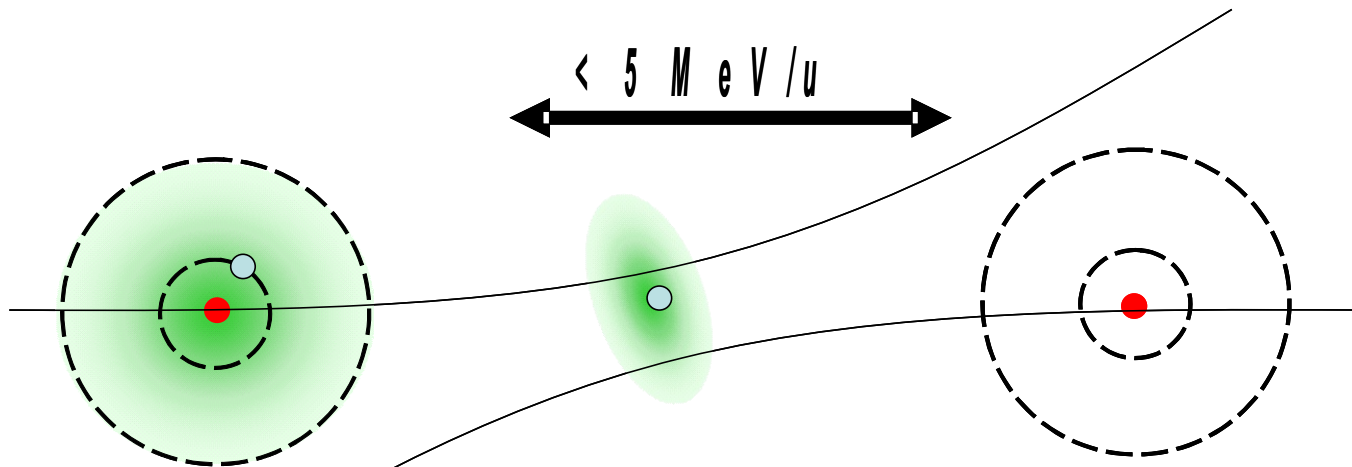




# Quasimolecular radiation in heavy-ion collisions

-- Two-center description

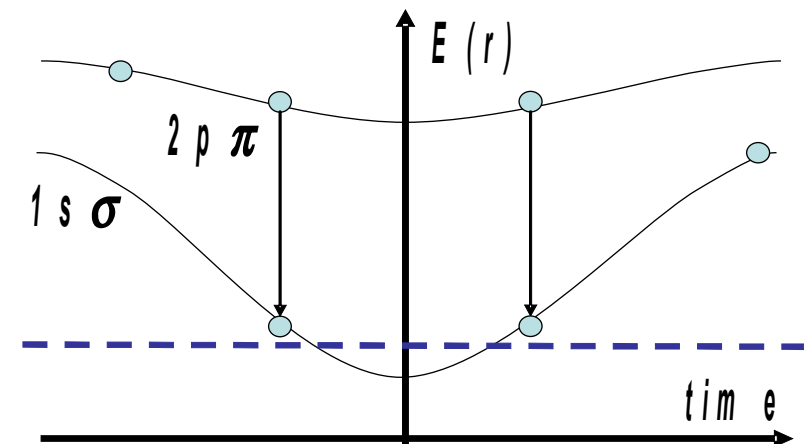
S. Fritzsche  
FIAS Frankfurt & GSI Darmstadt  
18<sup>th</sup> July 2008



Experiments 1977-1981

## Unique GSI/Unilac facility:

- (super-) strong em-fields
- $Z_{\text{united}} = Z_1 + Z_2 \sim 170..180$ , i.e. for  $Z\alpha > 1$
- collision times  $10^{-19} .. 10^{-21}$  s
- extremely short-lived superheavy „quasimolecules“
- closest approach  $< 150$  fm as typical for K-shell



