Precision Photo Electron Spectra

Discretization, Boundaries, Gauge

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Frontiers of Intense Laser Physics
KITP Santa Barbara, August 19, 2014

Munich Advanced Photonics
Excellence Cluster

Vienna Computational Materials Science
FWF Special Research Program

Correlated Multielectron Dynamics
in Intense Laser Fields

Marie Curie ITN

Vinay
Majety
2-electron
& molecules

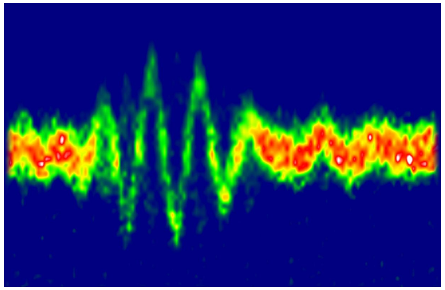
Mattia
Lupetti
Solids and
surfaces

Alejandro
“the convergator”
Zielinski
1-e elliptic
2-electron

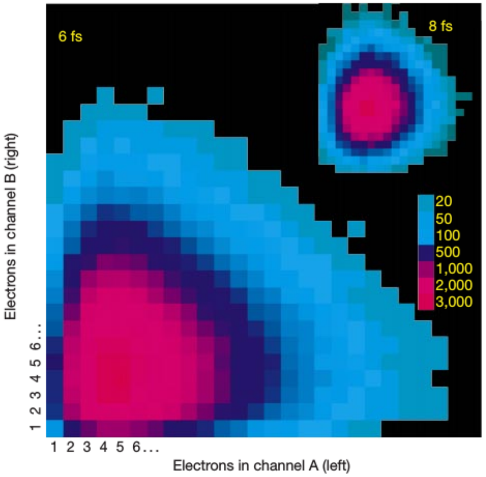
Jakob
Liss
Solids and
surfaces

A wealth of measured photo-electron spectra...

Few-cycle IR pulse

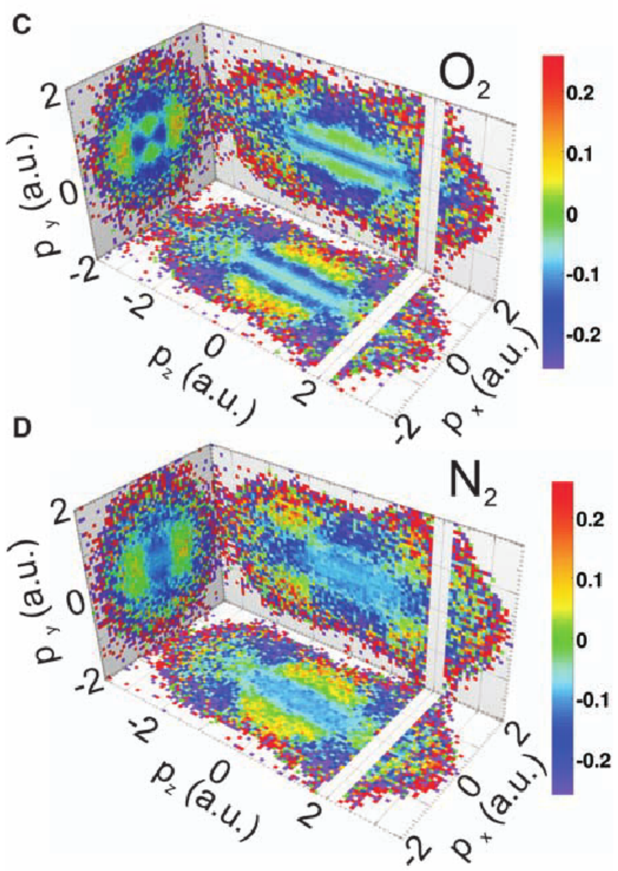


The first stereo-ATI result

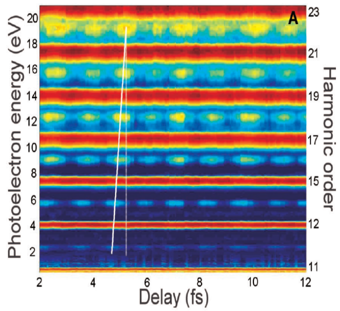


Laser-Induced Electron Tunneling and Diffraction

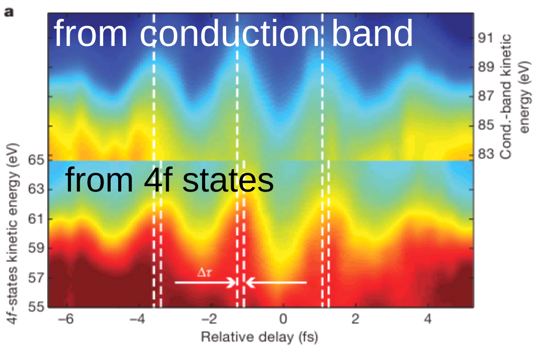
M. Meckel,[1,2] D. Comtois,[3] D. Zeidler,[1,4] A. Staudte,[1,2] D. Pavičić,[1] H. C. Bandulet,[3] H. Pépin,[3] J. C. Kieffer,[3] R. Dörner,[2] D. M. Villeneuve,[1] P. B. Corkum[1*]



RABITT spectrogram



Emission from surface

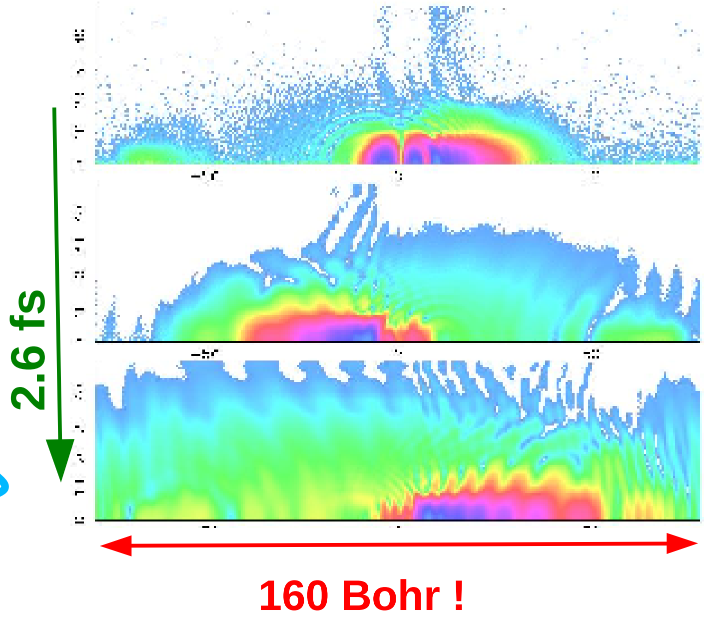


...but modelling and calculation are hard

Two main difficulties:

(1) solution covers large (phase) space
(2) complexity of few-electron calculations

Single electron density during 2.6 fs



Large box sizes due to ionization:

irECS perfect absorption method

Spectra from a truncated calcuation:

sTurff time dependent surface flux

Complexity of quantum chemistry wave function:

→ Integrate quantum chemisty with strong field dynamics

Messages: Methods

(1) Advertisement for the flexibility of finite element discretizations

(2) irECS - The problem of absorbing boundary conditions for the TDSE
is solved for all practical purposes

(3) tSURFF – computing photo-electron spectra
without spectral projections

(4) Mixing of length and velocity gauges in the same calculations
Unites numerical efficiency of length gauge
with intuitive modeling of length gauge
It is mandatory for numerical modeling using quantum chemical structure

Messages: Results & Code

(5) Single photo-electron spectra of He, H_2, N_2
converged @ 400 nm wave-length

(6) Fano line-shapes, IR control: numerics + analytic theory

(7) Double photo-electron spectra of He
converged at XUV wave length

(8) Correlation in double emission and its measure

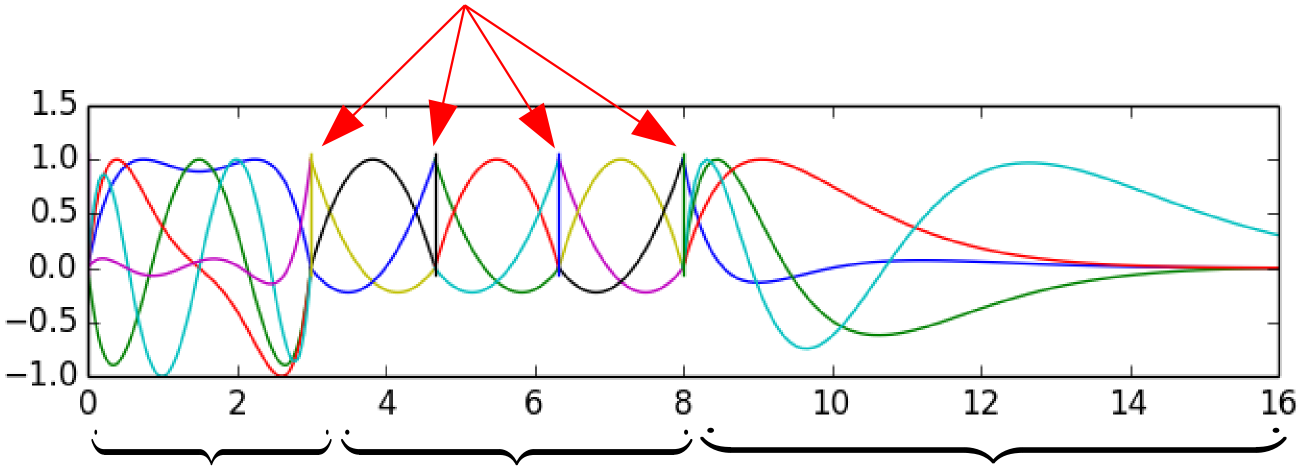
(9) tRecX – the code that does it all is available for use!

on the Discretization

(Finite Elements)

Finite elements

Approximation by piece-wise analytic functions (mostly polynomials)



Element boundaries
Functions continuous
Derivatives discontinuous

Polynomials
Degree 5

Polynomials
Degree 2

exp(-ar) x polynomials
extends to r = ∞

Flexible, can be adjusted to local properties of the solution

Discretization: why finite elements?

