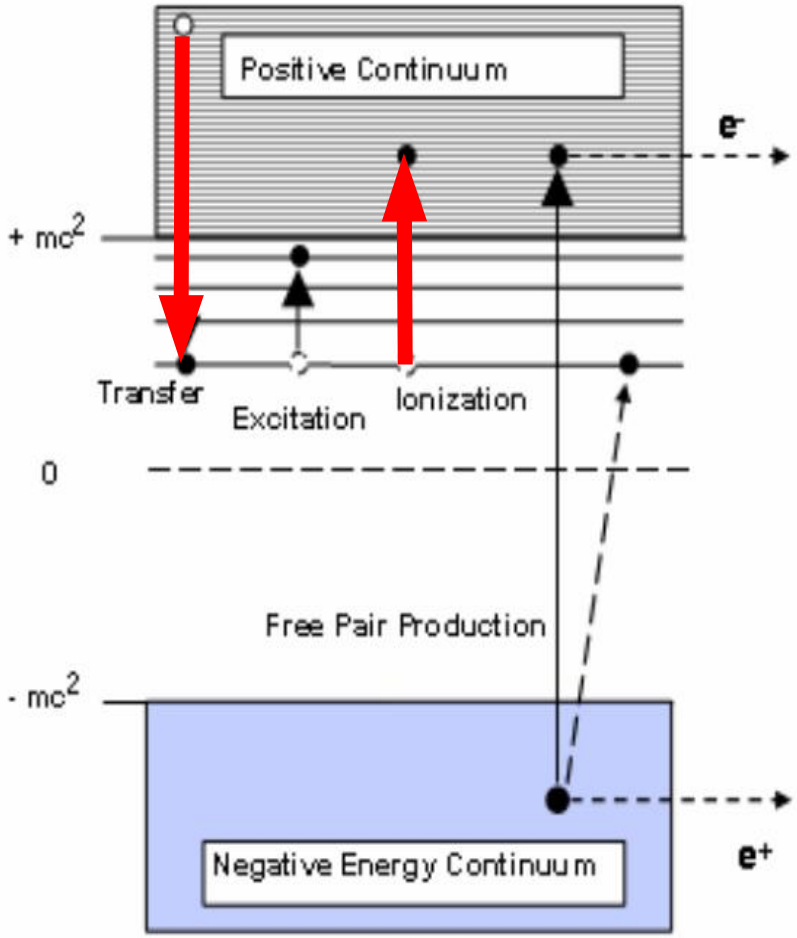
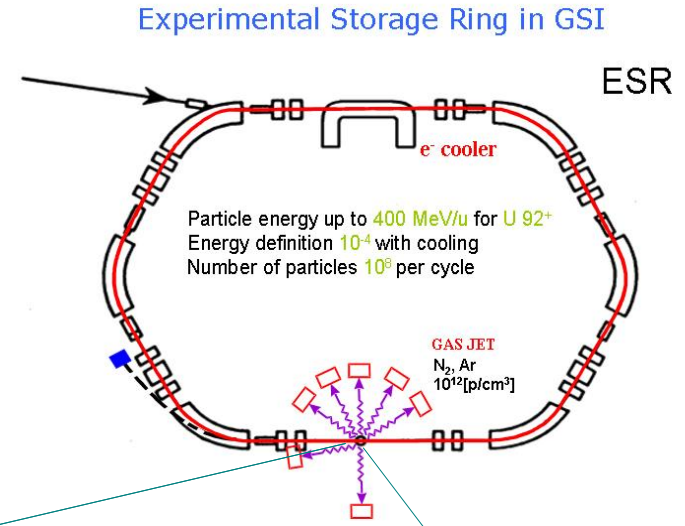
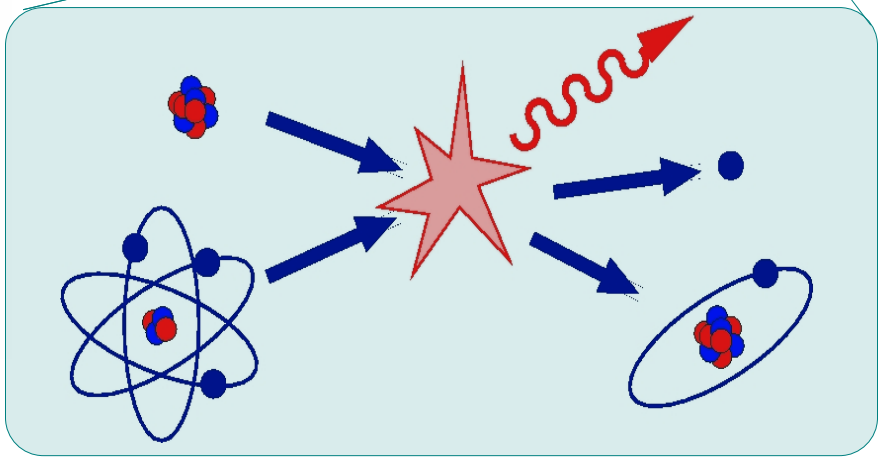
Accurate calculations of atomic structure and capture processes of high-Z ions

S. Fritzsche, T. Radtke and A. Surzhykov
GSI Darmstadt, 21. November 2006

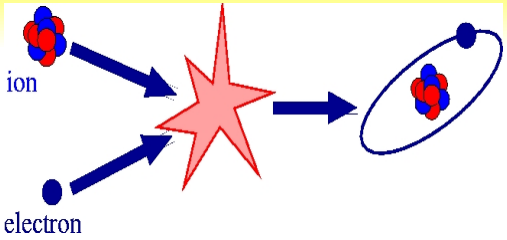




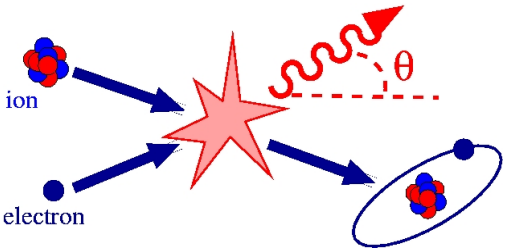


Electron capture at storage rings into high-Z ions

So far...

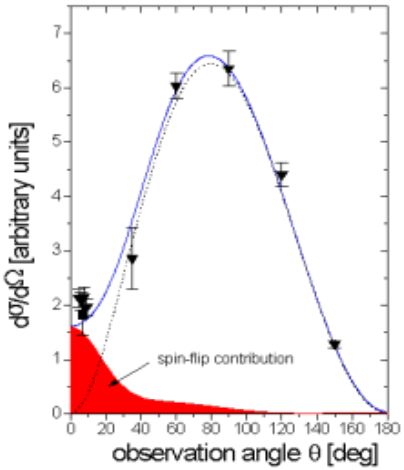


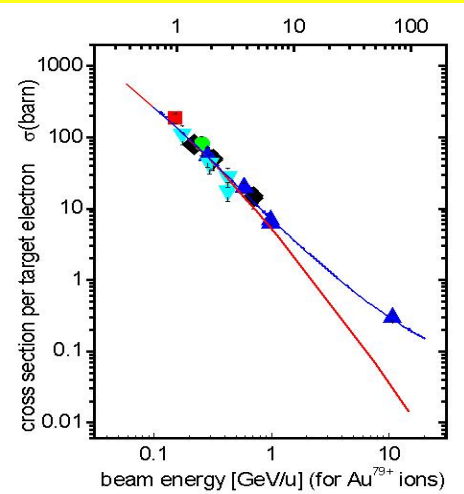
total cross sections



angular distributions

$$\sigma \sim \sum_{polarization} \int d\Omega |M|^2$$

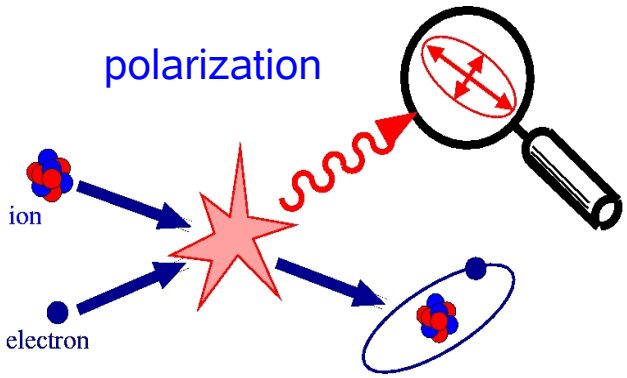


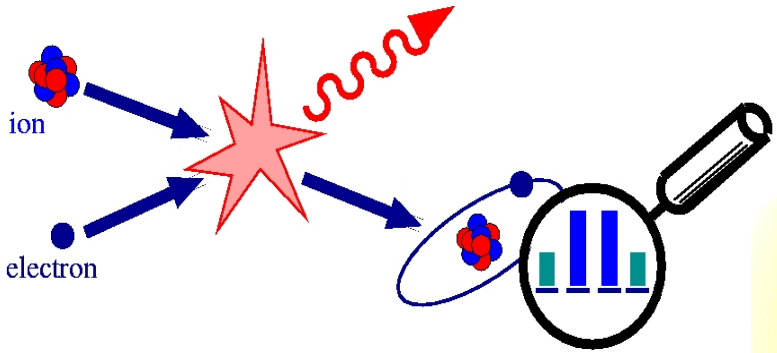


$$\frac{d\sigma}{d\Omega}(\theta) \sim \sum_{polarization} |M|^2$$

New directions ...

polarization





Alignment studies

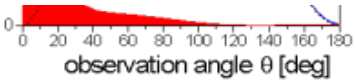
$$\sim |M|^2$$

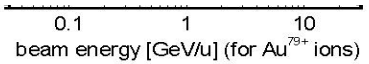
No summation over polarization states !

