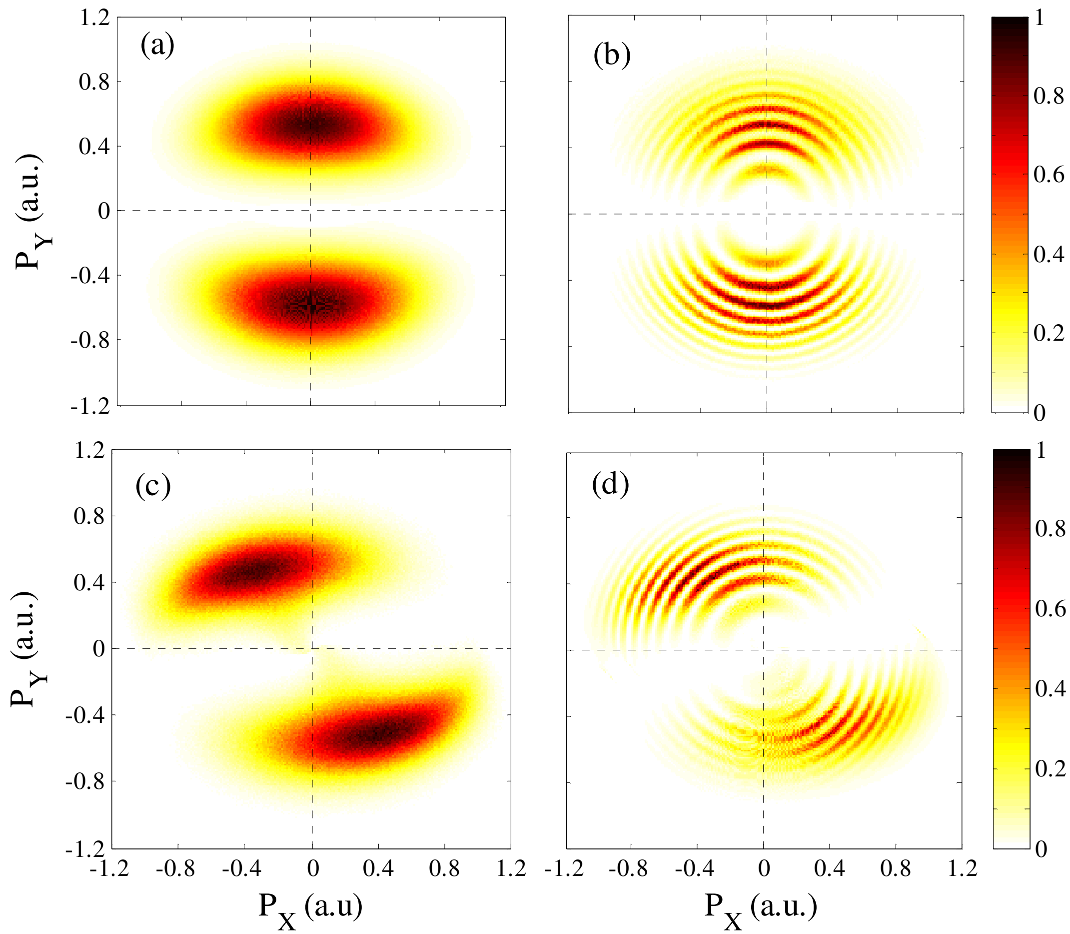


$$z_e \approx -\frac{I_p(F) + \sqrt{I_p^2(F) - 4ZF}}{2F}$$

$$w(t_0, p_\perp) \sim \exp\left(-\frac{2\kappa^3}{3F}\right)\exp\left(-\frac{\kappa p_\perp^2}{F}\right)$$