Required basis sizes

d degrees of freedom
phase space volume ***V***

$$N \gtrsim V/\hbar^d$$

There are no smart tricks to beat this number unless we have additional information

Additional information

E.g. perturbative ionization, i.e. initial state or free motion
or: SFA: initial state or Volkov wave packet
or: we "know" only bound states play a role or …

Basis sets

Pseudo-spectral (e.g. field-free eigenstates, momentum-space)

Build **energy or momentum** information into ansatz

Local basis sets (B-splines, finite-element, FEM-DVR)

Exploit **locality** of operators (differentiation, multiplication)
Numerically robust

High order finite elements

Locally adjustable (→ irECS)
Well-defined points of non-analyticity (element boudaries)
Rapid convergence due to high order (e.g. 10-20)

Boundary conditions

(aka Absorption)

Exterior complex scaling (ECS)

General principle for perfect absorbers (PML, ECS)

[A.S., H-P. Stimming, N. Mauser, J. Comp. Phys. 269, 98 (2014)]

Outside some inner region [0,R_0]

analytically continue a **unitary transformation U_λ** (e.g. coordinate scaling)

to **contractive** **(non-unitary)** U_Θ

$$i\frac{d}{dt}\Psi = H(t)\Psi \to i\frac{d}{dt}\Psi_\theta = U_\theta H(t) U_\theta^{-1}\Psi_\theta$$

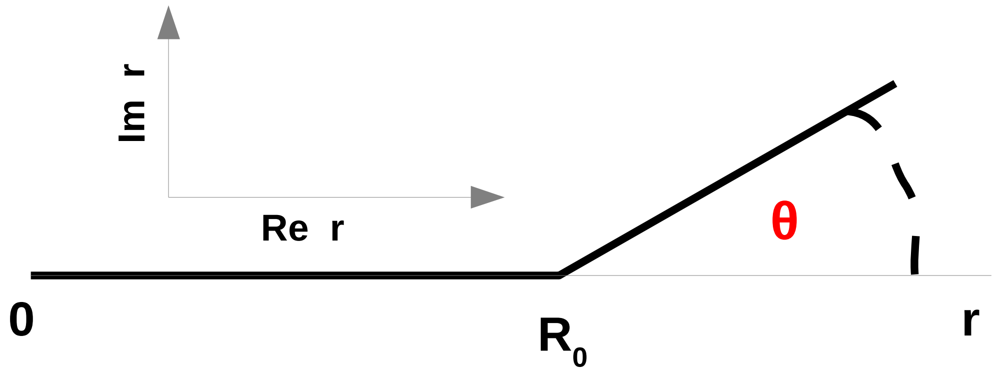
Unitarity + analyticity guarantee unchanged solution Ψ_θ on [0,R_0]

!!! Caution: Domain issues for $U_\theta H U_\theta^{-1}$!!!

Note: analytic continuation is $\lambda \to \theta$ (not in coordinate r)

Translates into:
Complex coordinates
beyond a finite distance R_0

r -> r for $r < R_0$
r -> $R_0 + e^{i\theta}(r-R_0)$ for $r > R_0$



Implementation of exterior complex scaling

Important technical complications

Bra and ket functions are not from the same set!!!

Exterior scaled Laplacian $\Delta_{R0,\Theta}$ is defined on discontinuous functions

$$\Psi(R_0-0)=e^{3i\theta/2}\Psi(R_0+0)$$

Discontinuity as we need unitarity for real transformation

Discontinuity is reversed for the left hand functions

$$\Psi^*(R_0-0)=(e^{-3i\theta/2}\Psi)^*(R_0+0)$$

Matrix elements of $\Delta_{R0,\Theta}$

are computed by piece-wise integration $[0,R_0]+[R_0,\infty)$

Conditions easy to implement with a local basis set

irECS – a perfect absorber

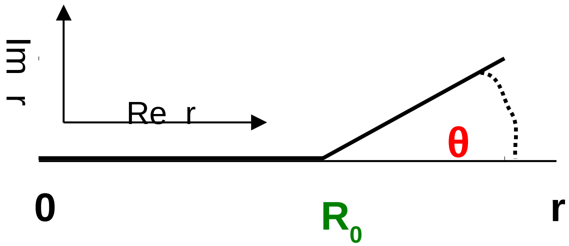
[A.S., Phys. Rev. A81, 53845 (2010)]

Infinite range Exterior Complex Scaling

ECS:

$r \rightarrow r$ for $r < R_0$

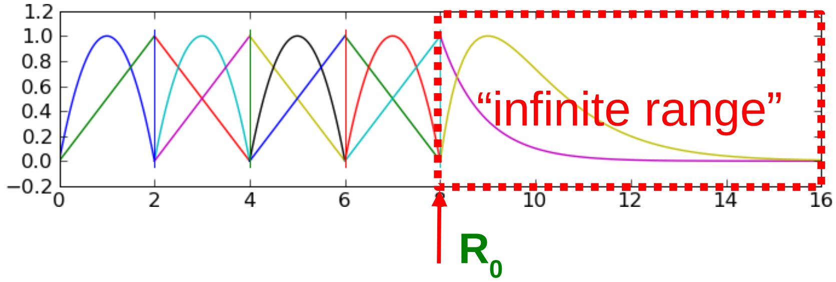
$r \rightarrow R_0 + e^{i\theta}(r-R_0)$ for $r > R_0$



Discretization

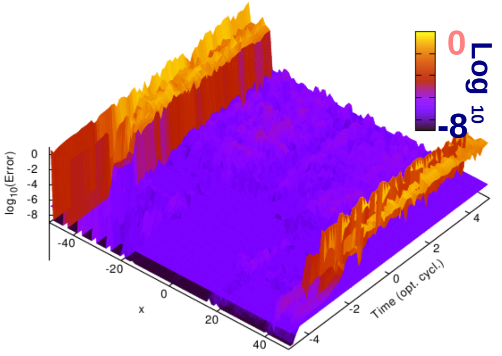
High (~8th) order finite elements

infinite size last element $[R_0,\infty)$



Accuracy

$|\Psi_{\theta R0}(x,t) - \Psi(x,t)| / |\Psi(x,t)|$

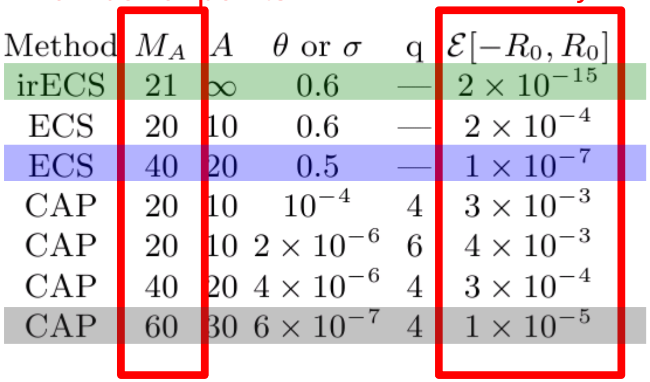


Accuracy inside R_0 ~ 10^{-7}

Efficiency

Number of points

Accuracy



Method	M_A	A	θ or σ	q	$\mathcal{E}[-R_0,R_0]$
irECS	21	∞	0.6	—	2×10^{-15}
ECS	20	10	0.6	—	2×10^{-4}
ECS	40	20	0.5	—	1×10^{-7}
CAP	20	10	10^{-4}	4	3×10^{-3}
CAP	20	10	2×10^{-6}	6	4×10^{-3}
CAP	40	20	4×10^{-6}	4	3×10^{-4}
CAP	60	30	6×10^{-7}	4	1×10^{-5}

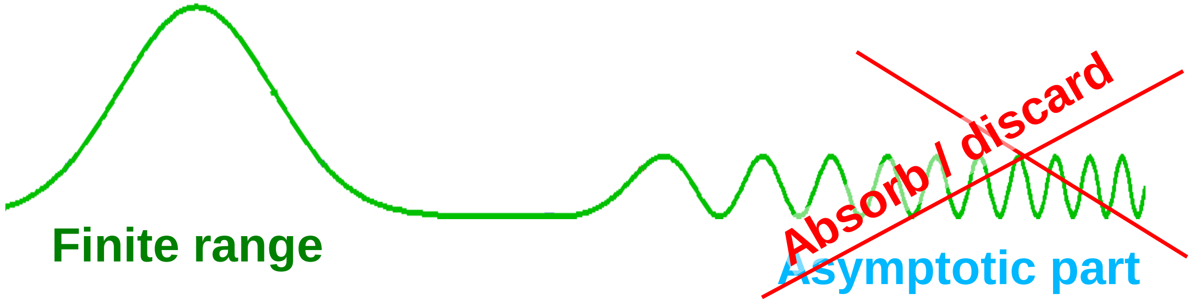
CAP = complex absorbing potential

Spectra

(tSURFF)

tSURFF – how to obtain spectra from a finite range wave function

Scattering spectra = asymptotic information by definition



If we solve only on a finite range, exactly the asymptotic information is **missing**

Solution:

Continue beyond the box using some **known solution - Volkov**

[Caillat et al., Rev. A 71 , 012712 (2005)]
[L. Tao and A.S., New. J. Phys. 14, 013021 (2012)]

How we usually calculate spectra from TDSE

Get Ψ(r,t) at the end of the pulse t=T: ***Ψ(r,T)*** **← problem 1** Needs very large box

Scattering solution ψ_k $$H(T)|\psi_{\vec{k}}\rangle = \frac{\vec{k}^2}{2}|\psi_{\vec{k}}\rangle$$ **← problem 2** Time-independent scattering

With asymptotics $$\psi_{\vec{k}}(\vec{r}) \sim (2\pi)^{-3/2}\exp(i\vec{k}\cdot\vec{r})$$

Spectrally analyze Ψ(x,t) $$b(\vec{k}) = \langle\psi_{\vec{k}}|\Psi(T)\rangle$$

Spectral density $$\boxed{\sigma(\vec{k}) \propto |b^2(\vec{k})|}$$

Solve by using additional information

(1) TDSE is a 2nd order PDE

Value and derivative at a surface $r = R_c$ suffice
to continue the solution beyond the surface

(2) Beyond distances $R_c \sim 50$ a.u. motion is ~ free

Use Volkov solution for free motion in the field instead of numerically solving

Compare R-matrix theory!

How things are done...

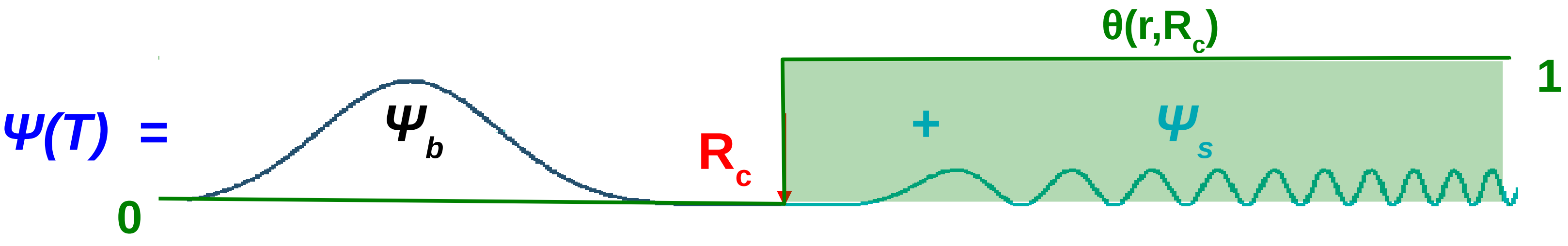
- for a given pulse, **solve** with irECS absorption (box size ~ 50 a.u., laser-dependent)
- save values and derivatives at surface(s) as function of time
- properly **time-integrate** surface values for asymptotic momenta ***p*** of your choice (one integration for each ***p*,** ordinary integrals, very cheap!)
- can zoom in onto areas of interest (important for 2-electron problems)
- Effort grows only linearly with pulse duration T (cf. $T^2 \sim T^4$ if time and box-size grow)

tSURFF – time-dependent surface flux method

[L. Tao and A.S., New. J. Phys. 14, 013021 (2012)]

Propagate until large T where bound Ψ_b and scattering Ψ_s parts separate

Beyond distance R_c scattering solutions χ_k are known



Spectral amplitude σ(k):

with *Volkov solutions* χ_k

$$\boxed{\sigma(\vec{k}) \propto \left|\langle\chi_{\vec{k}}|\theta(R_c)|\Psi(T)\rangle\right|^2}$$

Volume integral → Time-integral & surface integral

$$\langle\chi_k(T)|\theta(R_c)|\Psi_s(T)\rangle = i\int_0^T dt\, \langle\chi_k(t)| \left[-\frac{1}{2}\Delta + i\vec{A}(t)\cdot\vec{\nabla}, \theta(R_c)\right] |\Psi_s(t)\rangle$$