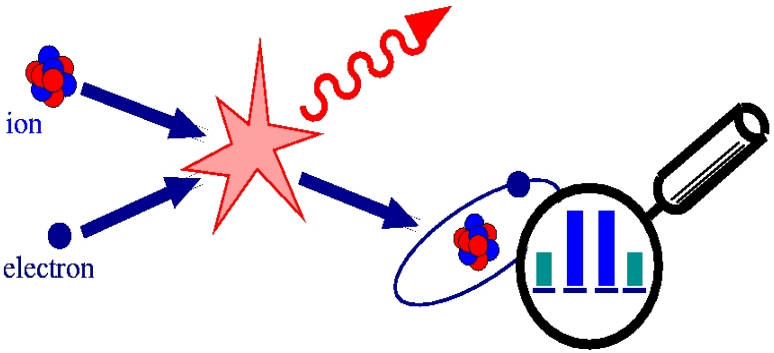
Electron capture at storage rings into high-Z ions

New directions ...

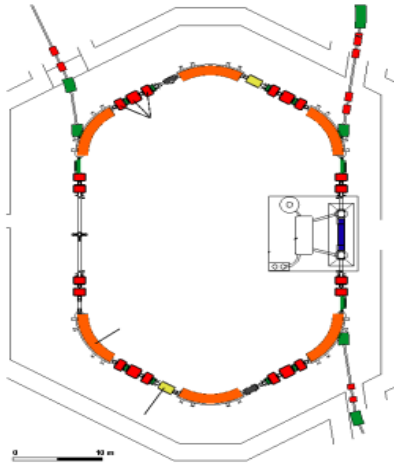
angular distributions

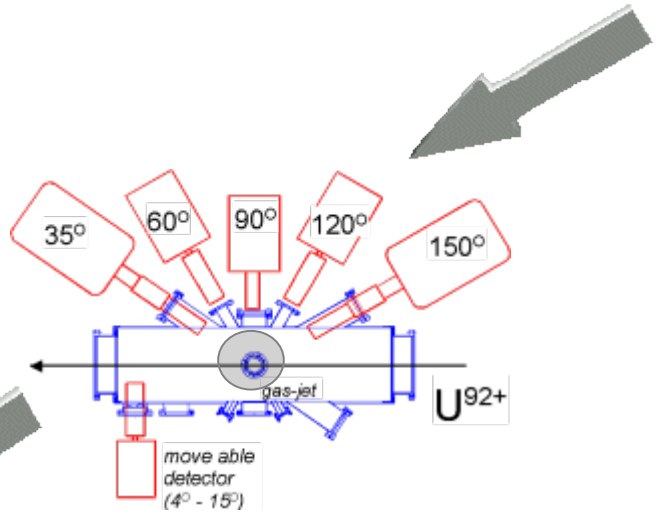


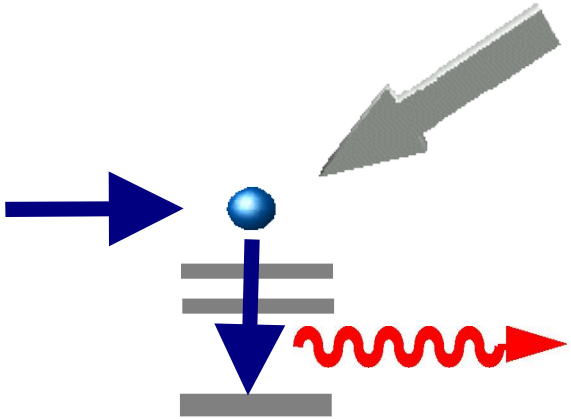




Alignment studies







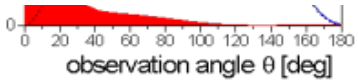
Experiments by Thomas Stöhlker and coworkers

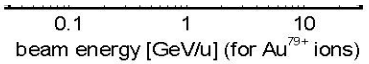
--> see talk by Andrey Surzhykov

Electron capture at storage rings into high-Z ions

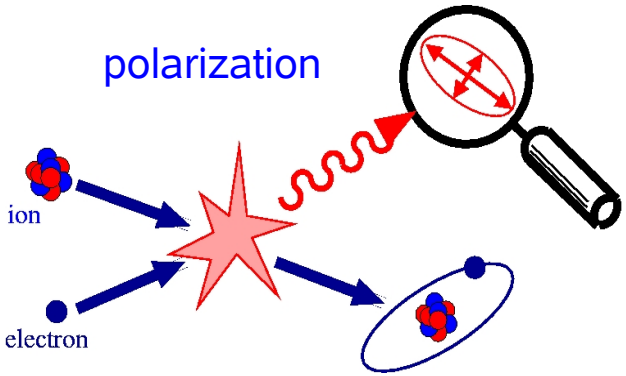
New directions ...

angular distributions

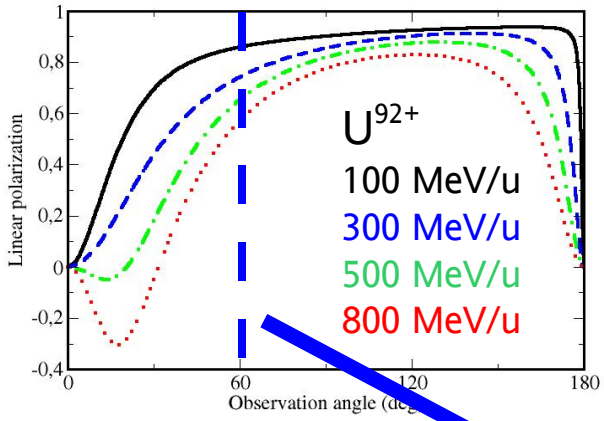




polarization

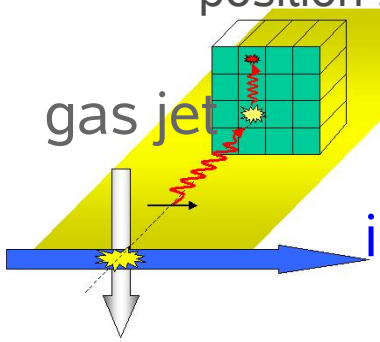


S. Tachenov et al., PRL (2006) in print

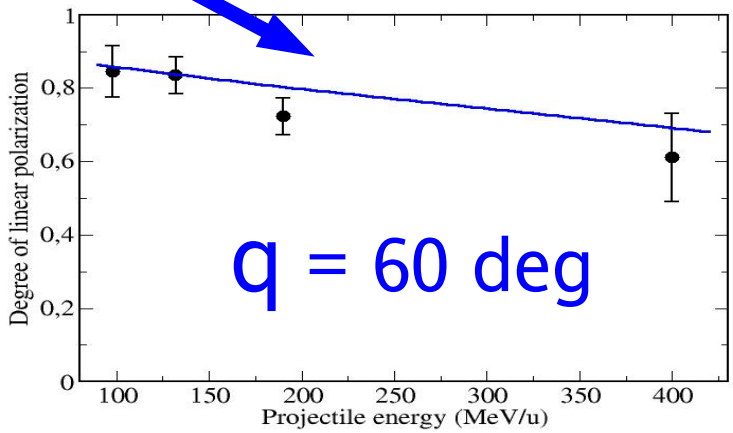


Excellent agreement with experimental data !

position sensitive detector



ion beam

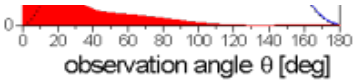


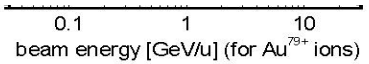
S. Tachenov/T. Stöhlker (2004)

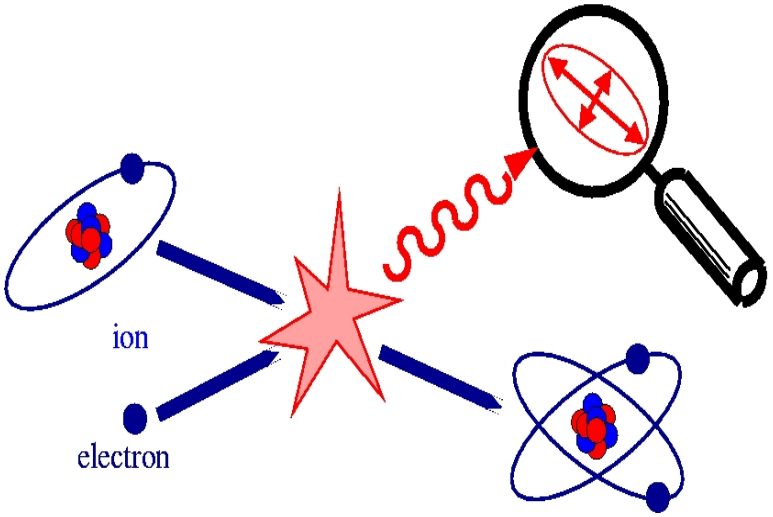
Electron capture at storage rings into high-Z ions

New directions ...