# Quasimolecular radiation in heavy-ion collisions

-- Two-center description

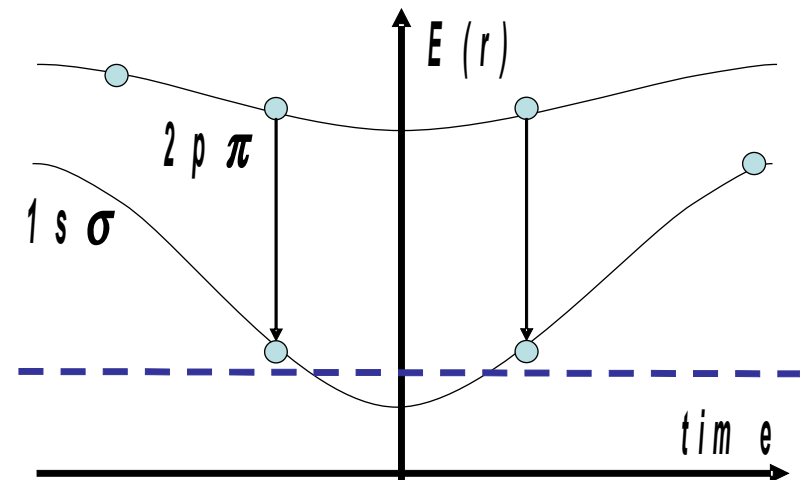
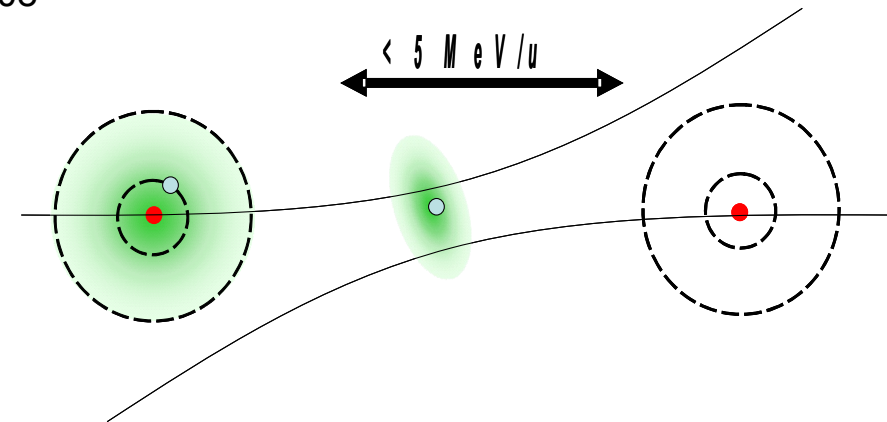
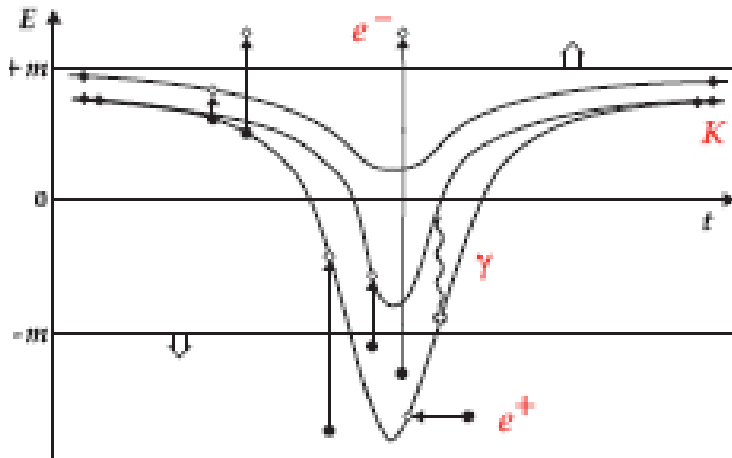
S. Fritzsche