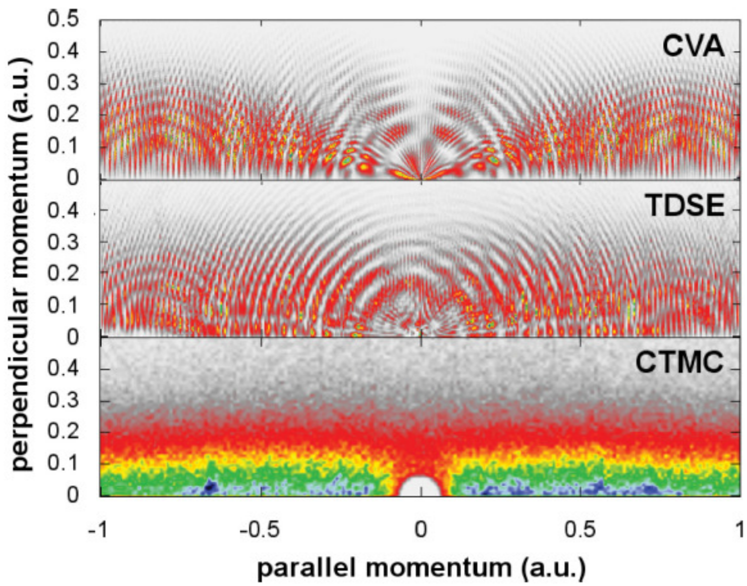
$$F = F(t_0),\ \kappa^2/2 = I_P$$

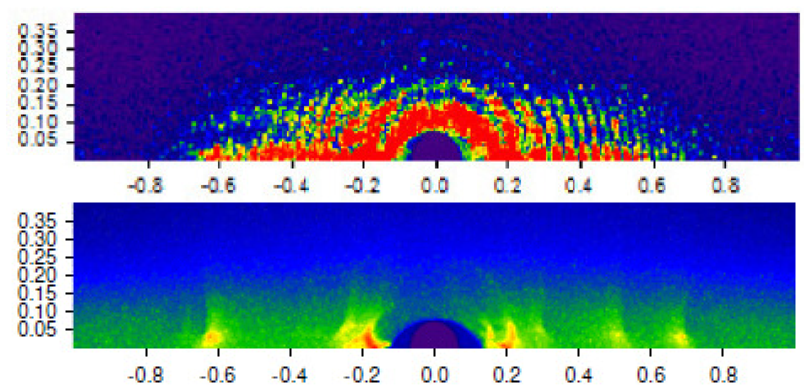
Momentum distributions of the photoelectrons for the H atom in the polarization plane using a laser pulse with wavelength λ=800 nm, peak intensity 2×10^{14} W/cm^2, ellipticity ε=0.5, and a laser pulse duration of n_p=6 cycles. Panels (a) and (b) show the distributions calculated ignoring the ionic potential after tunneling, when the tunneled electron moves in the laser field only. Panels (c) and (d) depict the same distributions, but with consideration for the Coulomb field. The distributions (b) and (d) are calculated taking into account quantum interference.