angular distributions

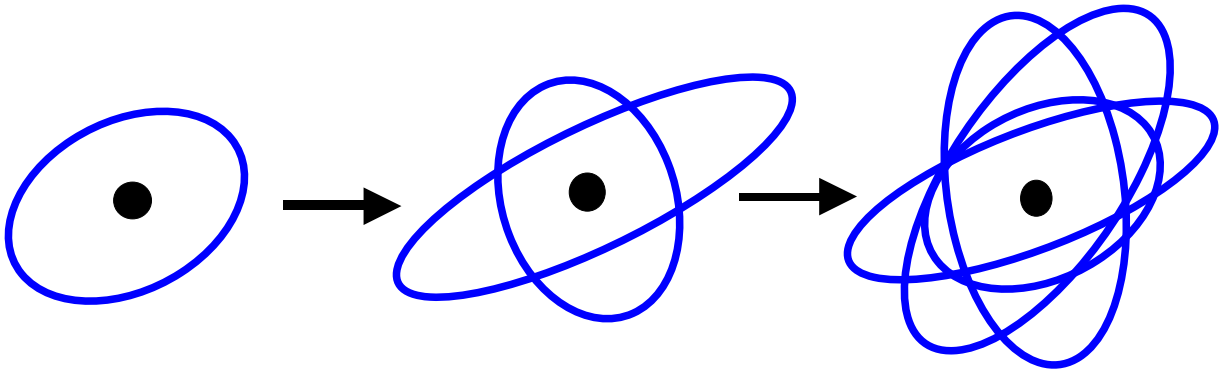






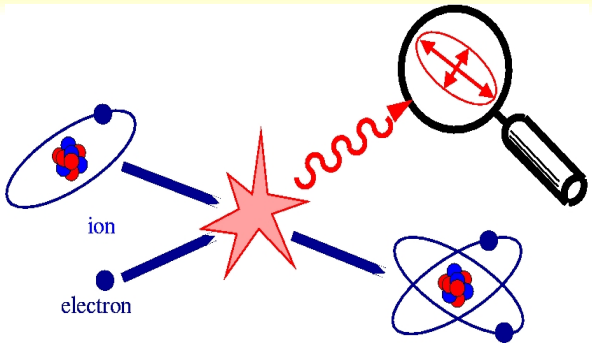
Many-particle character:

- e-e correlations in bound systems
- Free-bound interactions and correlations
- Effects of relativity and strong fields
- Resonance phenomena (Fano)



REC into high-Z, few-electron ions

--- first experimental studies



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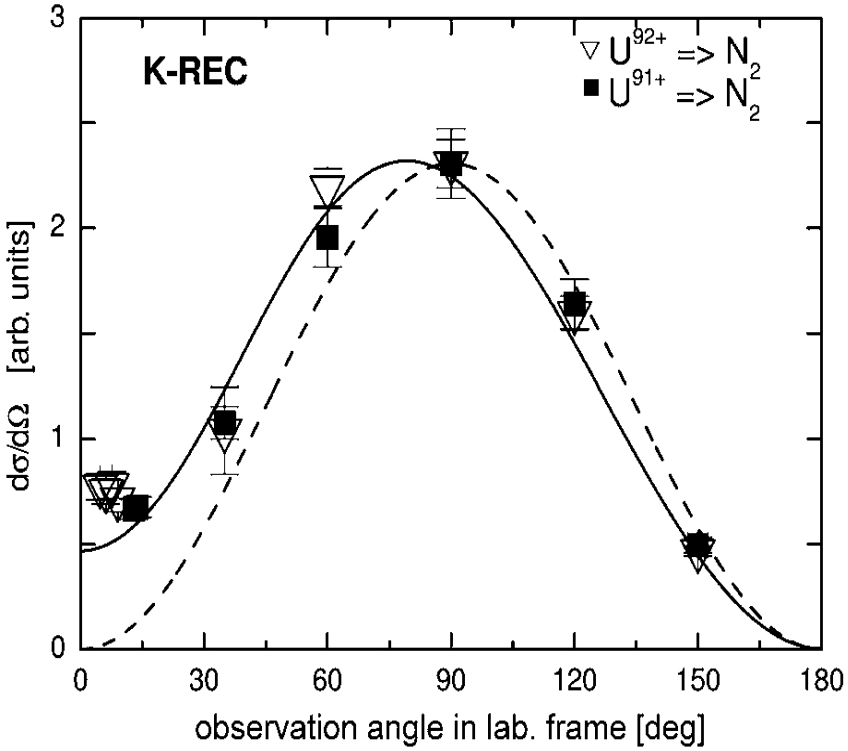
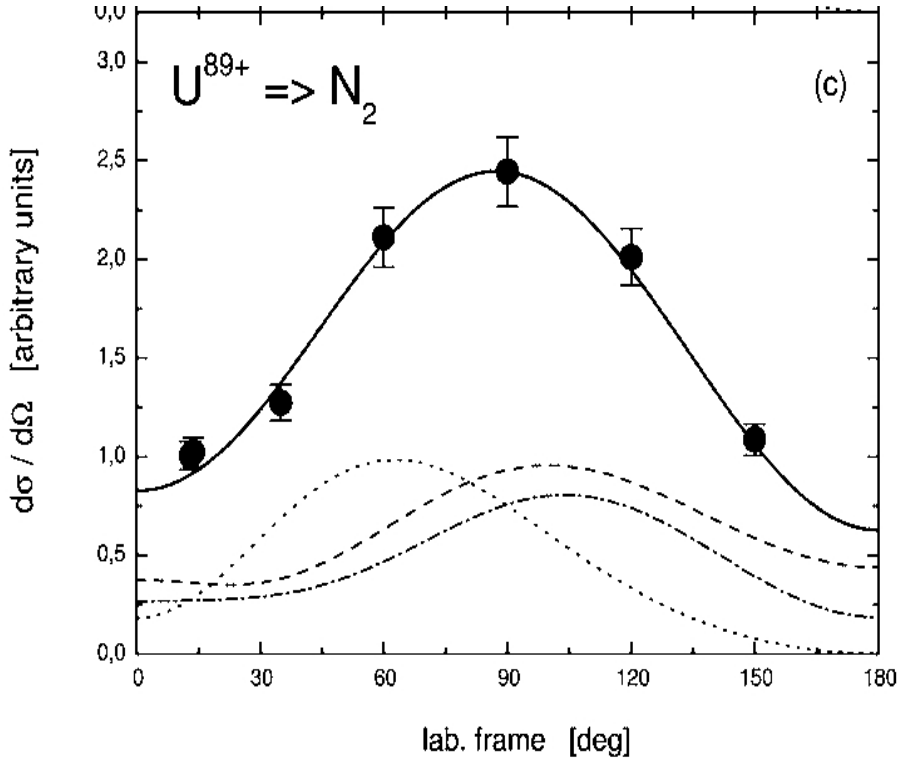




No effect on the REC for high collision energies

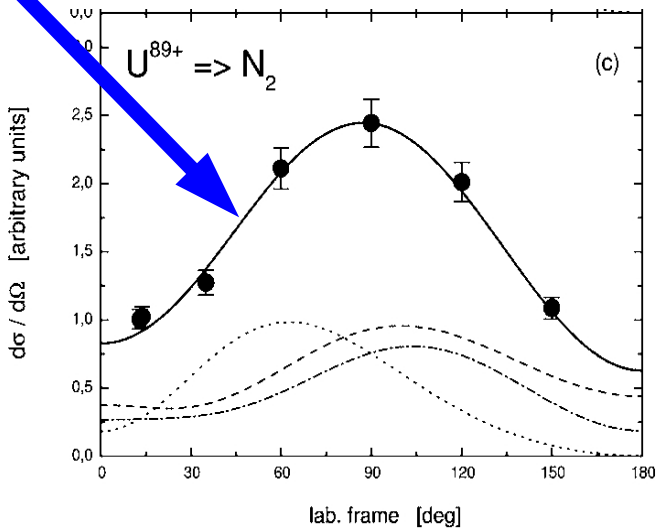
--> Need for decelerated ions !!

Effective „one-particle“ approximations

$$\Psi_{LM}(x_1, x_2) = \sum_{m_1 m_2} \langle l_1 m_1 l_2 m_2 | L M \rangle \begin{vmatrix} \phi_{l_1 m_1}(x_1) & \phi_{l_2 m_2}(x_1) \\ \phi_{l_1 m_1}(x_2) & \phi_{l_2 m_2}(x_2) \end{vmatrix}$$

Representation of the initial and final states of the collision process by means of Slater determinants

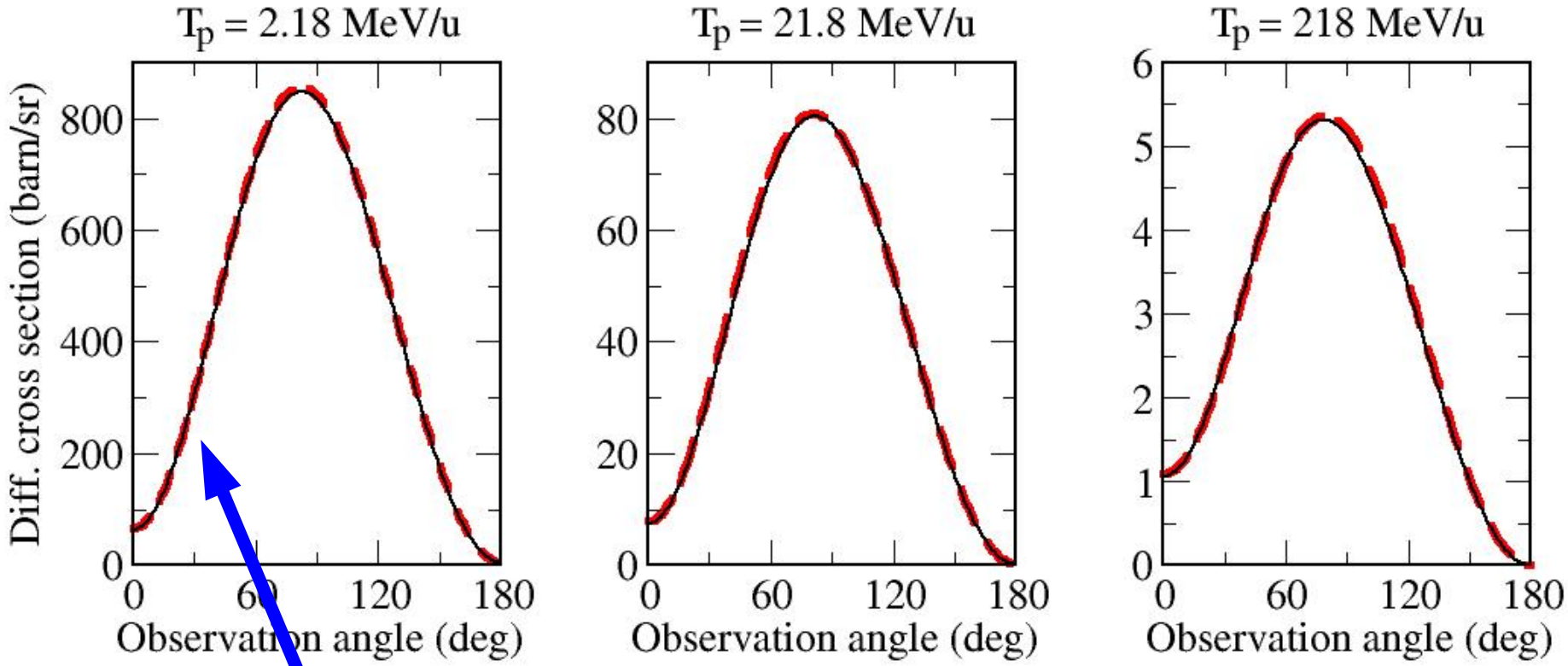
- Pauli principle
- Mean-field approximation
- Proper coupling of the angular momenta
- But no correlations !
- No systematic improvement of theory possible
- No coupling of different scattering channels
- …