FIAS Frankfurt & GSI Darmstadt

18<sup>th</sup> July 2008

## Creation of 'positrons'

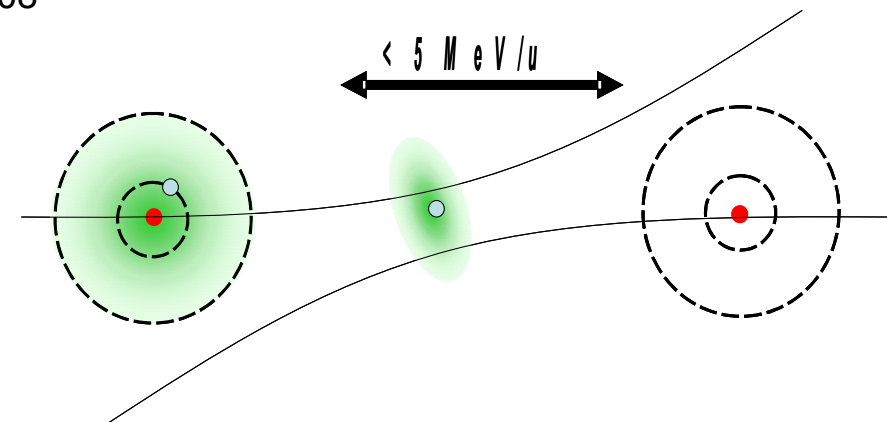
- spontaneous
- dynamical pairs (em field)
- induced by nuclear processes



# Quasimolecular radiation in heavy-ion collisions

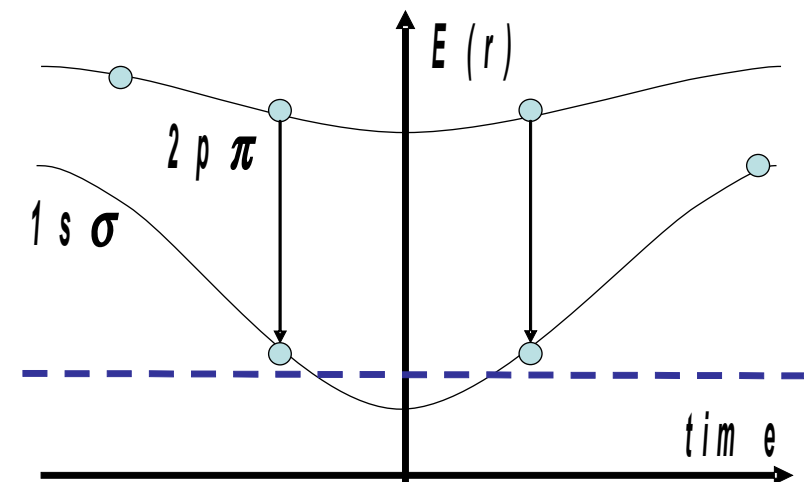
-- Two-center description

S. Fritzsche  
FIAS Frankfurt & GSI Darmstadt  
18<sup>th</sup> July 2008



## Outline of this talk:

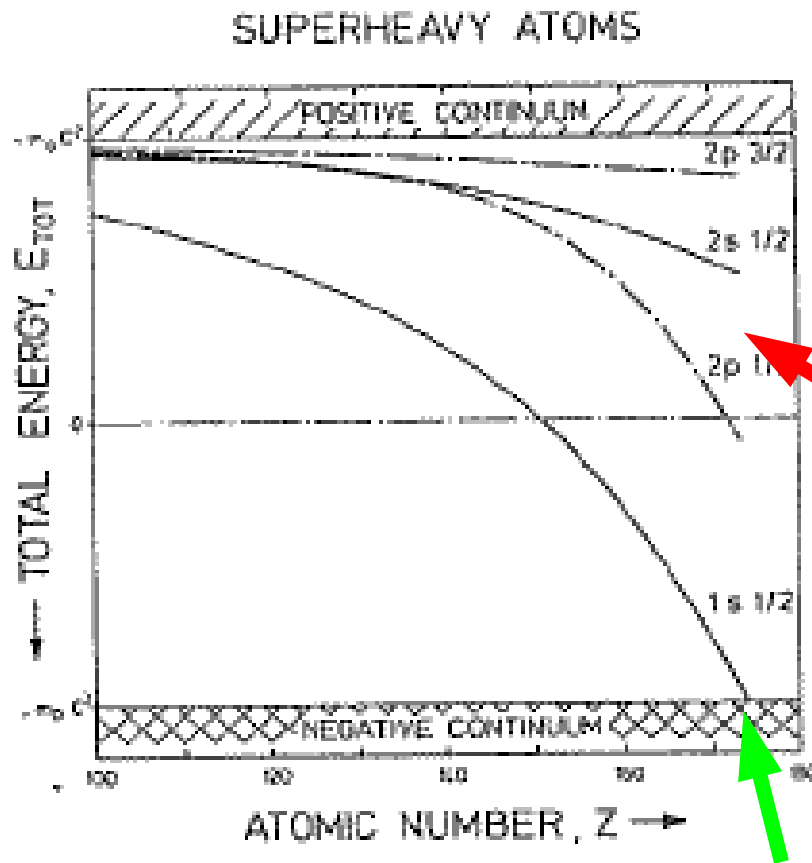
- i) Origin of quasi-molecular radiation
- ii) Formation of super-heavy quasimolecules
- iii) Adiabatic two-center description
- iv) Challenges and future chances