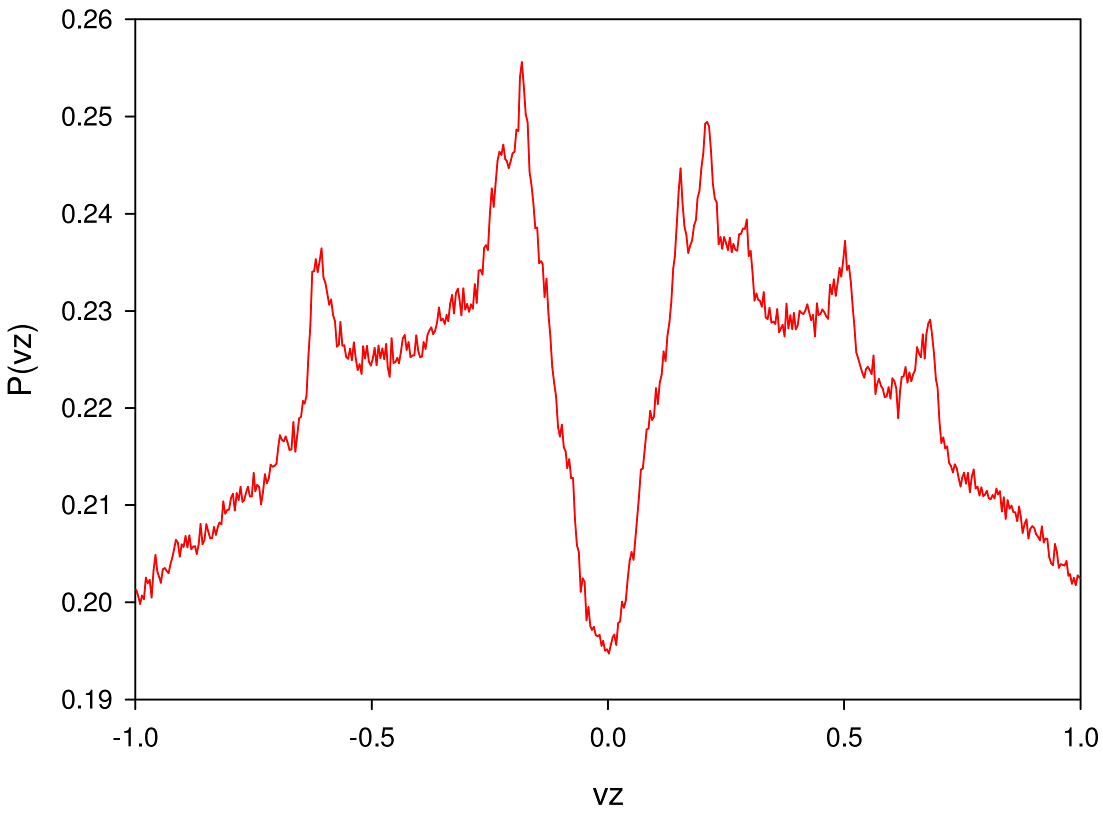
Linearly polarized field

$(I = 10^{14}\ \mathrm{W/cm^2})$ λ= 3200 nm



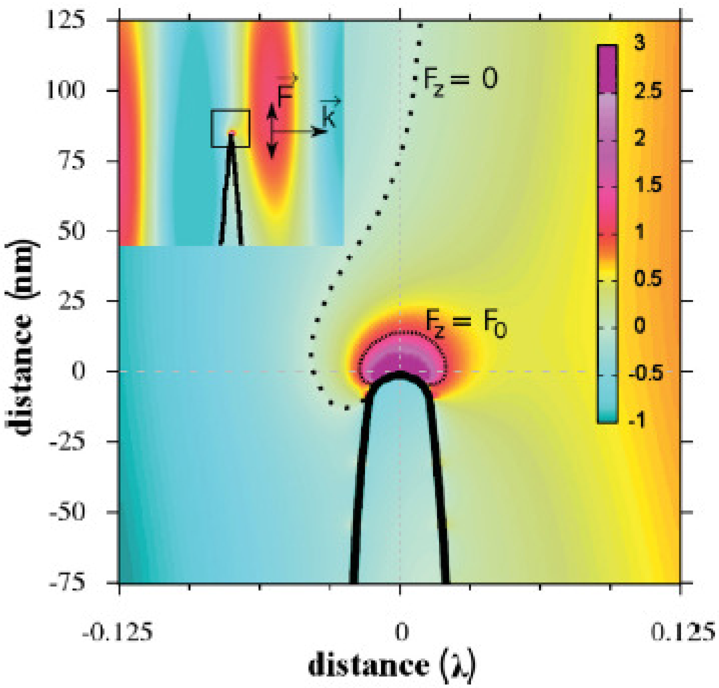


Longitudinal momentum distribution

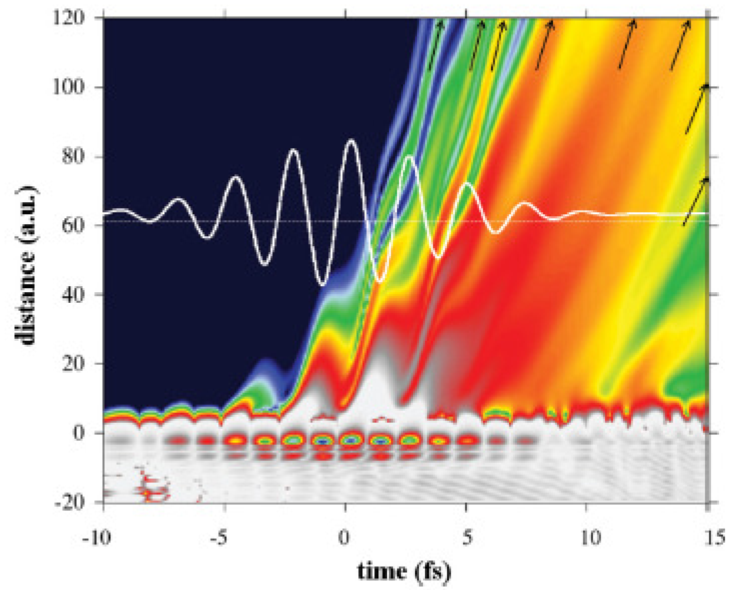


Future plan

Electron rescattering at metal nanotips



Time-dependent change in electron density

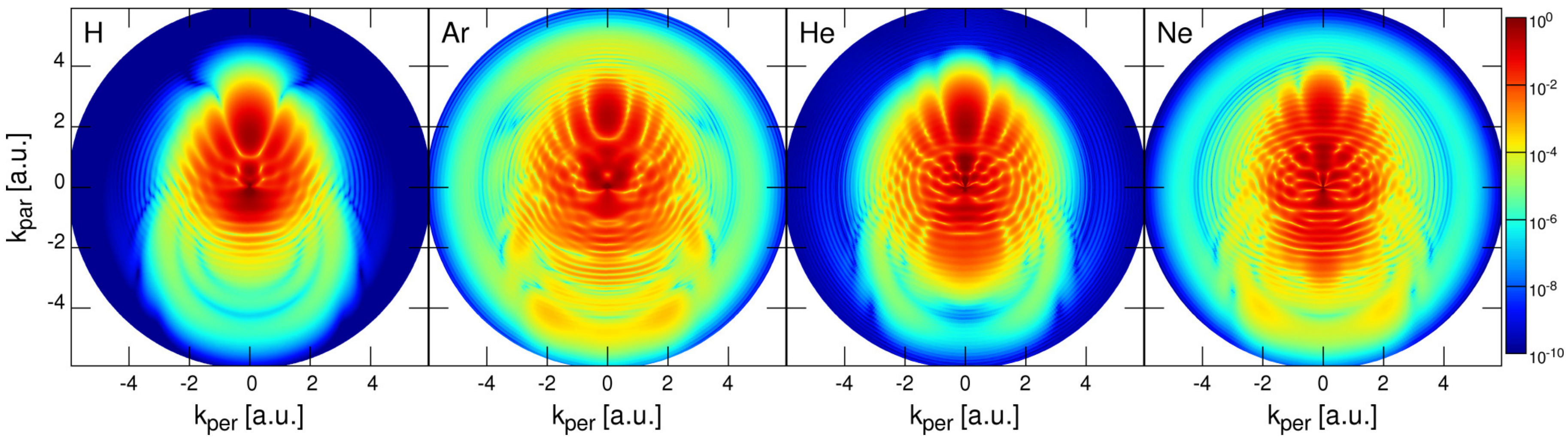


Field enhancements
Combining nano length scale with (sub)femto second time scale

G. Wachter, C, Lemell, J. Burgdörfer,M. Schenk, M. Krüger, and P. Hommelhoff,
PHYSICAL REVIEW B **86**, 035402 (2012).

Holographic mapping (HM) by ionization

Differences of the HM patterns



S. Borbély, A. Tóth, **K. Tőkési**, and L. Nagy, PHYSICAL REVIEW A **87**, (2013) 013405-1 - 013405-9.

Goals

- **The ultimate goal is not just to watch but to control and to influence the ultrafast motion for new technological applications.**
- **Attoscience promises to develop new technologies for the future.**
- **Combining the attosecond with nanometer scale opens new perspectives and promises new findings.**

Thank you!