Hydrogen-like ions

-- Capture into the $1s^2$ ground state

U^{91+}



1.2 keV

„Slow collisions“

120 keV

One-electron calculations

MCDF calculations

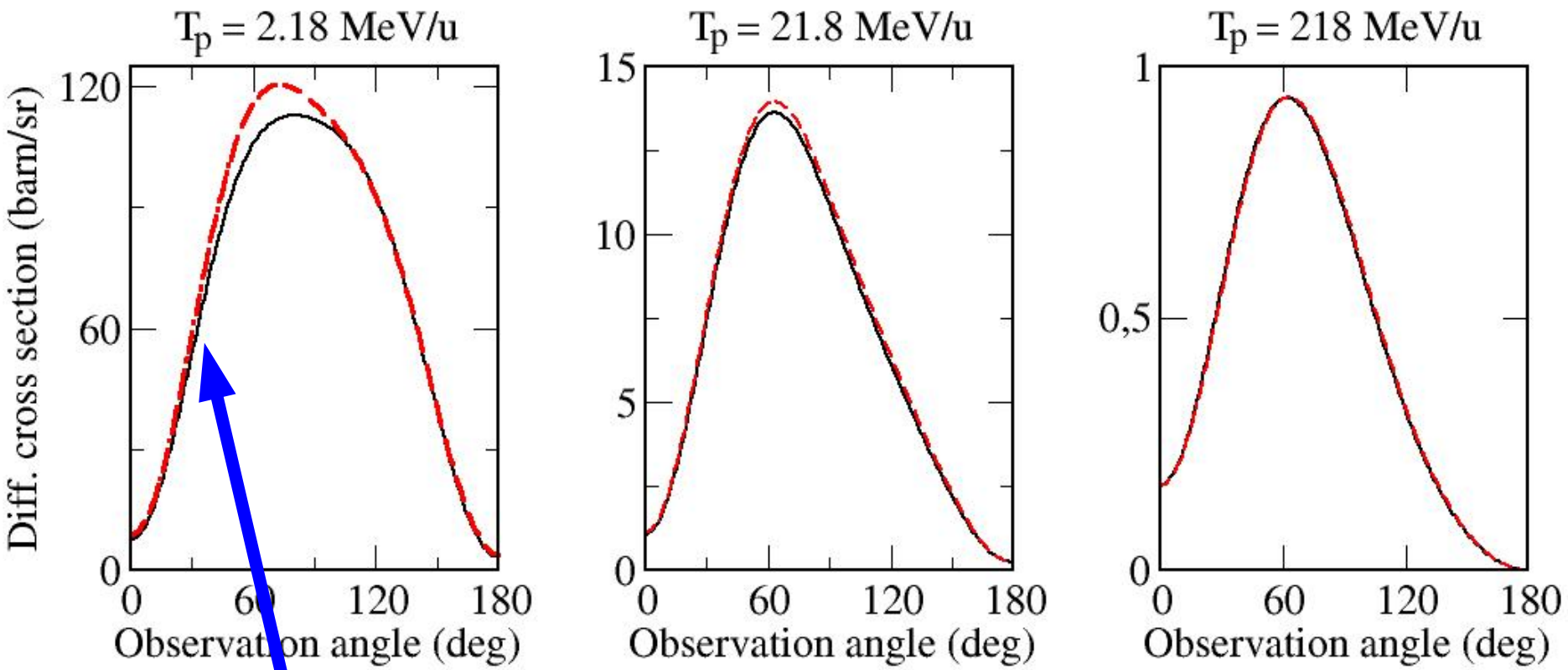
Binding energy: E_{1s} ~ 120 keV

S. Fritzsche et al., PRA 72 (2005) 012704 .

Lithium-like ions

-- Capture into the $1s^2 2s^2$ ground state

U^{89+}



1.2 keV „Slow collisions“ 120 keV

One-electron calculations
MCDF calculations

Binding energy: E_{2s} ~ 30 keV

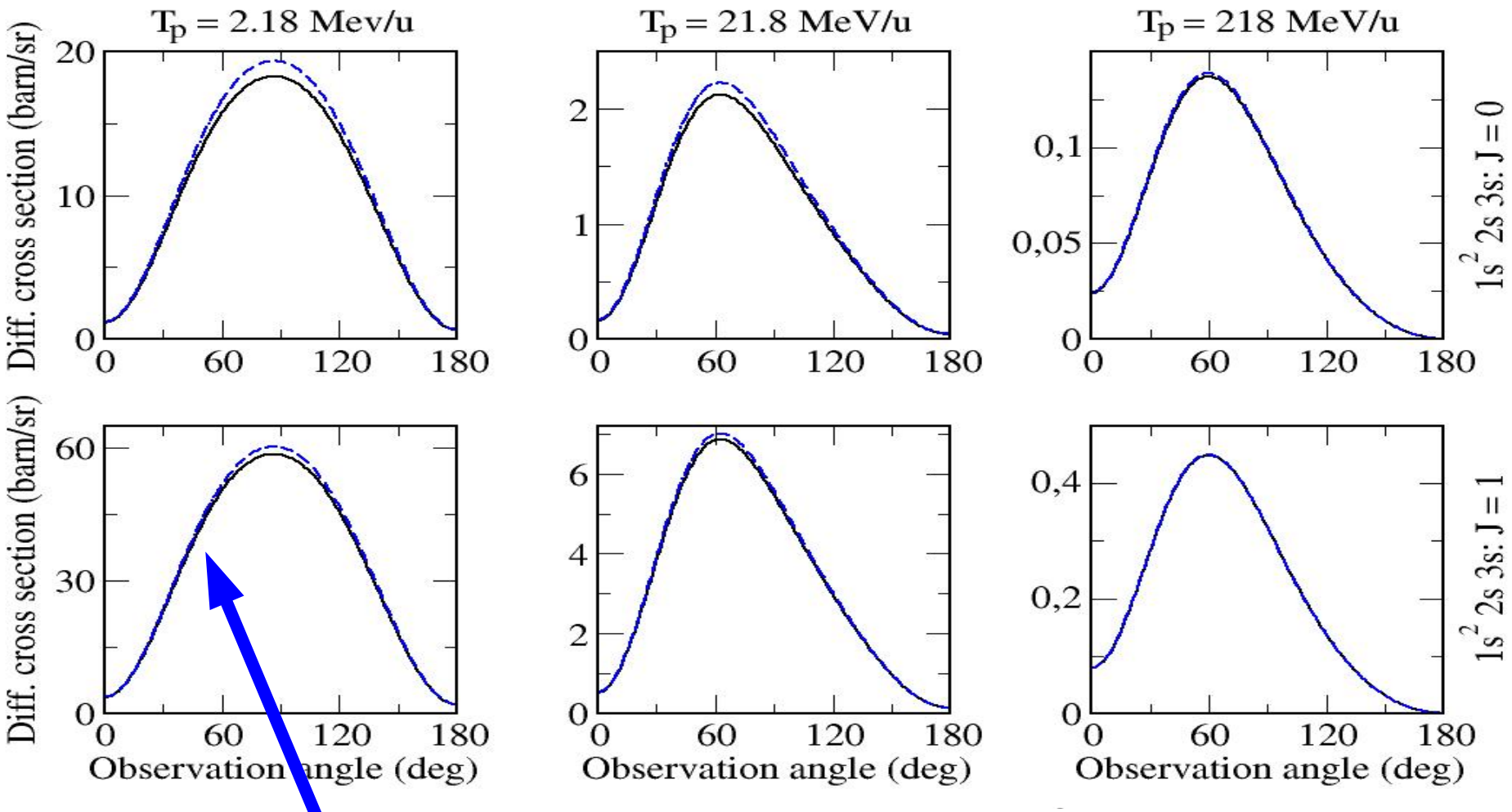
All results are virtually gauge independent !