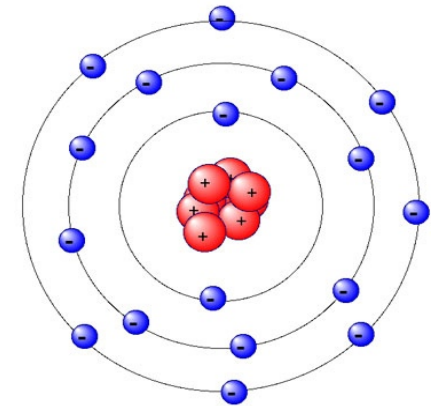
Thanks to: D. Liesen, F. Bosch & B. Fricke

# Supercritical „static“ fields for atoms (I)

-- Relativistic motion and atomic notations



strong spin-orbit splitting;  
swapped 'level order'



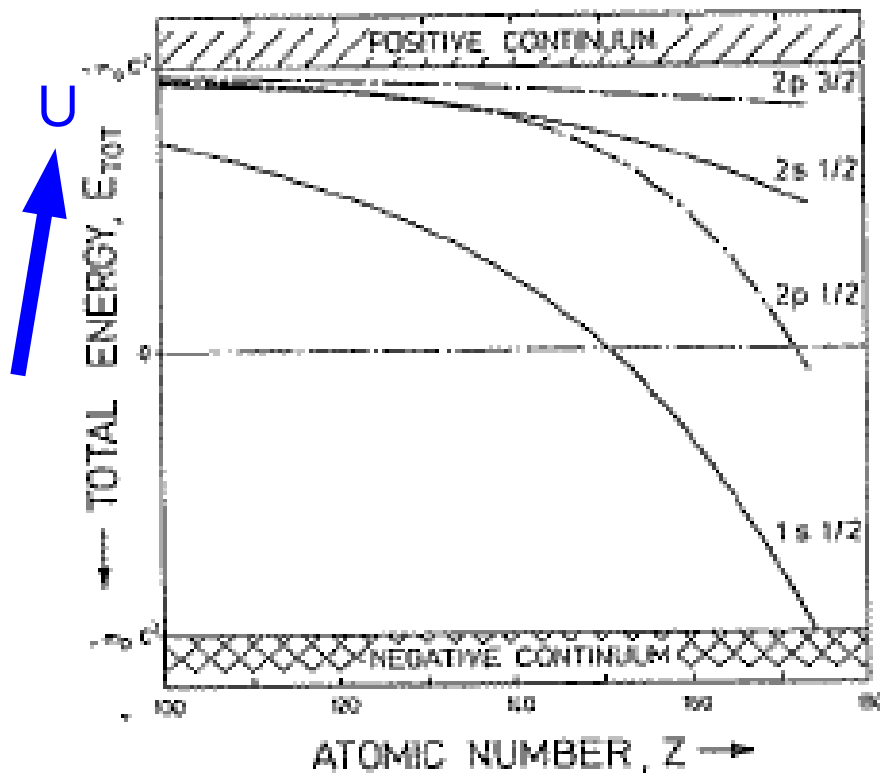
Fricke & Soff (1977)