Commutator depends only on *$\Psi(R_c,t)$ and $\partial\Psi(R_c,t)$*

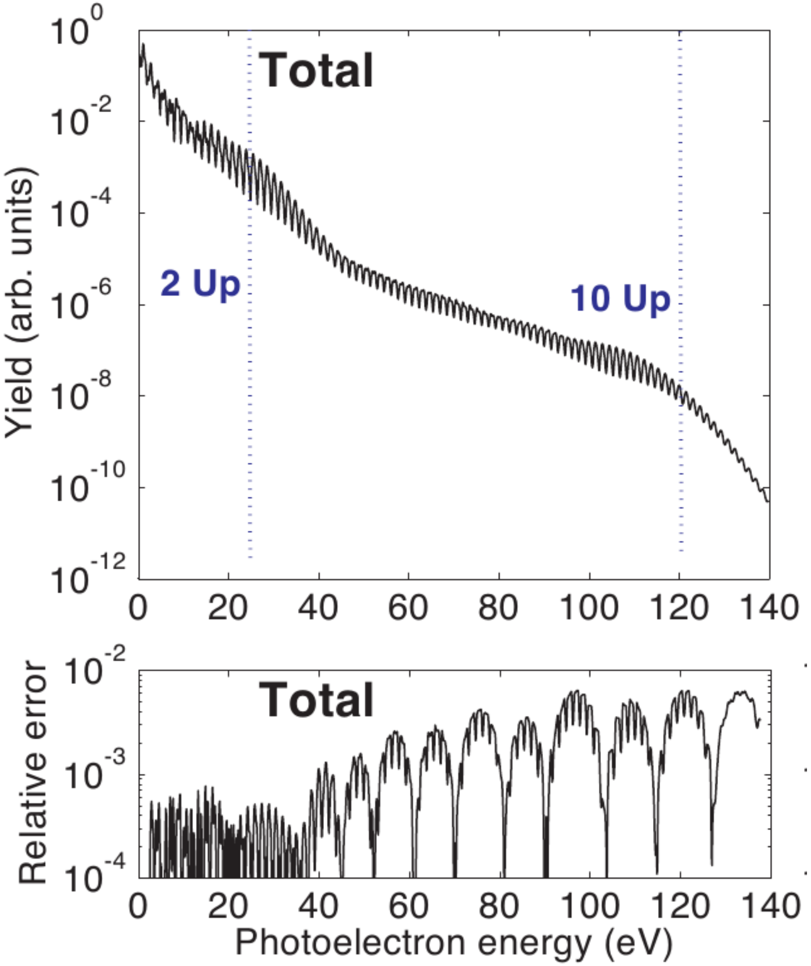
Note: need time-dependent bra-solutions ≈ ***Volkov (or better, if available)***

Single photo-electron spectra

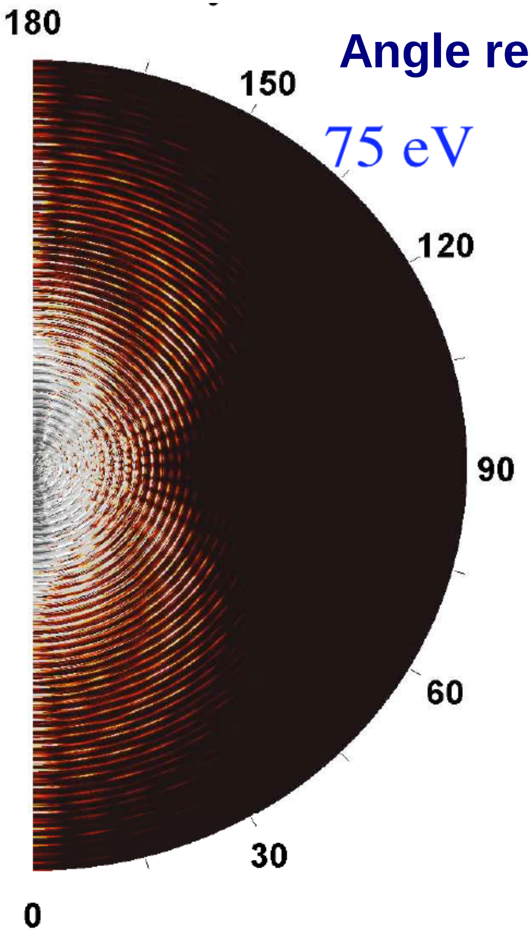
Photo-electron spectra – single electron, 3d

[L. Tao and A.S., New. J. Phys. 14, 013021 (2012)]

Hydrogen atom, Laser: 2 x 10^{14} W/cm^2 @ 800 nm, **20 opt.cyc. FWHM**
Linear polarization



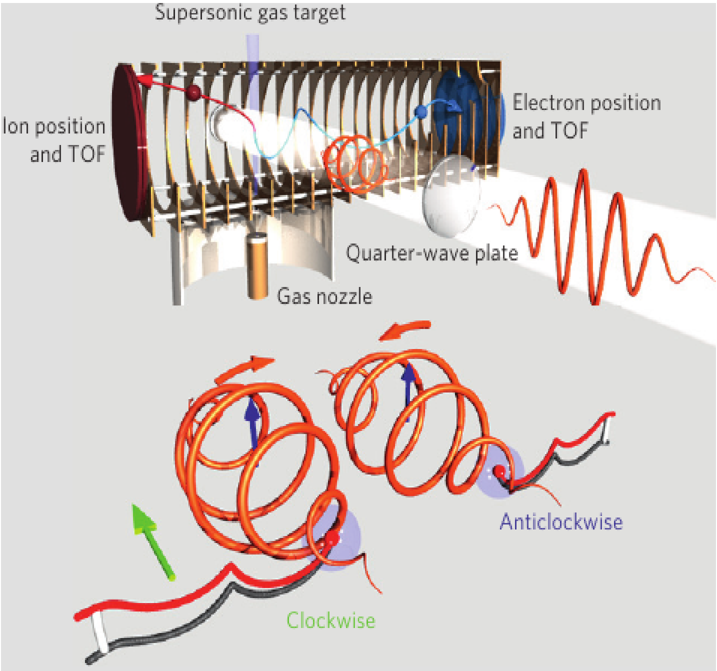
Angle resolved



90 radial discretization points, 30 angular momenta

Attoclock – ionization by elliptically polarized IR

[Pfeiffer et al, Nat. Phys. 8, 76 (2012)]

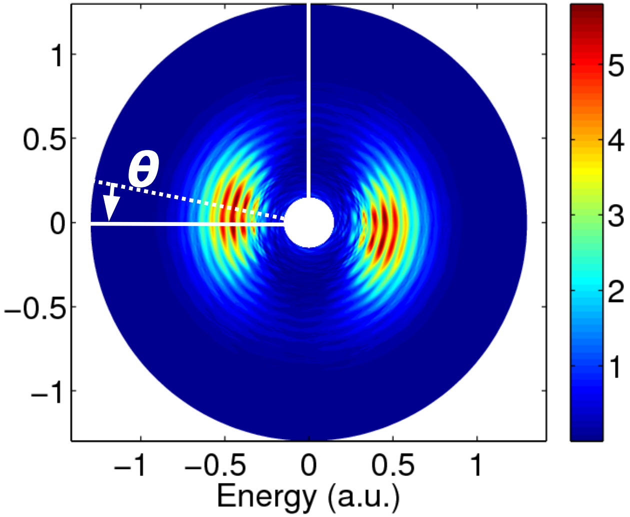


Angle-resolved photo-electron spectra

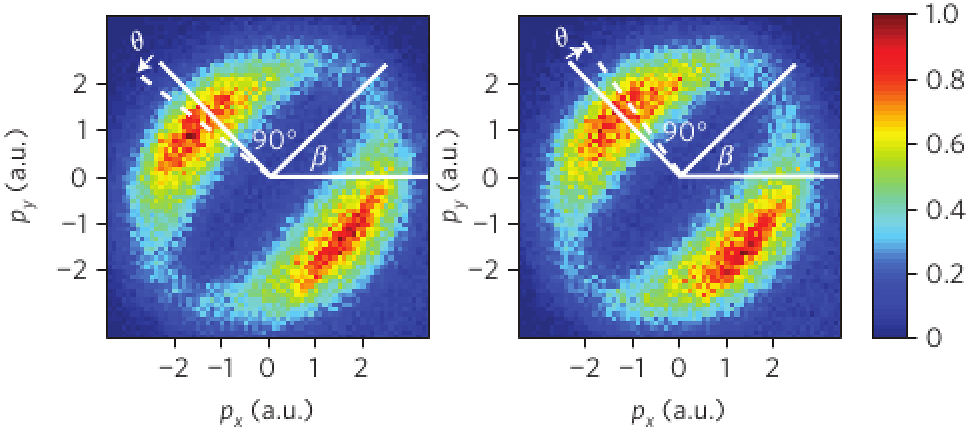
Peak emission direction
deviates from
Peak field direction

=> deduce delay in release of electron

Solution of the TDSE



Use oppositely handed polarizations
to calibrate peak field direction



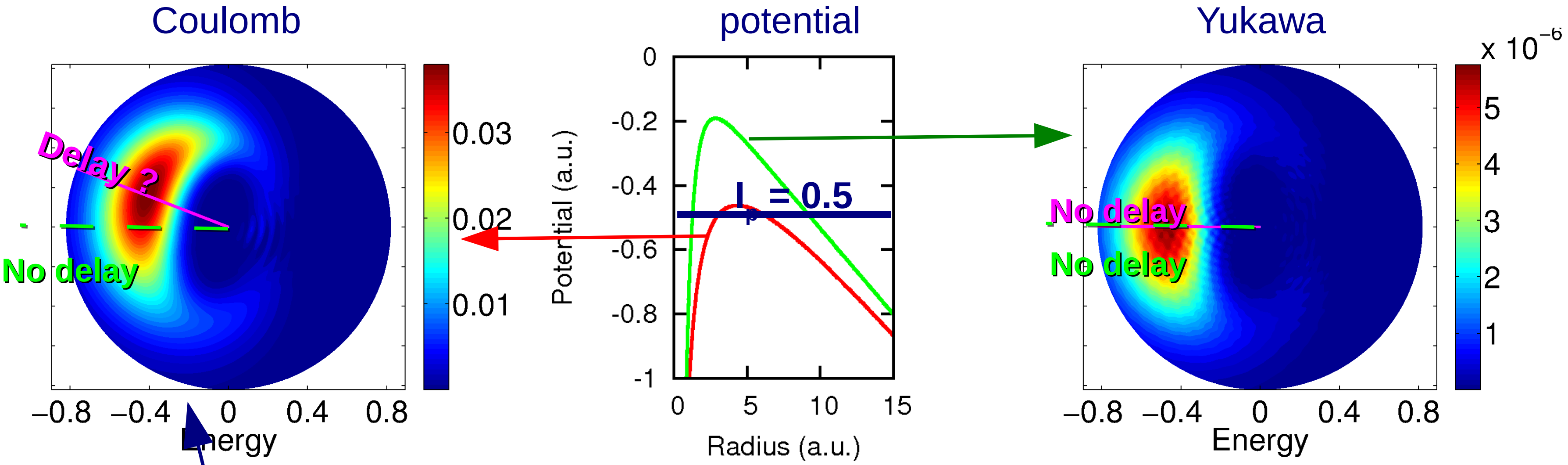
Tunneling times (?) in IR ionization

Is the offset angle θ related to a “tunneling time”?

If the time-delay is related to tunneling,
expect wider barrier longer tunneling delay?