S. Fritzsche et al., PRA 72 (2005) 012704 .

Lithium-like ions

-- Capture into the $1s^2\ 2s\ 3s$ excited states

U^{89+}



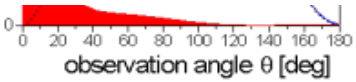
Velocity (Coulomb) gauge

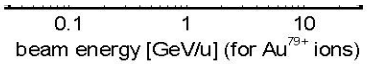
Length (Babushkin) gauge

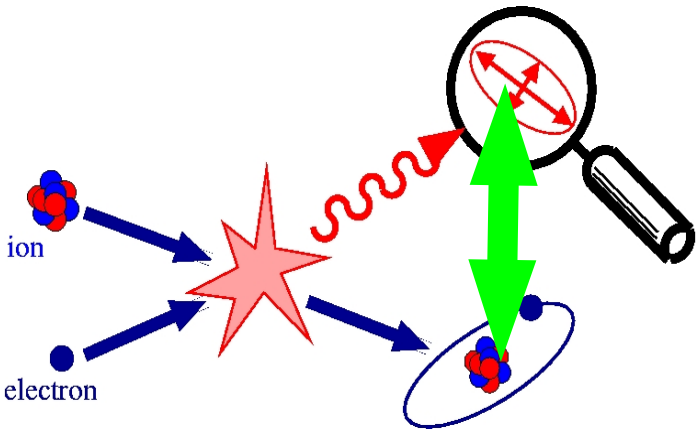
Electron capture at storage ringsinto high-Z ions

New directions ...

angular distributions



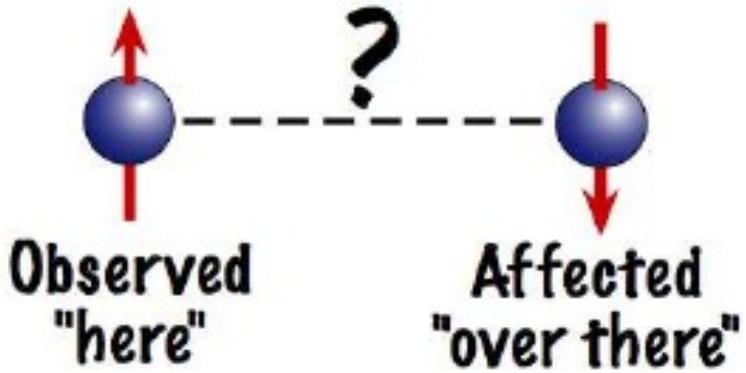




Quantum entanglement occurs when two or more particles interact in a way that causes their fates to become linked.

... Collectively they constitute a single quantum state.

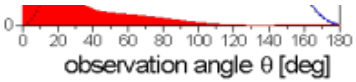
„...spooky action at a distance..." *(Einstein)*

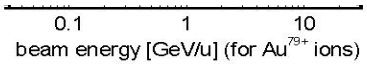


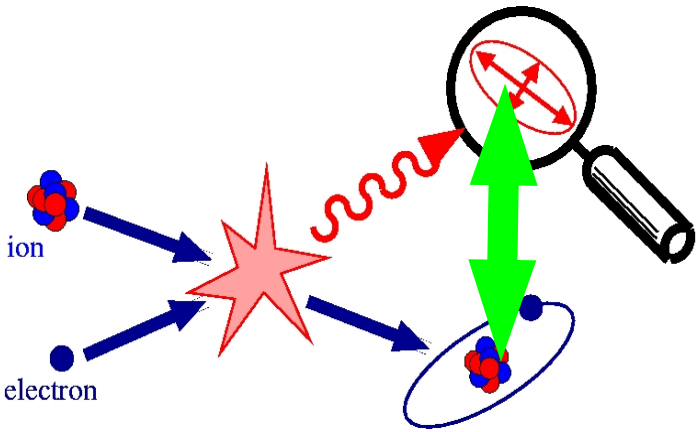
Electron capture at storage ringsinto high-Z ions

New directions ...

angular distributions







Quantum entanglement occurs when two or more particles interact in a way that causes their fates to become linked.

... Collectively they constitute a single quantum state.

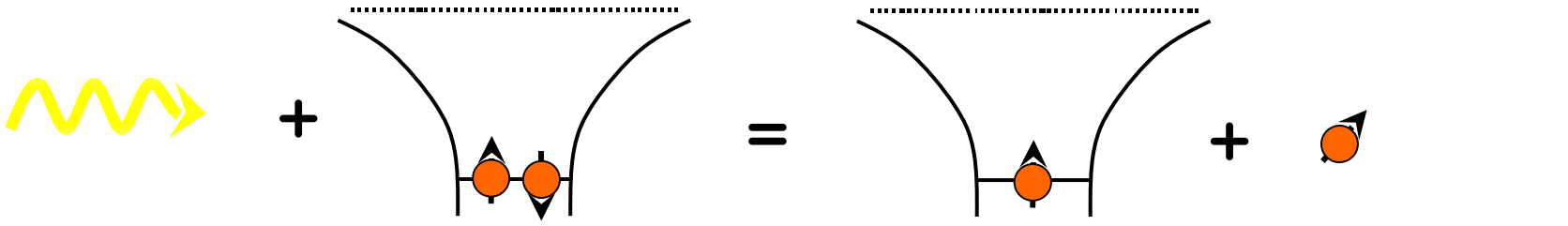
Applications of entanglement:

- superdense coding
- quantum state teleportation
- quantum cryptography (key distribution)
- efficient quantum algorithms

Search for physical processes where entanglement can be observed and manipulated !

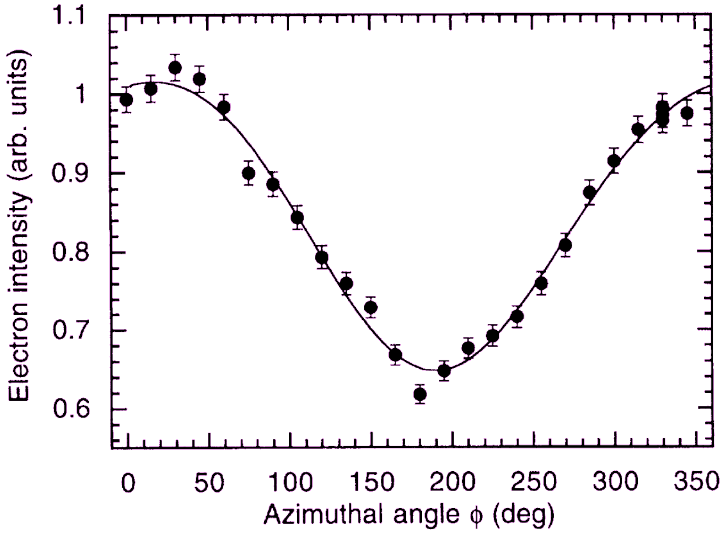
Change and control of entanglement in atomic photoionization

-- one of the most intensively studied processes



photon | atomic (ionic) bound state | residual ion | photoelectron in the continuum

$|\mathbf{k}\lambda\rangle$ $|\alpha_0 J_0 M_0\rangle$ $|\alpha_f J_f M_f\rangle$ $|\mathbf{p} m_s\rangle$

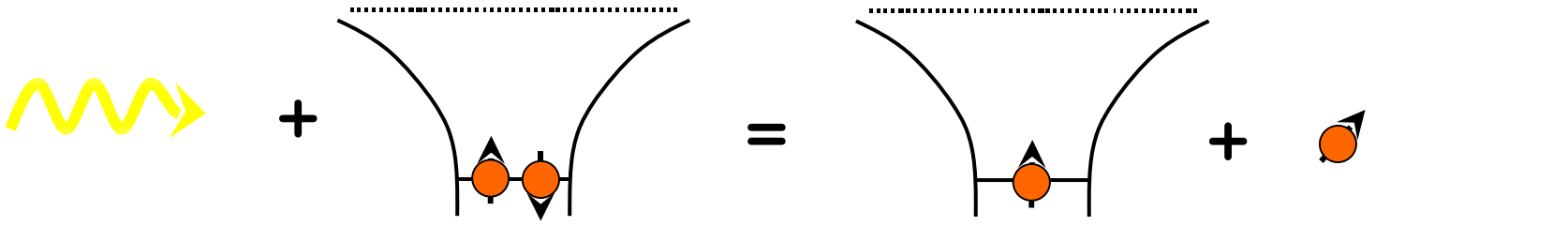


Studies on atomic photoionization

- (Total) cross section
- Angular distributions
- Spin-polarization
- Entanglement as additional resource

Change and control of entanglement in atomic photoionization

-- one of the most intensively studied processes



photon | atomic (ionic) bound state | residual ion | photoelectron in the continuum

$|\mathbf{k}\lambda\rangle$ $|\alpha_0 J_0 M_0\rangle$ $|\alpha_f J_f M_f\rangle$ $|\mathbf{p}m_s\rangle$

Degree of entanglement: Concurrence $0 \leqslant C(\rho) \leqslant 1$

$C = max(0,\ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$ are eigenvalues of $\rho\bar{\rho} = \rho(\sigma_y^A \otimes \sigma_y^B)\rho^*(\sigma_y^A \otimes \sigma_y^B)$

Examples:

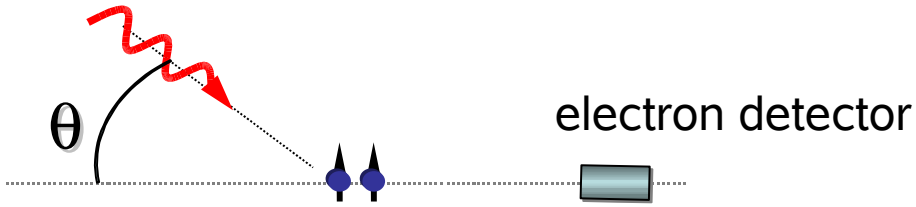
Bell state $|\Psi^+> = \dfrac{|01> + |10>}{\sqrt{2}} \longrightarrow C(\Psi^+) = 1$

Product state $|\Psi> = |00> \longrightarrow C(\Psi) = 0$

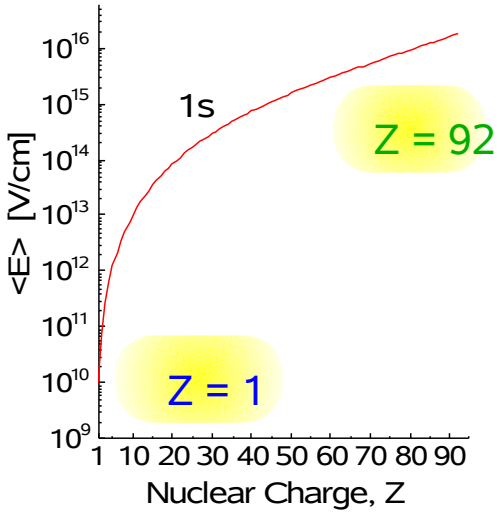
T. Radtke et al., Phys. Lett. A 347 (2005) 73.