$Z \sim 173$

# Supercritical „static“ fields for atoms (I)

-- Relativistic motion and atomic notations

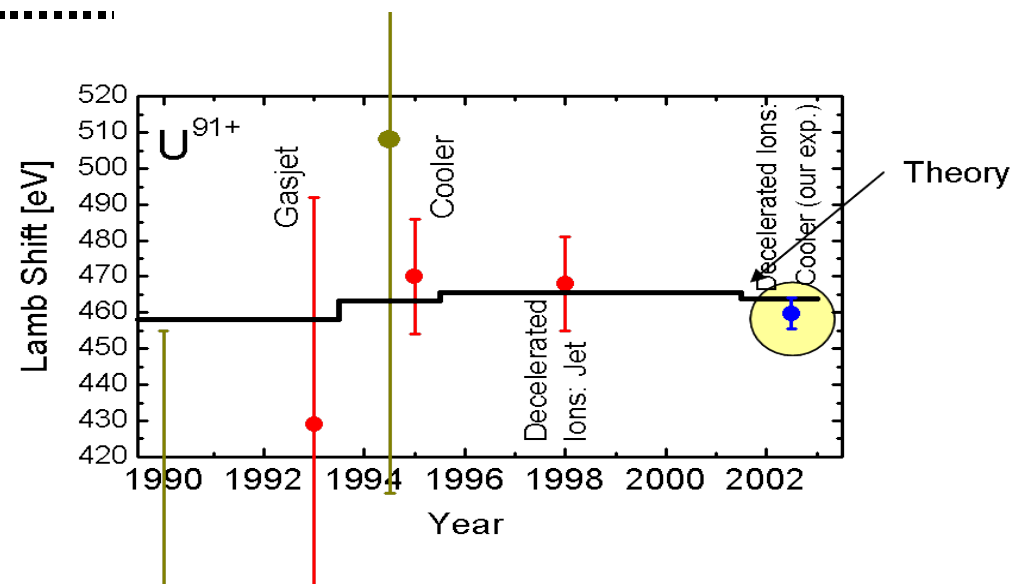
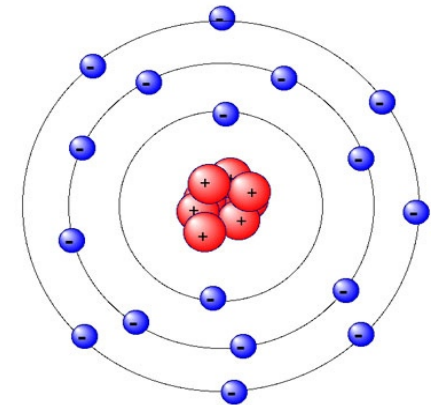
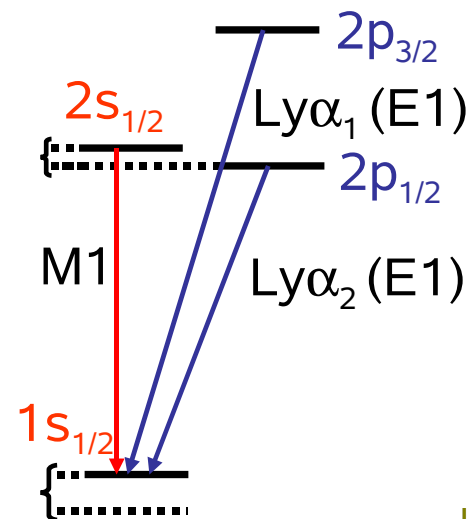
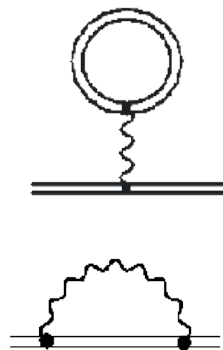
## SUPERHEAVY ATOMS



Fricke & Soff (1977)

### Main QED contributions:

- Electron self-energy (SE)
- Vacuum polarization (VP)
- Finite-size effects (FS)
- Higher-order contributions