Numerical result

Laser: 800nm, single cycle, 10^{14}W/cm^2, ellipticity as in Pfeiffer et al.
Ionization potential: 0.5 a.u. (Hydrogen)



No evidence for “tunneling time” in this setting

(Reasons for the observed delay in Coulomb – long range correction)

Comparison theory and experiment

Angles of peak photo-emission

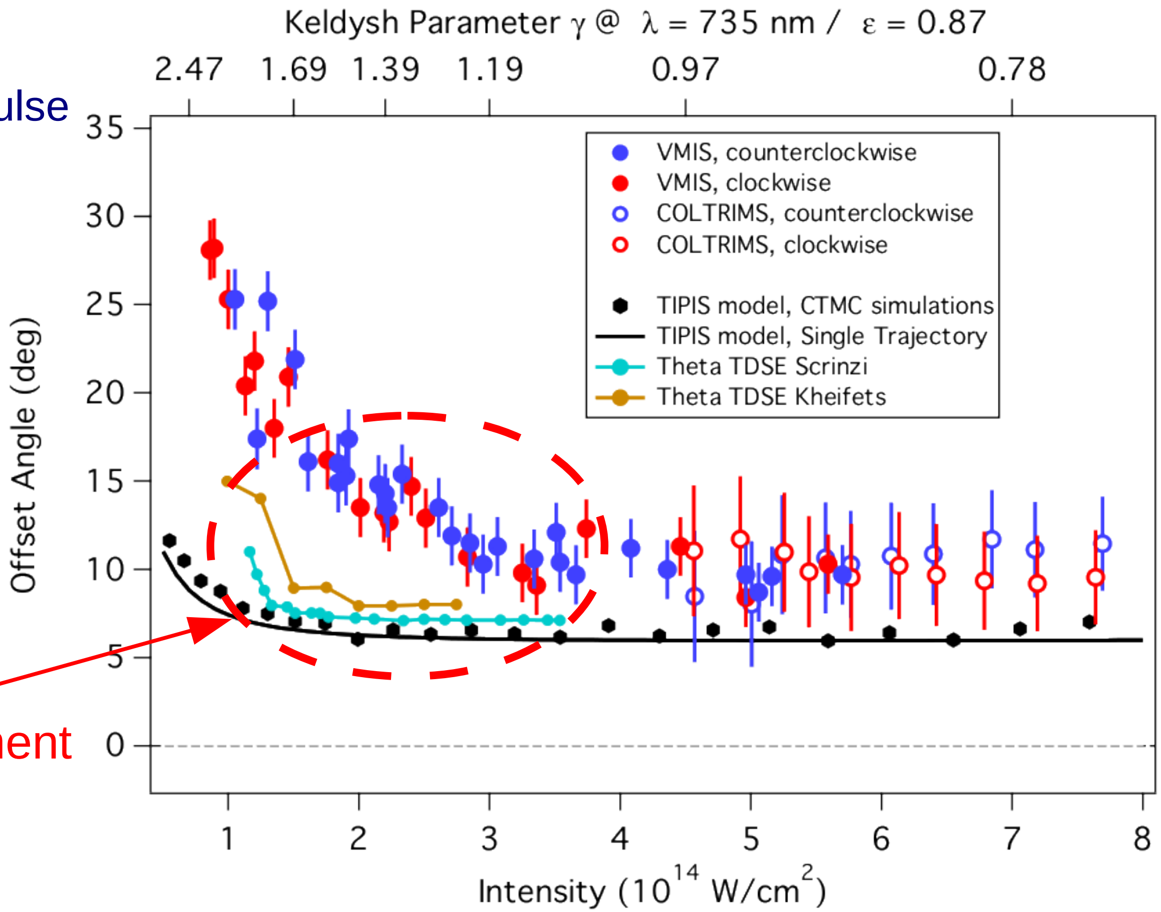
Helium, elliptically polarized pulse

Measurements:

C. Cirelli et al. ETH

Calculations:

L. Madsen(TIPIS)
Kheifets/Ivanov
A. Zielinski/A.S.



Very disquieting disagreement

Note: calculations are all single-electron...

Multi-electron effects?

Two-electron systems

- ✔ Extension of tSURFF to multi-channel emission
- ✔ Extension to double-emission
- ✔ Technical remarks
- ✔ Fano-resonances, correlation in double emission

tSURFF for 2-electron systems

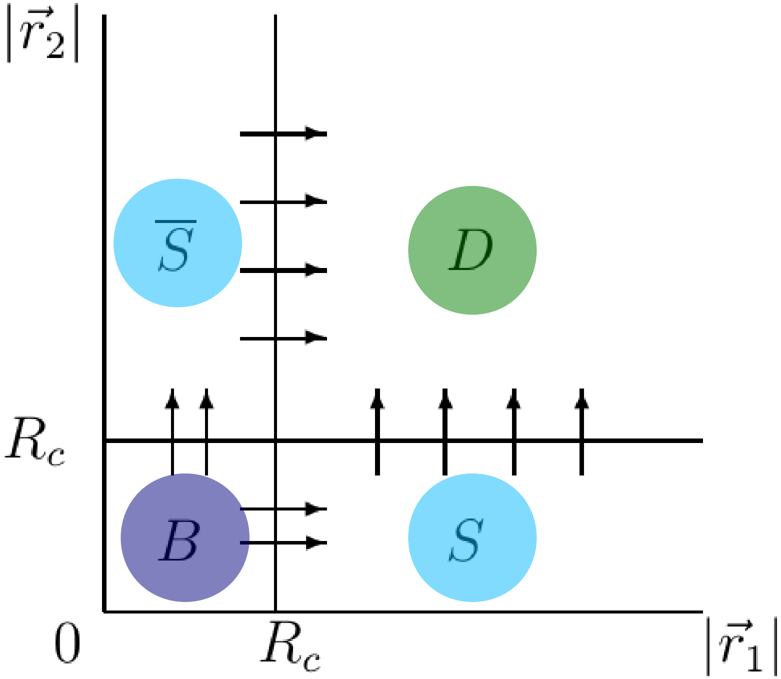
[A. S., New. J. Phys., 14, 085008 (2012)]

Split two-electron coordinate space

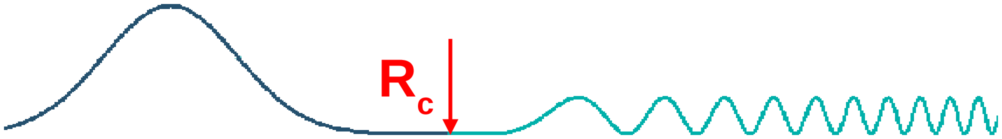
B... $|\mathbf{r}_1|,|\mathbf{r}_2| < R_c$ “bound” region
Numerical solutions on $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$

S... $|\mathbf{r}_2| < R_c$, $|\mathbf{r}_1| > R_c$ “singly asympotic” region
Numerical ionic solution on $\boldsymbol{r}_2$: $\Phi_c(\boldsymbol{r}_2,t)$
Volkov solution on $\boldsymbol{r}_1$

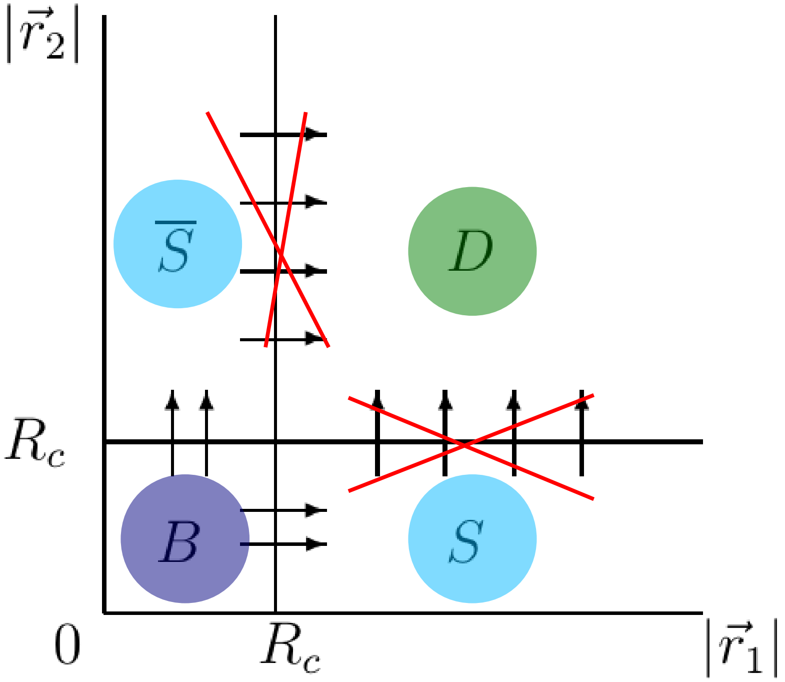
D... $|\mathbf{r}_1|,|\mathbf{r}_2| > R_c$ “doubly asymptotic” region
Volkov solutions on $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$



R_c as before:



Multi-channel single emssion



If one can neglect double ionization

Computational tasks for ionic channels reduces to:

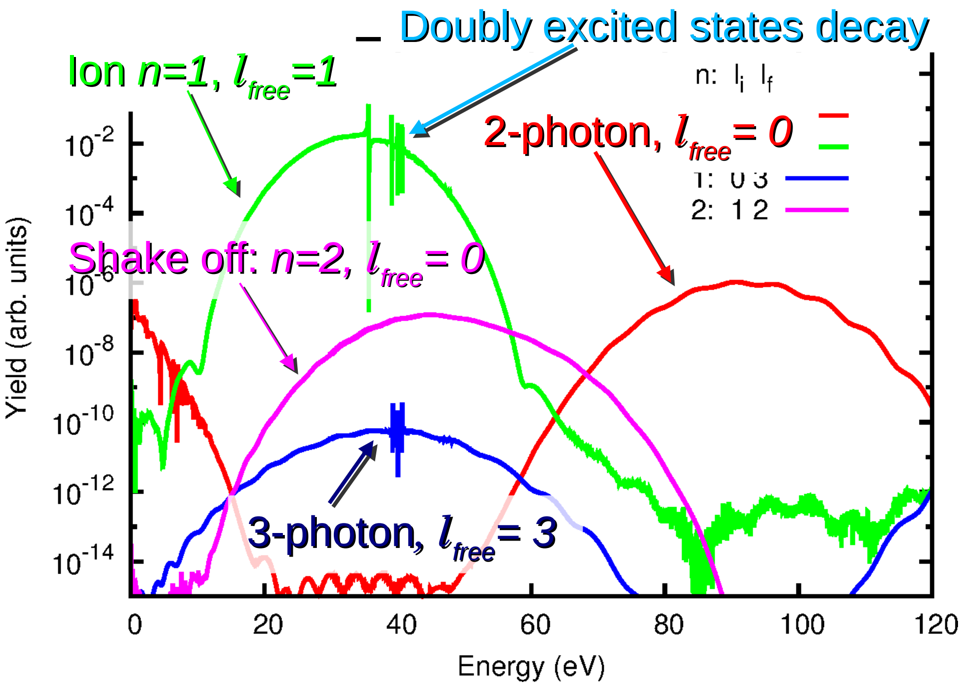
- solve full 2-electron problem on B

- for each single ionization channel, solve a single **ionic problem in [0,R_c]**

3d He: shake up photo-electron spectra @ XUV

Ionic channels & partial waves

(Laser: 2 opt.cyc. FWHM @ hυ=54eV, perturbative intensity regime)