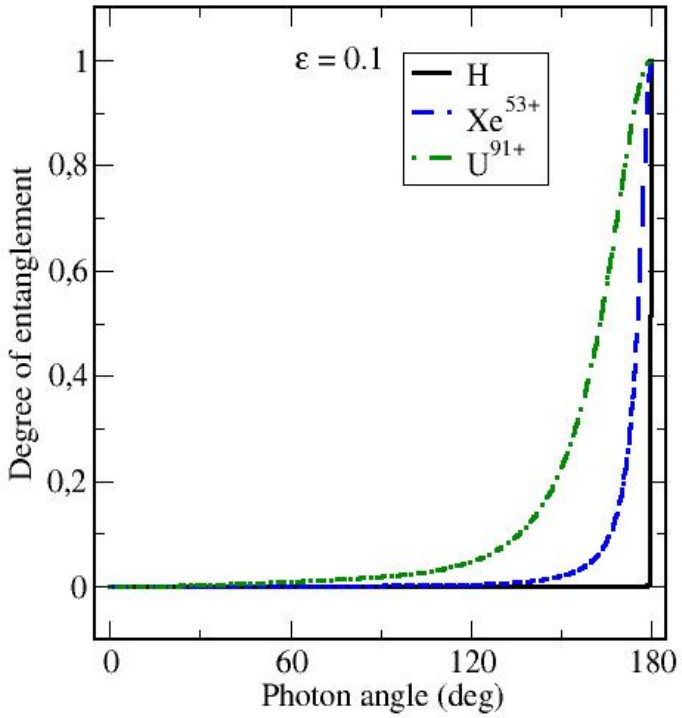
Change of entanglement in atomic photoionization

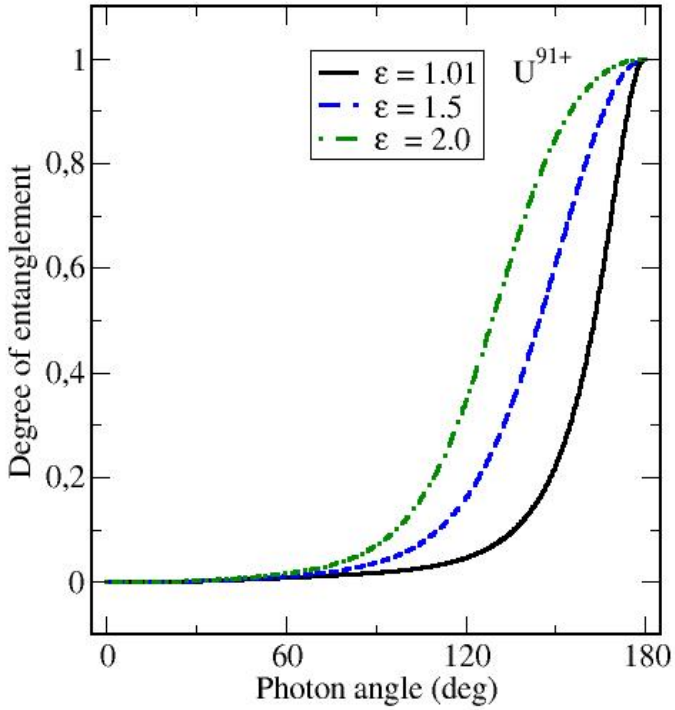
-- entanglement as function of the photon angle



Calculations are performed for the relative photon energy $\varepsilon = E_\gamma / E_{1s}$ where E_{1s} is the 1s ionization threshold.







Relativistic effects result in a change of entanglement !

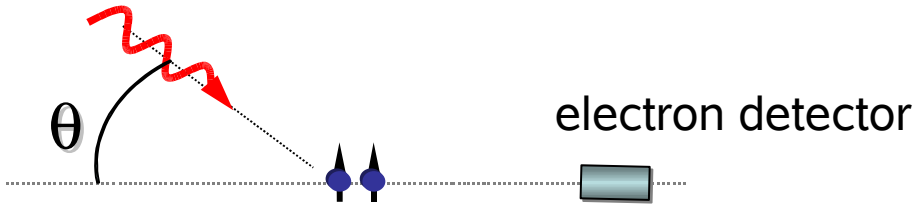
T. Radtke et al., Phys. Lett. A 347 (2005) 73.

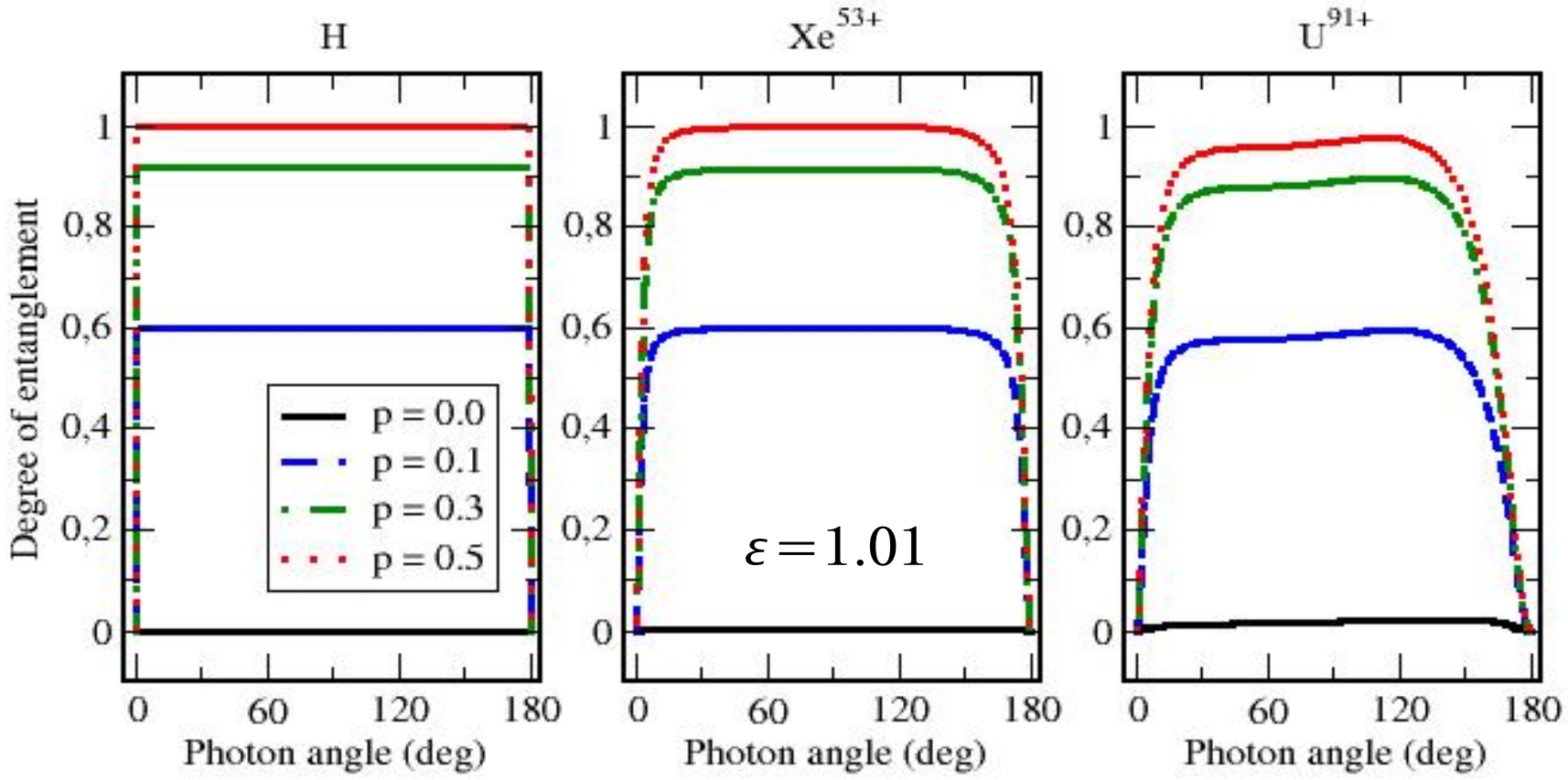
Change of entanglement in atomic photoionization

-- entanglement as function of the initial 2-qubit state

Calculations are performed for the initial state:

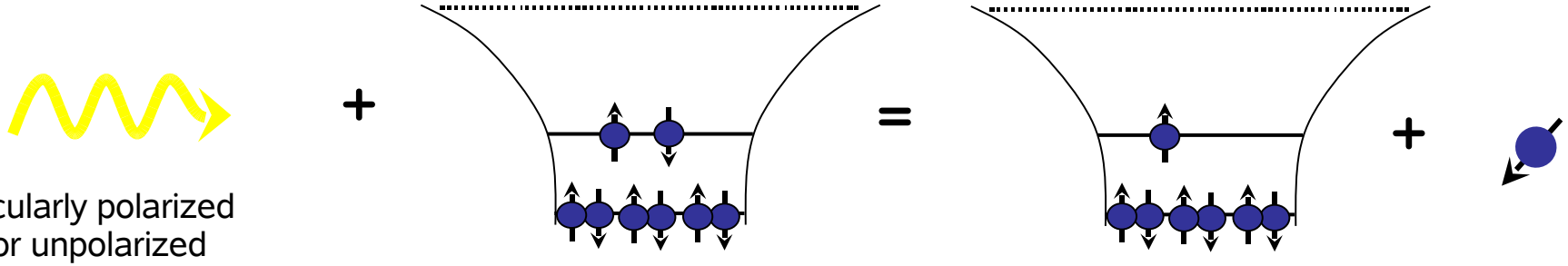
$$|\Psi> = \sqrt{p}|01> + \sqrt{1-p}|10>$$