Doubly excited states decay

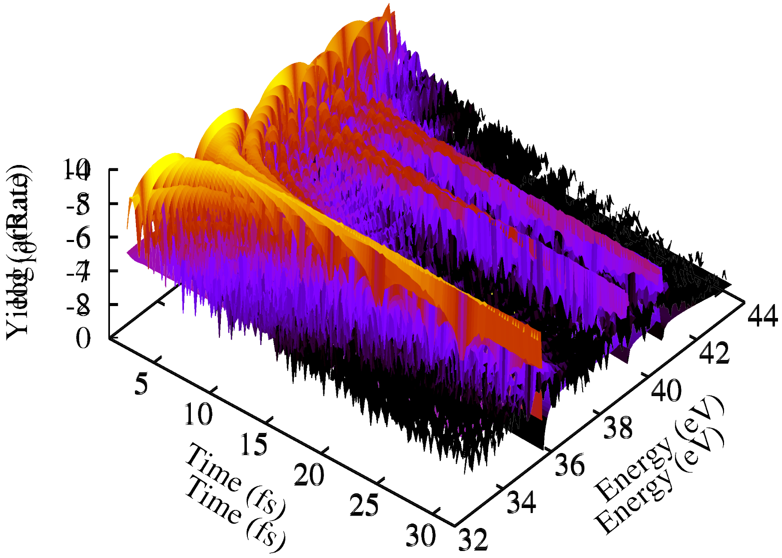
Ion *n*=1, l_{free}=1

2-photon, l_{free} = 0

Shake off: *n*=2, l_{free} = 0

3-photon, l_{free} = 3

Buildup cftEand/dtso(Eat)ces



Note:

Doubly excited content after the end of the pulse
can also be obtained by projection / window operator

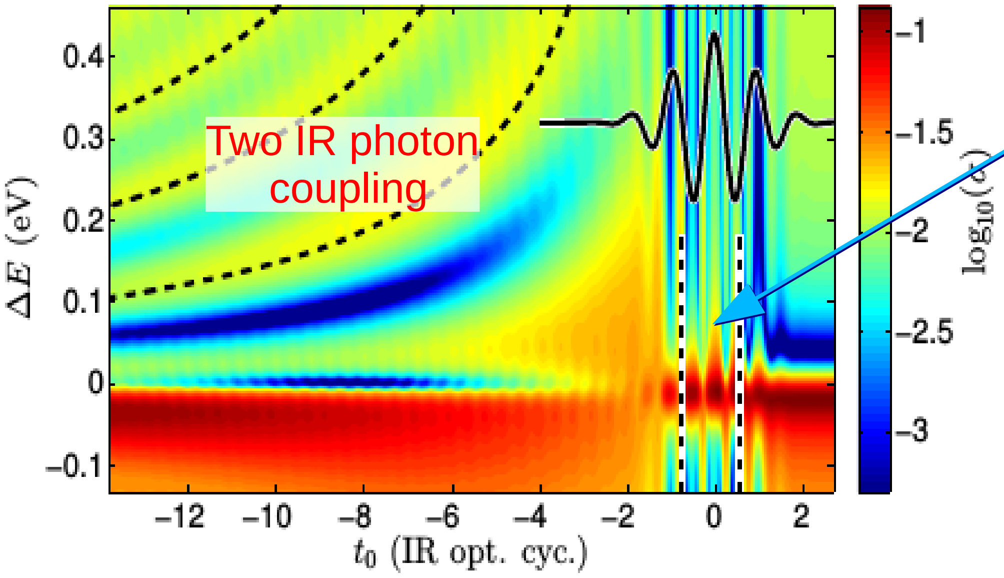
Control of a Helium Fano line shape by IR

[A. Zielinski et al., arXiv:1405.4279]

Pulse parameters

XUV @ 21 nm, 150 as duration
Time-delayd 800 nm few-cycle IR probe
Intensity 2 x 10^{12} W/cm^2

Photo-electron spectrum



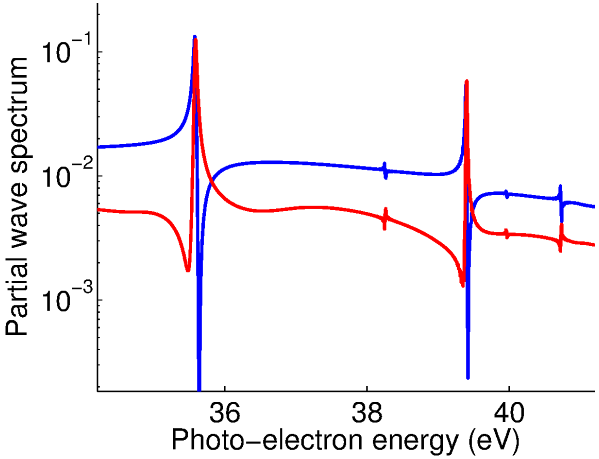
IR after XUV

Overlap

Line-shape modulations

Fano / anti-Fano

(No IR / peak IR)



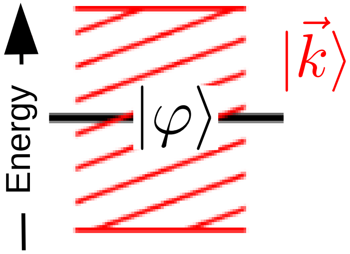
Compare experiment by Ott et al. Science 340, 716 (2013)

Modified Fano theory

[A. Zielinski et al., arXiv:1405.4279]

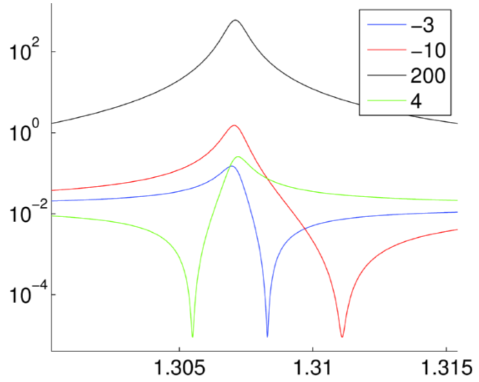
Standard Fano Hamiltonian – resonant state |φ> embedded in continuum |k>

$$H = \underbrace{|\varphi\rangle E_\varphi \langle\varphi| + \int \mathrm{d}k^3\, |\vec{k}\rangle \frac{\vec{k}^2}{2} \langle\vec{k}|}_{H_0:\ \text{interaction-free eigenstates}} + \int \mathrm{d}k^3\, \underbrace{\left(|\vec{k}\rangle V(\vec{k}) \langle\varphi| + |\varphi\rangle V(\vec{k})^* \langle\vec{k}|\right)}_{V:\ \text{coupling}}$$



Lineshape:

$$\sigma := \frac{|\mathcal{E} + q|^2}{\mathcal{E}^2 + 1}$$



Modification during IR

Neglect coupling: $V = 0$

Effects of IR:

$$H_0 \rightarrow H_{IR}(t) = |\varphi\rangle \underbrace{E_\varphi(t)}_{\text{Stark shift}} \langle\varphi| + \int \mathrm{d}^3k\, \underbrace{|\vec{k} - \vec{A}_{IR}(t)\rangle \frac{(\vec{k} - \vec{A}_{IR})^2}{2} \langle\vec{k} - \vec{A}_{IR}(t)|}_{\text{free motion in IR / Volkov}}$$

Modified Fano parameter q → q_{IR}

Complex Fano q-parameter

[A. Zielinski et al., arXiv:1405.4279]

Modification of Fano q-parameter

IR-induced phase shifts

IR streaking

$$q_{\mathrm{IR}} = q + \alpha \left[e^{-i \int_{t_0}^{t_1} dt \left(E_\varphi(t) - E_\varphi^{(0)} \right) + \frac{i}{2} \int A_{IR}^2} / \mathcal{J}(A_{\mathrm{IR}}, k) - 1 \right]$$

coupling

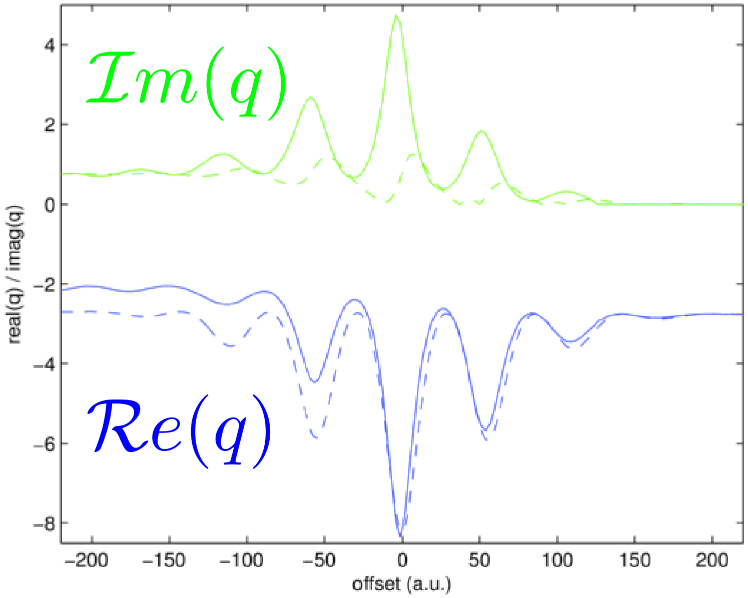
Click for details...

Model vs. TDSE

Solid: fit to full 2-electron TDSE
Dashed: q_{IR}

Need complex q_{IR} !

(no time-reversal symmetry)

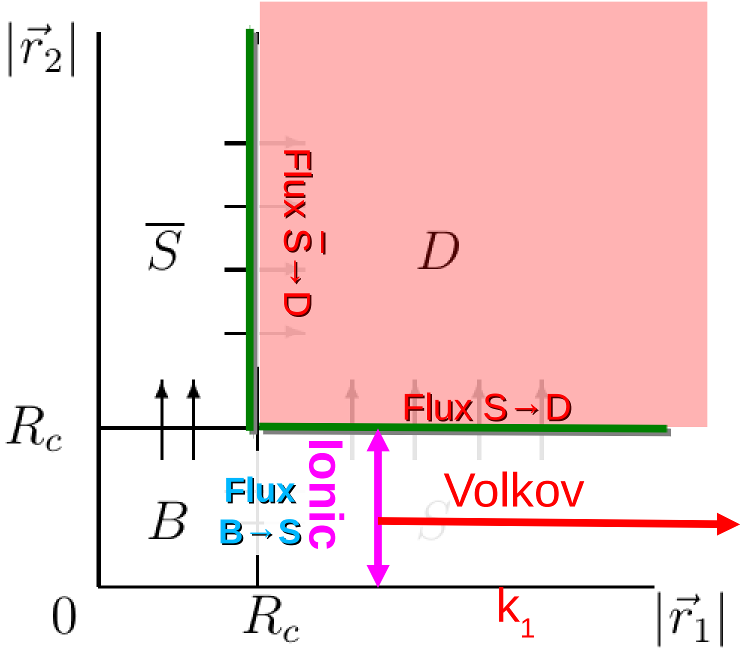


Double-ionization

t-SURFF for two-electron systems: double ionization

[A. S., New. J. Phys., 14, 085008 (2012)]

Spectrum in D – integrate flux S → D



S-D-surface values/derivatives

Need solution in region ***S***

Dynamics is entangled:

Independently for each Volkov $\boldsymbol{k}_1$,

solve one ionic problem in $[0,R_c]$

(perfectly parallelizable)

Similar for flux $\bar{S}$ → D

Equations on *S*

$b(k_1,n,t)$ … coefficients for ionic basis $|\xi_n>$ in $[0,R_c]$

$$i\frac{d}{dt}b(\vec{k}_1,n,t) = \sum_m \langle\xi_n|H_{ion}(t)|\xi_m\rangle b(\vec{k}_1,m,t)$$