5s photoionization of atomic strontium (Z=38)

$$Sr\,(5s^2\ {}^1S_0) + h\nu \rightarrow Sr^+\,(5s\ {}^2S_{1/2}) + e^-$$



circularly polarized
or unpolarized

the 2 valence electrons are
maximally entangled

$J_f = 1/2$

$s=1/2$

composite system
of two qubits:
Photoion + electron

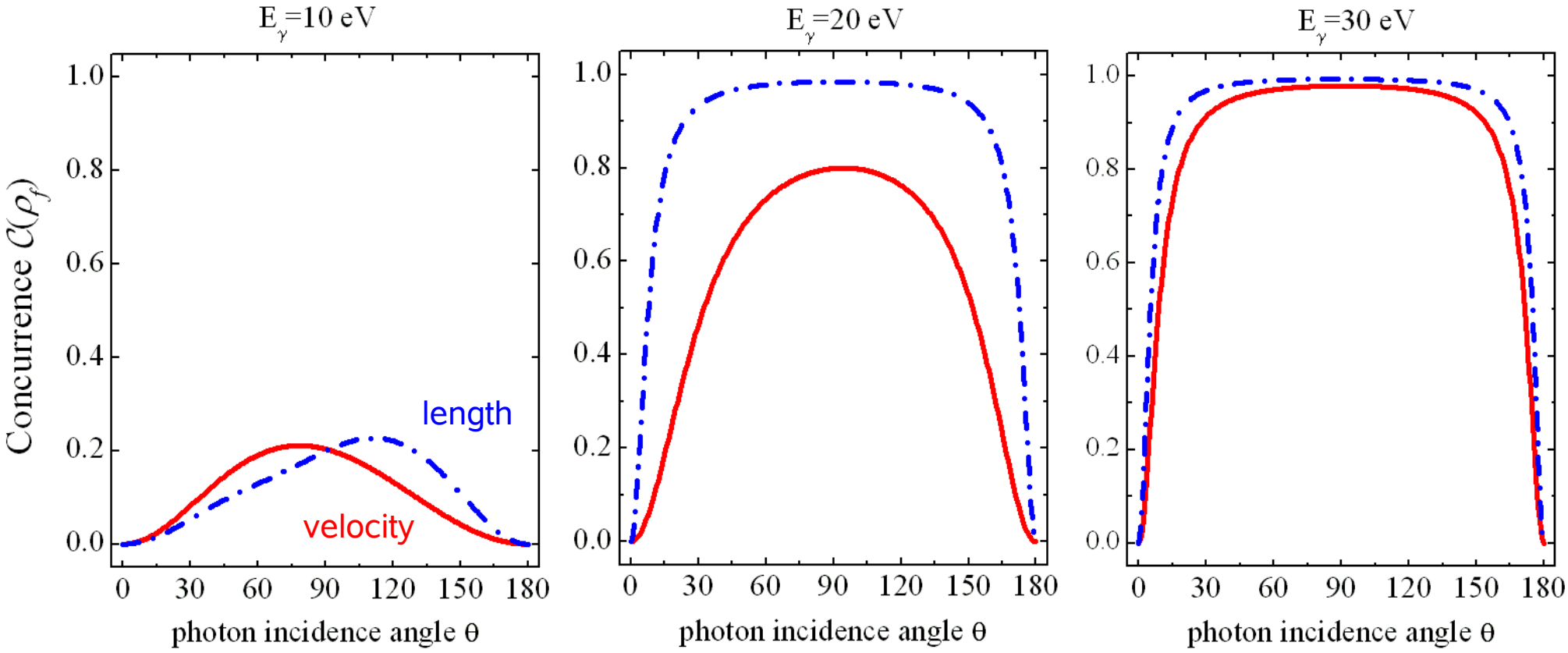
$$\left\langle \alpha_f J_f M_f, \mathbf{p} m_s \middle| \rho_f \middle| \alpha_f J_f M_f', \mathbf{p} m_s' \right\rangle \propto \sum W \left\langle (\alpha_f J_f, \varepsilon \kappa j)\, J_{tot} \middle\| \boldsymbol{\alpha} \mathcal{A}_L^{(\lambda)} \middle\| \alpha_0 J_0 \right\rangle$$
$$\times \left\langle (\alpha_f J_f, \varepsilon \kappa' j')\, J'_{tot} \middle\| \boldsymbol{\alpha} \mathcal{A}_{L'}^{(\lambda)} \middle\| \alpha_0 J_0 \right\rangle^*$$

lenghty geometric factor
(Clebsch-Gordans, D-matrix etc.)

T. Radtke et al., PR A 74 (2006) 032709

Final-state entanglement as function of the photon angle

-- comparison of length and velocity gauge

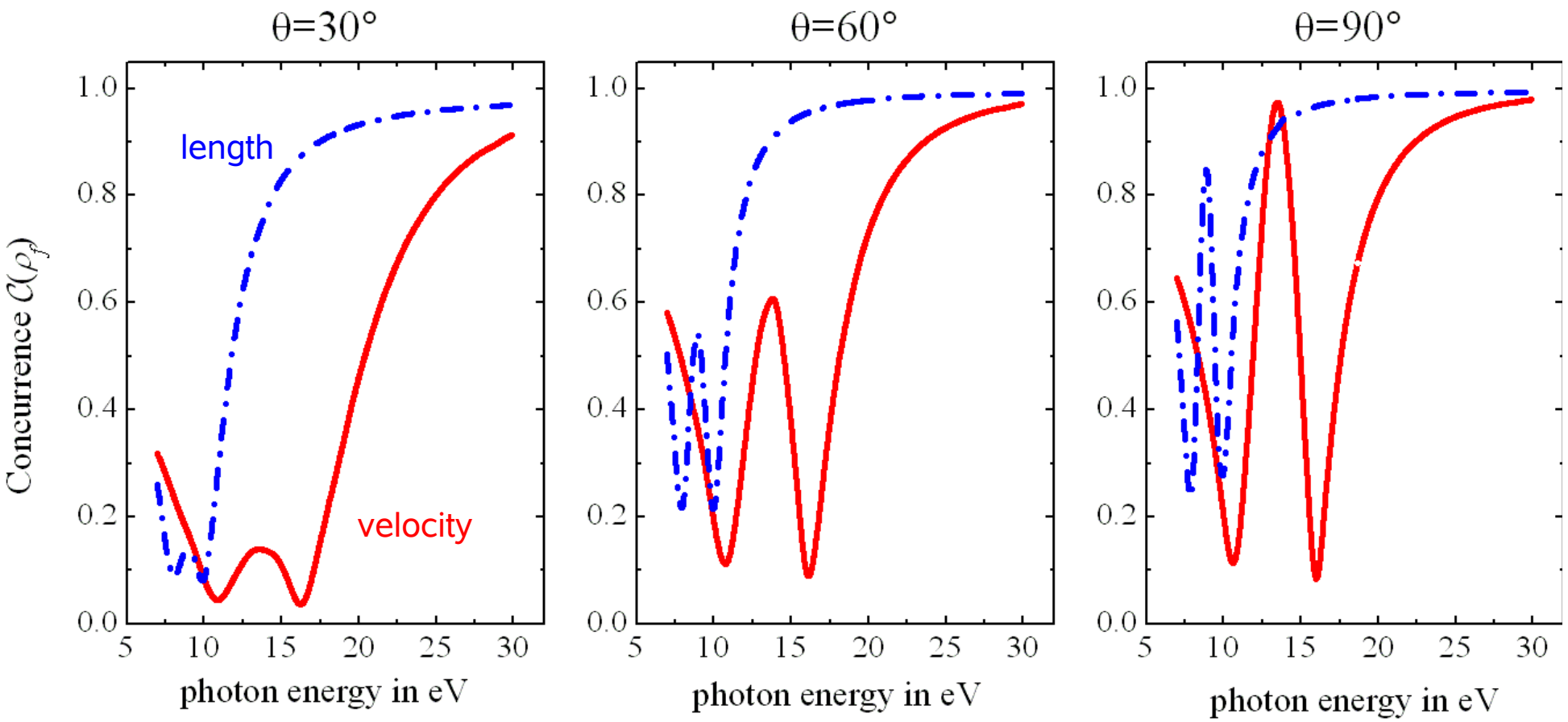


Angular distribution similar to IPM results, but much lower values near to the ionization threshold.

T. Radtke et al., PR A 74 (2006) 032709

Final-state entanglement as function of the photon energy

-- with right-circular polarized light



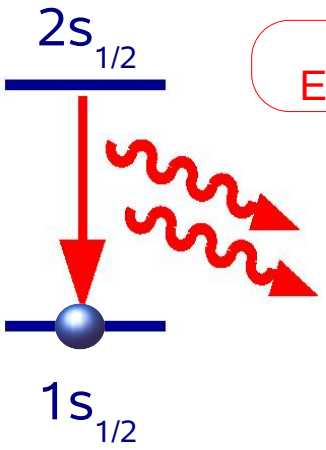
Good agreement with IPM results for high photon energies.

Entanglement can be observed and manipulated in atomic photoionization

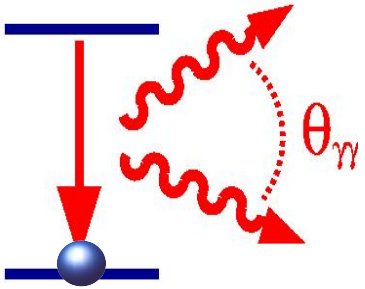
- sensitive to relativistic/multipole effects
- strongly sensitive to many-particle effects

A.Surzhykov et al. PRA71 (2004) 012034

Two-photon decay of highly-charged ions



E1E1 + E1M2 + M1M1+E2E2 + E2M1....

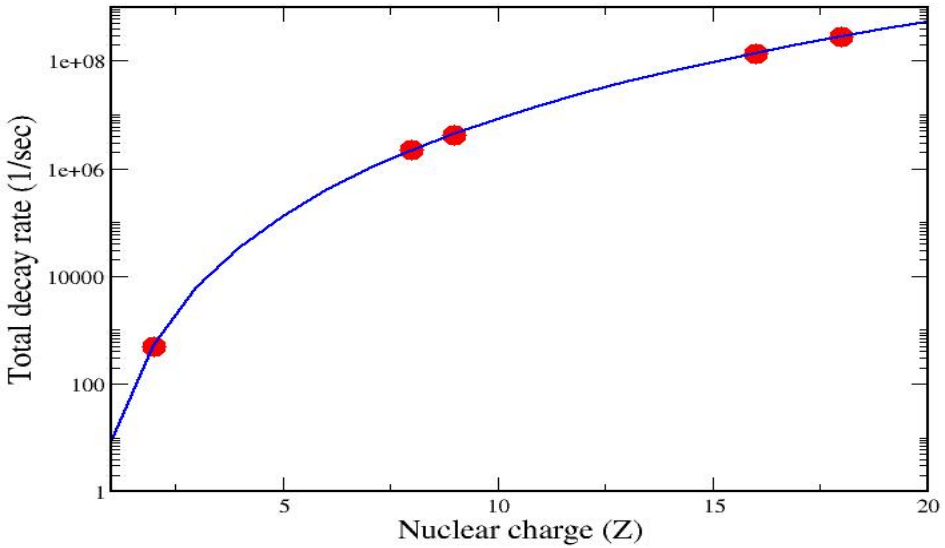


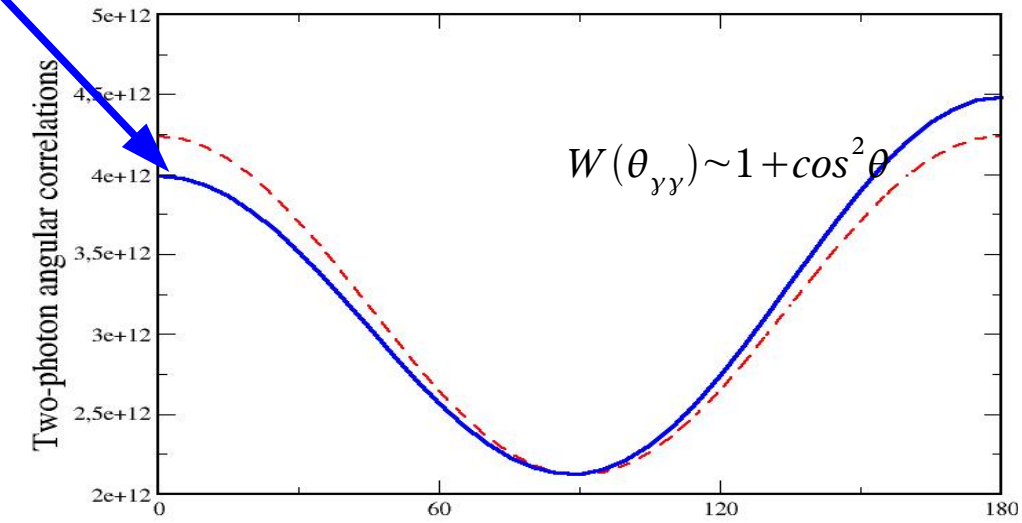
?

Higher multipoles give rise to an asymetrical shift

Spin-spin correlations & concurrence

$$\Gamma_{tot} \approx \Gamma_{E1E1} = 8.229 \cdot Z^6$$





Atomic and heavy-ion theory within the SPARC collaboration

-- Requirements and present capabilities

Letter of Intent:

- Test of quantum electrodynamics in strong fields
- Relativistic collision dynamics in strong electromagnetic fields
- Atomic physics techniques applied to nuclear physics
- Test of fundamental interactions and symmetries beside of QED
- Interaction of ions with intensive (laser) light

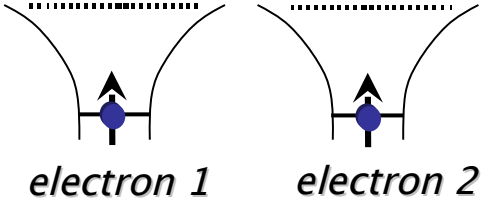
Which theoretical support is needed by experiment
What should be 'measured' from the viewpoint of theory

Theory group: Structure & Dynamics

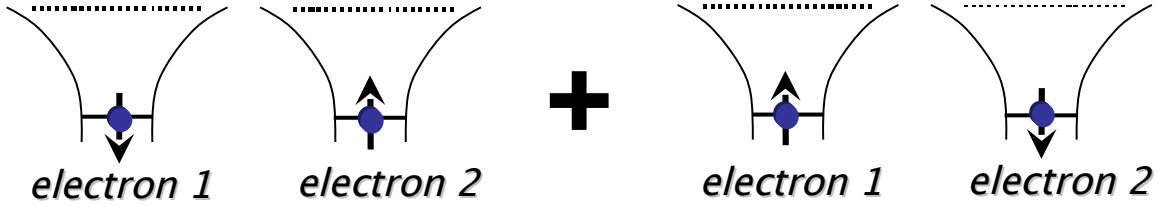
Change of entanglement in atomic photoionization

-- entanglement of two electron spins

Electron spins form a two-qubit system:



$$|\Psi> = |00>$$



$$|\Psi^{+}> = \frac{|01> + |10>}{\sqrt{2}}$$

From: www.labs.nec.co.jp/ Eng/innovative/E3/03.html

S. Fritzsche, JESRP 114-116 (2001) 1155; Phys. Scr. T100 (2002) 46

RATIP

Relativistic Atomic Transition and Ionization Properties

(CPC library)

$$\psi_\alpha(PJM) = \sum_r^{n_c} c_r(\alpha) \left|\gamma_r PJM\right\rangle$$

Relativistic CI wave functions including QED estimates and mass polarization

RELCI, CPC 148 (2002) 103

LSJ spectroscopic notation from jj-coupled computations

LSJ, CPC 157 (2003) 239

Auger rates, angular distributions and spin polarization; level widths

AUGER

Photoionization cross sections and (non-dipole) angular parameters

PHOTO

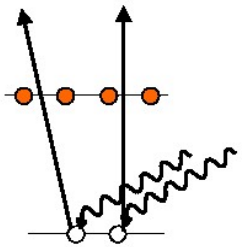
Radiative and dielectronic recombination; angle-angle correlations

REC

...

Many-electron basis (wave function expansions)

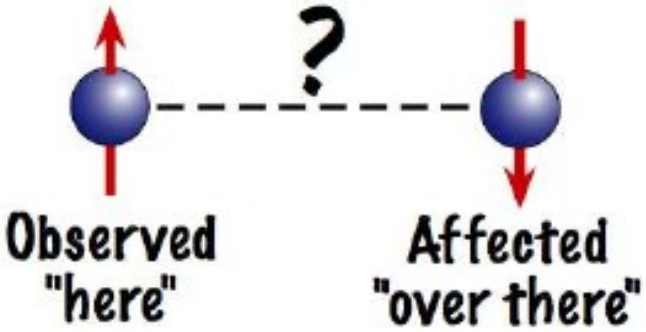
- Construction and classification of N-particle Hilbert spaces
- Shell model: Systematically enlarged CSF basis
- Interactions
  - Dirac-Coulomb Hamiltonian
  - Breit interactions + QED
  - Electron continuum; scattering phases
- Coherence transfer and Rydberg dynamics



Entanglement in quantum systems

-- nonlocal correlations between two or more subsystems

Quantum entanglement occurs when two or more particles interact in a way that causes their fates to become linked. ... Collectively they constitute a single quantum state.



„...spooky action at a distance..." (Einstein)

Quantification of entanglement remains in general unsolved; already the decision for density matrix about being separable or entangled is NP-hard.

Applications of entanglement:

- superdense coding
- quantum state teleportation
- quantum cryptography (key distribution)
- efficient quantum algorithms

Search for physical processes where entanglement can be observed and manipulated !

Entanglement in quantum systems

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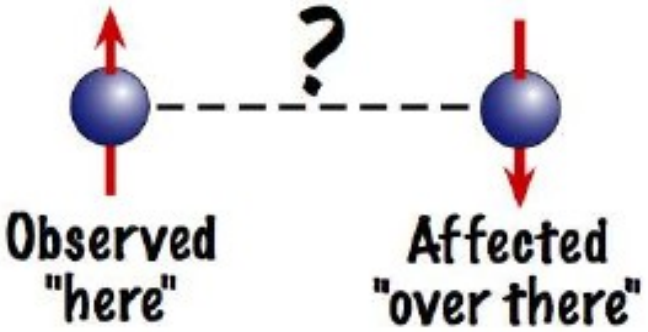

„...spooky action at a distance..." (Einstein)

Quantification of entanglement remains in general unsolved; already the decision for density matrix about being separable or entangled is NP-hard.

Degree of entanglement:

Concurrence $0 \leqslant C(\rho) \leqslant 1$

$C = max(0,\ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$ are eigenvalues of $\rho\bar{\rho} = \rho(\sigma_y^A \otimes \sigma_y^B)\rho^*(\sigma_y^A \otimes \sigma_y^B)$

Examples:

Bell state $|\Psi^+> = \frac{|01> + |10>}{\sqrt{2}} \longrightarrow C(\Psi^+) = 1$

Product state $|\Psi> = |00> \longrightarrow C(\Psi) = 0$