…ionic time-evolution

$$-\langle\vec{k}_1,t|[H_v(t),\theta_1]\langle\xi_n|\Psi(t)\rangle\rangle$$

…flux B → S

Double-ionization of Helium at XUV wave length

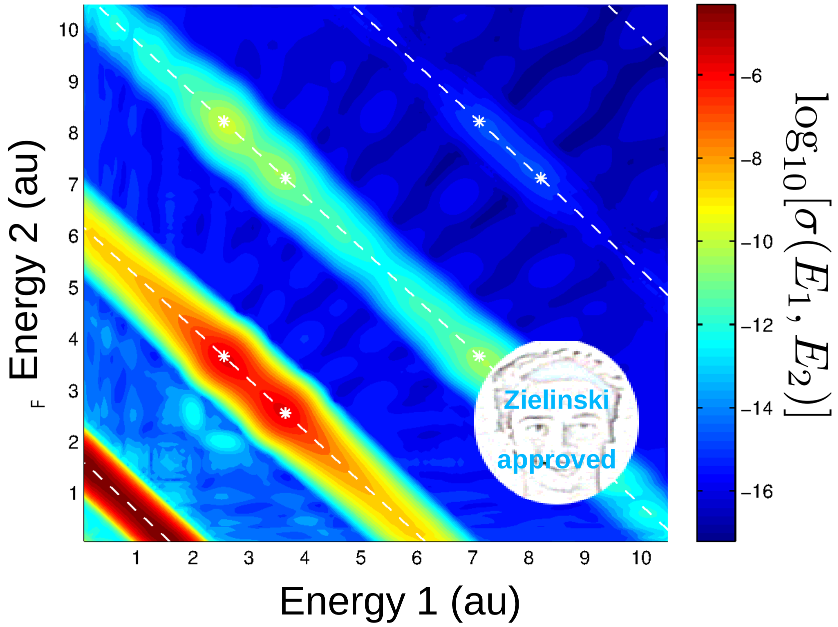
Helium atom

XUV pulse 10nm
Duration 8 cycles
Intensity 10^{15}W/cm^2

Discretization

Simulation volume: 15 au
Angular momenta: 16
Radial basis functions: 56 per electron & ang.mom.
Propagation time: 400 optical cycles

Angle-integrated spectrum



Matches in detail with calculations by S. Nagele et al., box size ~ 1000 au

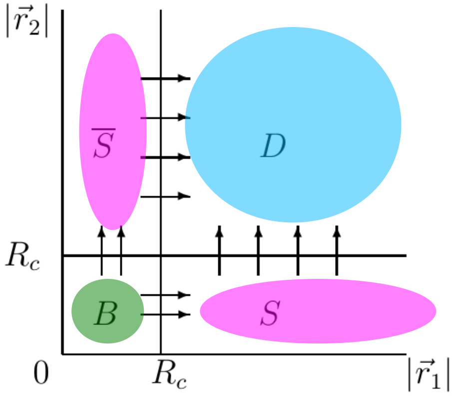
Run time:
4 hours on 16 CPUs (2-electron part)
3* hours on 128 CPUs (spectra from surfaces)

(*)Spectral calculation is fully parallel, effort $\propto \sqrt{\text{number of spectral points}}$

Effort for two-electron calculations

Inner region (B)

Box sizes R_c x R_c ~ 20 x 20 a.u.
Radial discretization points N_1 x N_2 ~ 40 x 40
Angular momenta: wave-length dependent
XUV: M x L_1 x L_2 ~ 2 x 4 x 4
NIR: M x L_1 x L_2 ~ 4 x 40 x 40



Single ionization spectra (S)

Solve one (hydrogen-like) ionic TDSE
for each channel ***c***

$$i\frac{d}{dt}\Phi_c(\vec{r}_1) = H_{ion}(\vec{r}_1)\Phi_c(\vec{r}_1)$$

One time-integral
for each momentum ***p*** in the channel

$$\int dt\ \mathrm{f}[\vec{p}, \Phi_c(|\vec{r}_1| = R_c)]$$

Double ionization spectra (D)

One ionic TDSE with source term
for each momentum $\boldsymbol{p}_2$,

$$i\frac{d}{dt}\Phi_{\vec{p}_2}(\vec{r}_1) = H_{ion}(\vec{r}_1)\Phi_{\vec{p}_2}(\vec{r}_1) + S_{\vec{p}_2}(\vec{r}_1)$$

One time-integral
for each momentum pair ($\boldsymbol{p}_1$,$\boldsymbol{p}_2$)

$$\int dt\ \mathrm{g}[\vec{p}_1, \Phi_{\vec{p}_2}(|\vec{r}_1| = R_c, t)]$$

Complex atoms and small molecules

- ✔ Integration with quantum chemistry (COLUMBUS)
- ✔ Technical remarks
- ✔ Emission from Ar and N_2

Ionic core dynamics (quantum chemical)

for molecular photo-emission...

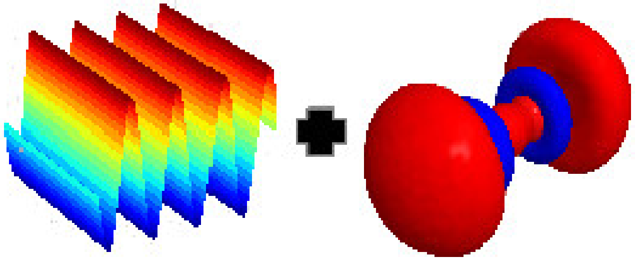
Combine complex scaled basis χ_i
with ionic CI functions Φ_c (COLUMBUS)

Goals:
Reliable strong-field ionization rates
Accurate photo-electron spectra

Anti-symmetrize

$$\psi_{i,c}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n) = \mathcal{A}\left[\chi_i(\vec{r}_1)\,\Phi_c(\vec{r}_2, \ldots, \vec{r}_n)\right]$$

$$\boxed{\Psi = \sum_{c=1}^{N_{core}} \sum_i C_{i,c}(t)\psi_{i,c}}$$



Difficulties:

Get CI wave function (solved)
Basis size (endless story)
Messy matrix elements (solved)
Over-completeness issues (solved)
Gauge (solved)

Many thanks for access to
COLUMBUS wave functions
H. Lischka
Th. Müller
J. Pittner

Core-dynamics Anti-Symmetrization Gauge

Gauge dependence of the approach

Idea of the quantum chemistry basis

Core electron dynamics largely within field free bound states Ψ_i

Length gauge:

x and p have their standard meaning
Functions Ψ_i correspond to field free states also in presence of IR

Velocity gauge:

Corresponds to a time-dependent boost $p \to p + eA(t)/c$
Functions $e^{-i\vec{r}\cdot\vec{A}(t)}\Psi_i(\vec{r})$ correspond to field free state

At strong IR fields exp[-irA(t)] can strongly differ from 1 across the Ψ_i

(Compare the debate about the “correct” gauge in SFA)

Computations more efficient in velocity gauge
=> local gauge transform on the bound state range
(tricky business)

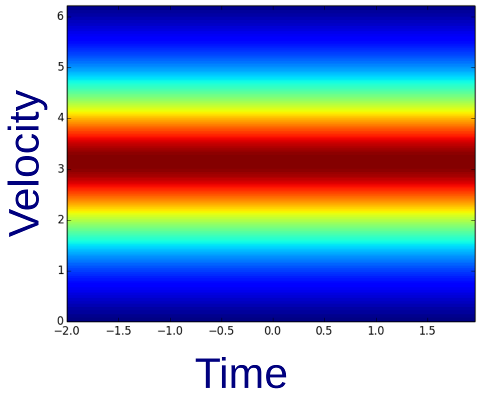
Physics implications of gauge

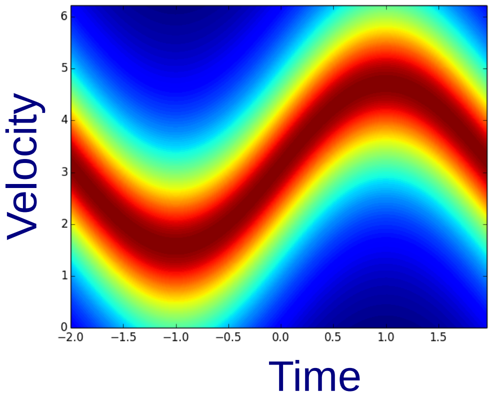
Gauge is nothing but math – multiply everything by $U(t) = \exp[-i\vec{A}(t)\cdot\vec{r}]$

Velocity gauge is an accelerated frame of reference

Change of momentum coordinate $\vec{p} \to \tilde{\vec{p}} = \vec{p} + \vec{A}(t)$

Velocity distribution of $\Phi_0(\vec{r}) = \exp(-r)$


Length gauge


Velocity gauge

So, which distribution is your choice?

Length gauge is the natural* choice IF we believe the system remains close to Φ_0

(*) for SFA, Coupled-Channels, R-matrix,...

Numerical aspects of gauge

While length gauge may be more “natural”…

Velocity gauge is “better” for numerical calculations

Smaller momenta

When the laser-imposed boosts become
comparable to the initial state momentum spread

the canonical momentum-range covered is smaller
→ Fewer phase-wiggles in your wave-function
→ Fewer angular momenta $L = \vec{r} \times \vec{p}$ - important at large |r|

Efficient absorption

irECS – the by far most efficient (and the only exact)
absorption method for TDSE
requires velocity gauge

Break the spell – mix the gauges!

Issues: rapid, time-dependent change or
discontinuity of solution
in the transition region length ←→ veloctiy

Core-discretization is gauge sensitive

Non-interacting system $H(x,y) = h(x) + h(y)$

Ansatz + exchange (triplet) $\Psi(x,y,t) = \phi(x,t)\chi(y,t) - \chi(x,t)\phi(y,t)$

Matrix element
$$\langle\Psi|H|\Psi\rangle = \langle\phi|\phi\rangle\langle\chi|h|\chi\rangle + \langle\phi|h|\phi\rangle\langle\chi|\chi\rangle$$
$$\underbrace{-\langle\chi|\phi\rangle\langle\phi|h|\chi\rangle - \langle\chi|h|\phi\rangle\langle\phi|\chi\rangle}$$

$\langle\chi(t)|\phi(t)\rangle = 0$ for exact time-evolution

$\langle\chi(t)|\phi(t)\rangle \neq 0$ for approximate evolution of $|\phi(t)\rangle$

Importance of the effect

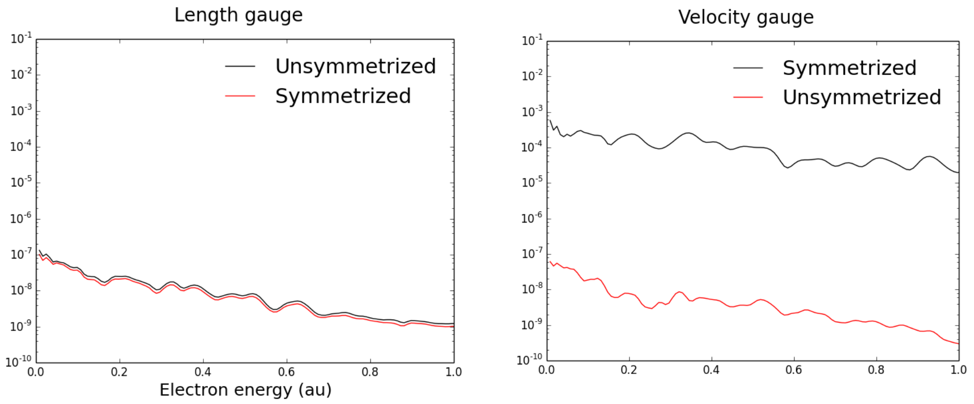
System: non-interacting He

Pulse: 1 x 10^{15} W/cm^2

400 nm

Discretization:

4 coupled channels



**** Minimize core-polarization (→ length gauge)**

**** Describe remaining polarization correctly:**

e.g. xSCF, small phase-space grid for one more electron

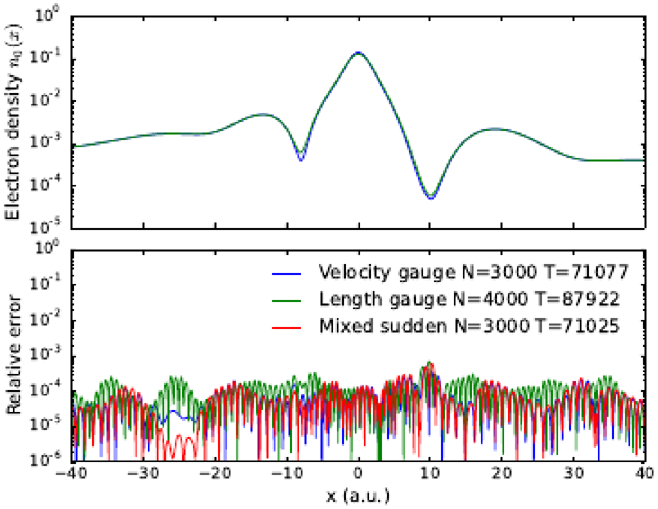
**** Possibly: separate spin from exchange symmetry (?)**

Numerical efficiency of gauges – single electron

1d model electron density

Single-cycle pulse,
800 nm, 25% ionization
No absorption (large box)

Discretization adjusted
for 10^{-4} relative error

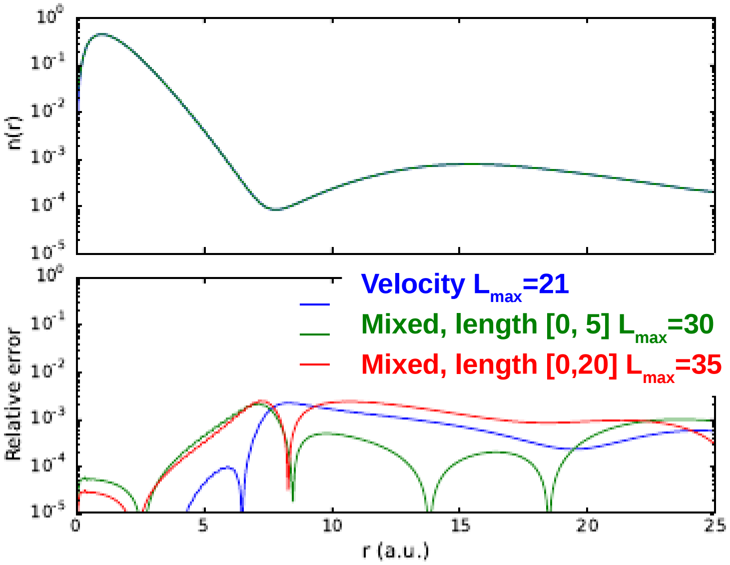


**Velocity and mixed comparable
Length less efficient**

3d H-atom electron density

3-cycle pulse,
800 nm, 16% ionization
irECS absorption (box 30 au)

Discretization adjusted
For ~ 10^{-3} relative error



Penalty for size of length-gauge region

Numerical efficiency of gauges – He and H_2

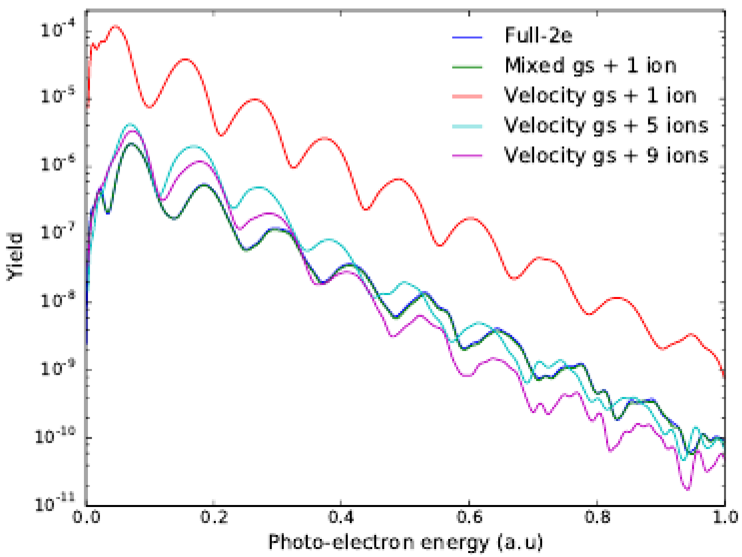
Total photoelectron spectra

3-cycle pulse, 400 nm, 10^{14} W/cm^2

Compare

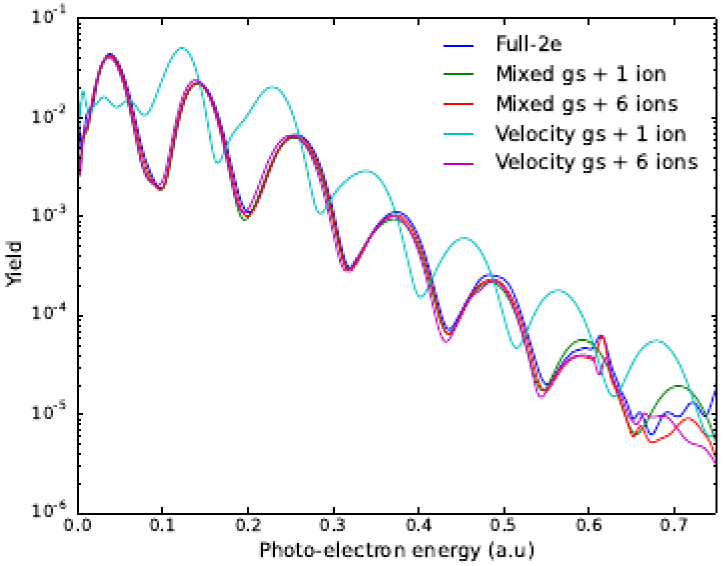
Converged 2-electron calculation
with ionic core dynamics calculations
in velocity and mixed gauges

Helium



Mixed gauge converges with 1 ion state
Velocity gauge not converged with 9 ion states

H_2 molecule



Mixed gauge converges with 1 ion state
Velocity gauge barely converged with 6 ion states

A flavor of the complexity of matrix elements

Two-particle (electron-electron) interaction: $H_2 = \sum_{i,j,i<j} h_{ij}$

Electron + ion basis function:

$$\psi_{i,I} = \mathcal{A}\left[\chi_i(\vec{r}_1)\Phi_I(\vec{r}_2 \ldots \vec{r}_n)\right]$$

Matrix element:

$$\begin{aligned}
\langle\psi_{i,I}|H_2|\psi_{j,J}\rangle = &(n-1)\sum_{kl}\langle\phi_k\chi_i|\phi_l\chi_j\rangle\rho^{(1)}_{kl;IJ} \\
&+\frac{(n-1)(n-2)}{2}\langle\chi_i|\chi_j\rangle\sum_{klmn}\langle\phi_k\phi_l|\phi_m\phi_n\rangle\rho^{(2)}_{klmn;IJ} \\
&-(n-1)\sum_{kl}\langle\phi_k\chi_i|\chi_j\phi_l\rangle\rho^{(1)}_{kl;IJ} \\
&-(n-1)(n-2)\sum_{klmn}\langle\phi_k\chi_i|\phi_m\phi_n\rangle\rho^{(2)}_{klmn;IJ}\langle\phi_l|\chi_j\rangle \\
&-(n-1)(n-2)\sum_{klmn}\langle\phi_k\phi_l|\chi_j\phi_n\rangle\rho^{(2)}_{klmn;IJ}\langle\chi_i|\phi_m\rangle \\
&-\frac{(n-1)(n-2)(n-3)}{2}\sum_{abcdef}\langle\phi_a\phi_b|\phi_d\phi_e\rangle\boxed{\rho^{(3)}_{abcdef;IJ}}\langle\chi_i|\phi_f\rangle\langle\phi_c|\chi_j\rangle
\end{aligned}$$

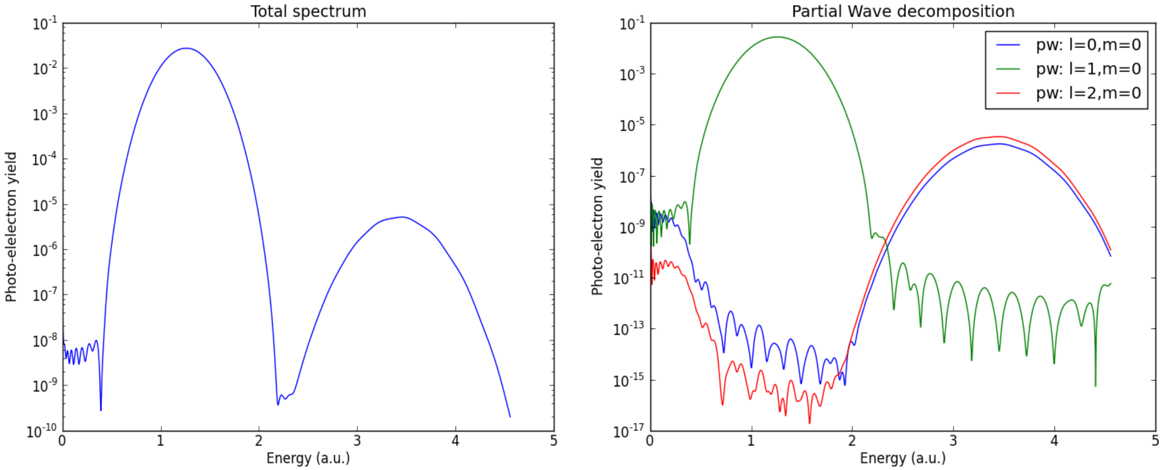
Non-standard 3-particle reduced density matrix for ionic states Φ_I,Φ_J

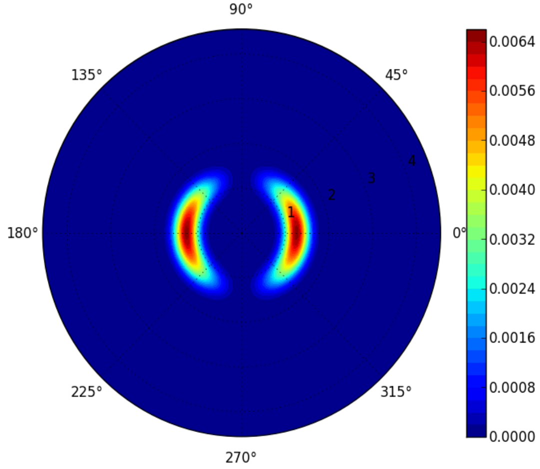
Photo-electron spectra of He, H_2, N_2

XUV photo-ionization of Helium

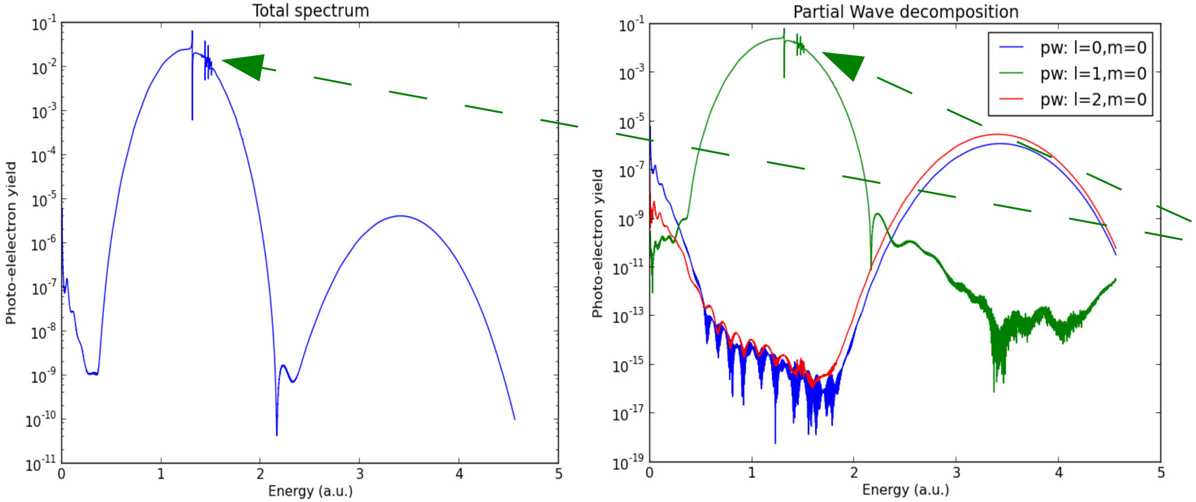
Pulse parameters: λ = 21nm, 3-cycle, $\cos^8$ envelope, linear polarization

1 ionic state





6 ionic states



Doubly excited states / Fano resonances

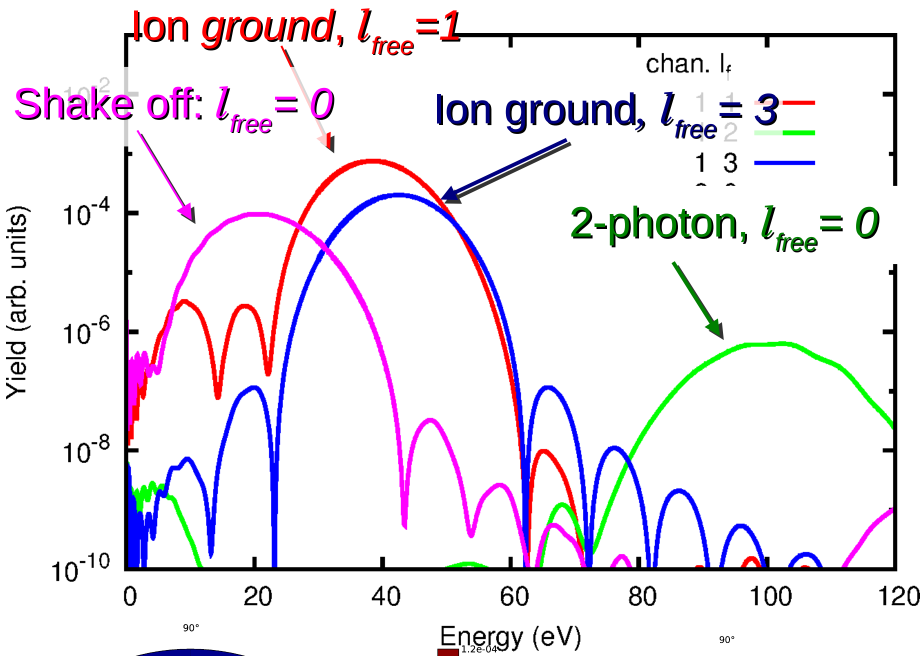
State	Literature[a]	Calculation
2s 2p	1.307	1.313
2s 3p	1.436	1.441
2s 4p	1.466	1.474

[a] J Chem. Phys. 139, 104314 (2013)

Photo-ionization of H_2 and N_2

H_2 XUV photo-ionization

Pulse: 21 nm, 3 cycle FWHM, 10^{15}W/cm^2


Ion ground, l_{free}=1

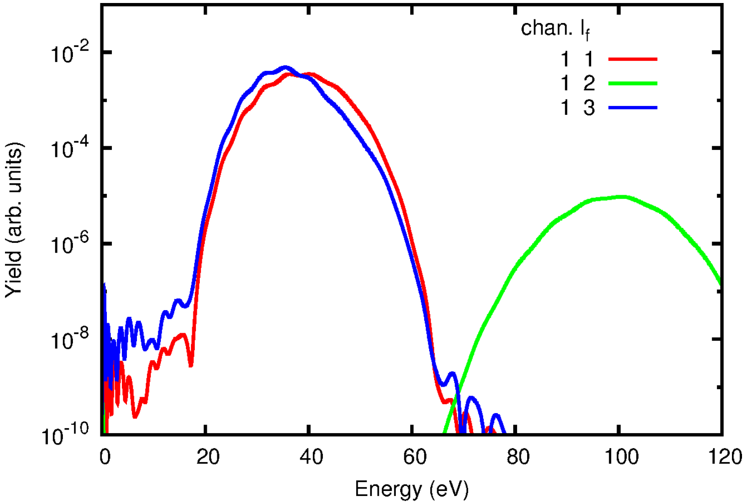
Shake off: l_{free} = 0

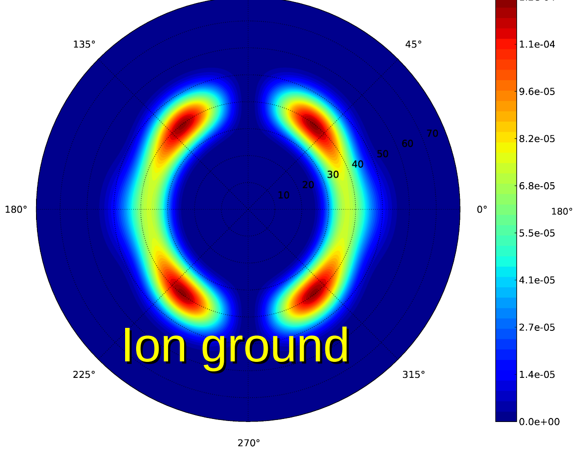
Ion ground, l_{free} = 3

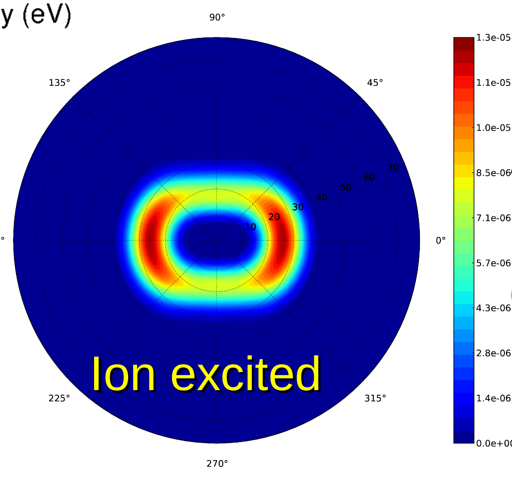
2-photon, l_{free} = 0

N_2 XUV photo-ionization

More of the same...




Ion ground


Ion excited

Angle-resolved spectra

H_2 ionic channels
(disc diameter=80 eV)

Team

Vinay Majety
2-electron
& molecules

Mattia Lupetti
Solids and
surfaces

Alejandro “the convergator” Zielinski
1-e elliptic
2-electron

Jakob Liss
Solids and
surfaces

Publications

[A.S., Phys. Rev. A81, 53845 (2010)]
[L. Tao and A.S., New. J. Phys. 14, 013021 (2012)]
[A. S., New. J. Phys., 14, 085008 (2012)]
[A.S., HP. Stimming, N. Mauser, J.Comp.Phys 269, 68 (2014)]

Finances

MAP
Munich Advanced Photonics
Excellence Cluster

ViCoM
Vienna Computational Materials Science
FWF Special Research Program

CORINF
Correlated Multielectron Dynamics
in Intense Laser Fields
Marie Curie ITN

Code: tRecX = tSURFF + irECS (working title)

All codes united in a single, C++ code based on recursive structures

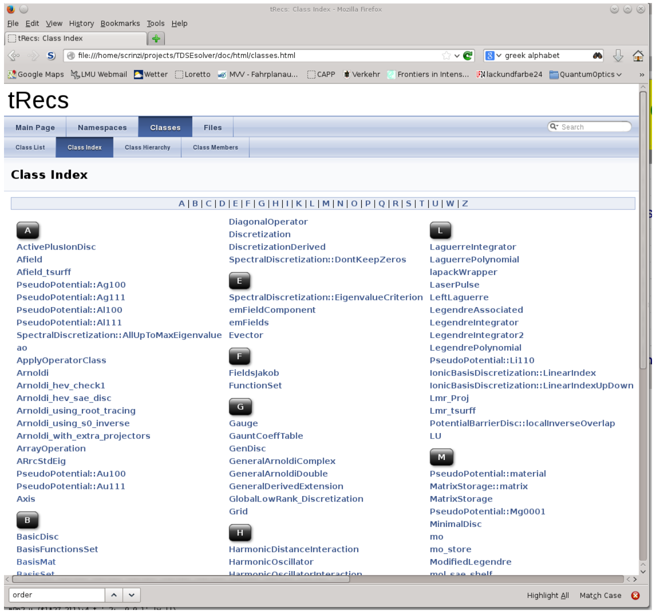
General dimensions and coordinate systems

PDEs of the form $\boxed{d/dt\Psi = D\Psi}$

(includes e.g. Maxwell's equations)

Preparing for public access
Can be made available for collaborations immediately

Doxygen documentation



tRecs

Class Index

A | B | C | D | E | F | G | H | I | K | L | M | N | O | P | Q | R | S | T | U | W | Z

A
ActivePlusIonDisc
Afield
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PseudoPotential::Ag111
PseudoPotential::Al100
PseudoPotential::Al111
SpectralDiscretization::AllUpToMaxEigenvalue
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Arnoldi_hev_sae_disc
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Arnoldi_using_s0_inverse
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SpectralDiscretization::DontKeepZeros

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GeneralArnoldiDouble
GeneralDerivedExtension
GlobalLowRank_Discretization
Grid

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HarmonicOscillator

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LegendreAssociated
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IonicBasisDiscretization::LinearIndexUpDown
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Lmr_tsurff
PotentialBarrierDisc::localInverseOverlap
LU

M
PseudoPotential::material
MatrixStorage::matrix
MatrixStorage
PseudoPotential::Mg0001
MinimalDisc
mo
mo_store
ModifiedLegendre

tRecX demo input

```
--- coordinates and discretization ---
Axis: coordinate,nCoefficients,lower end, upper end,functions,order
 M,1
 Eta,3
 R,120,0.,60.,legendre,20

--- Hamiltonian for the Hydrogen atom ---
Operator: Hamiltonian
<1><1><1/2.dJd-Jr>+<1><1/2.dJ1q2d><rJr>

--- laser pulse definition ---
Laser: shape, I(W/cm2), FWHM, lambda(nm),phiCEO
gauss, 0.5e14, 110., 100000.,0

--- what to plot along which coordinates ---
Plot: coordinate,points,lowerBound,upperBound
      R,51,0.,12.
      Eta,21,-1.,1.
```