# Supercritical „static“ fields for atoms (II)

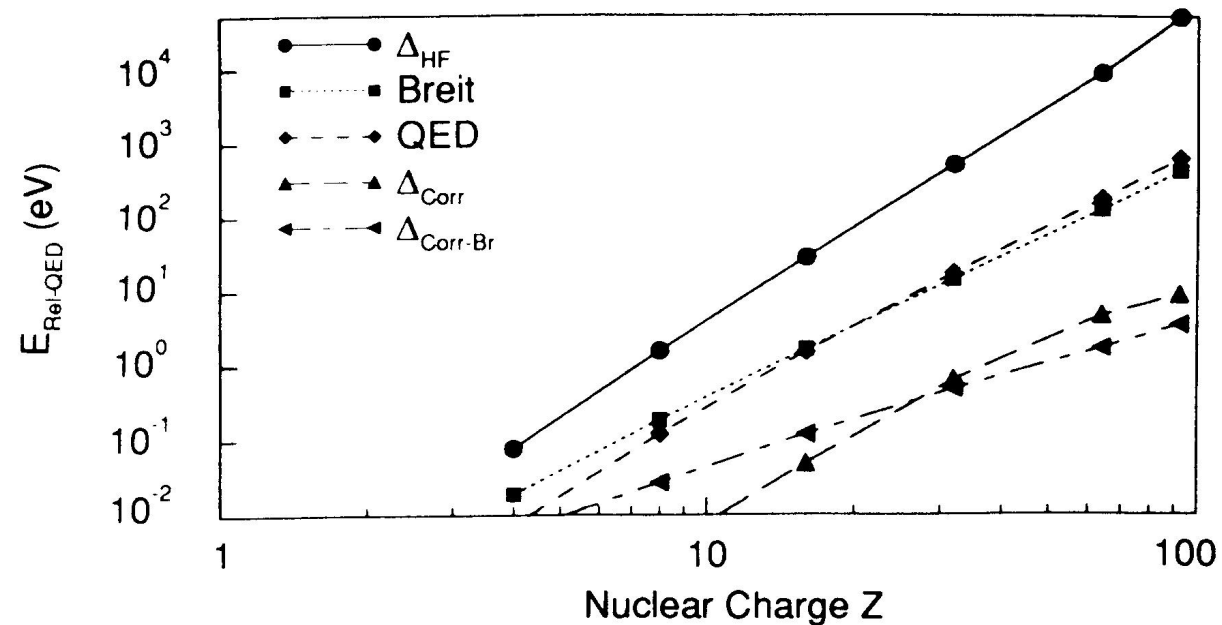
## -- Relativistic motion and atomic notations

„Dirac see“ is visible in different properties

- energies
- transition probabilities (M1, ...)
- x-ray emission (angles & polarization)
- ...

Relativistic and correlation contributions to  
the ground-state energy of Be-like ions

W. R. Johnson (1994)

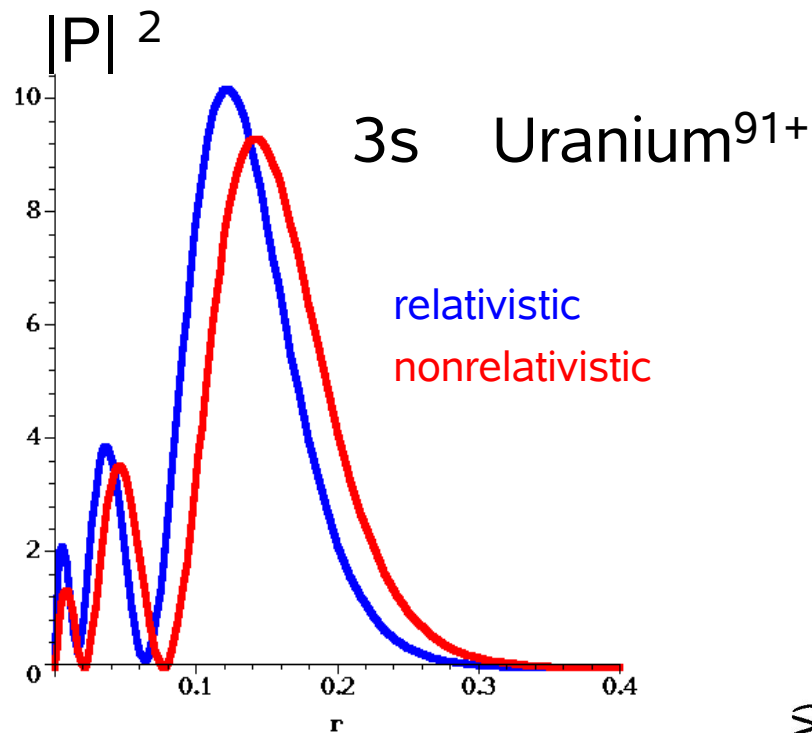


# Supercritical „static“ fields for atoms (II)

## -- Relativistic motion and atomic notations

„Dirac see“ visible in different properties

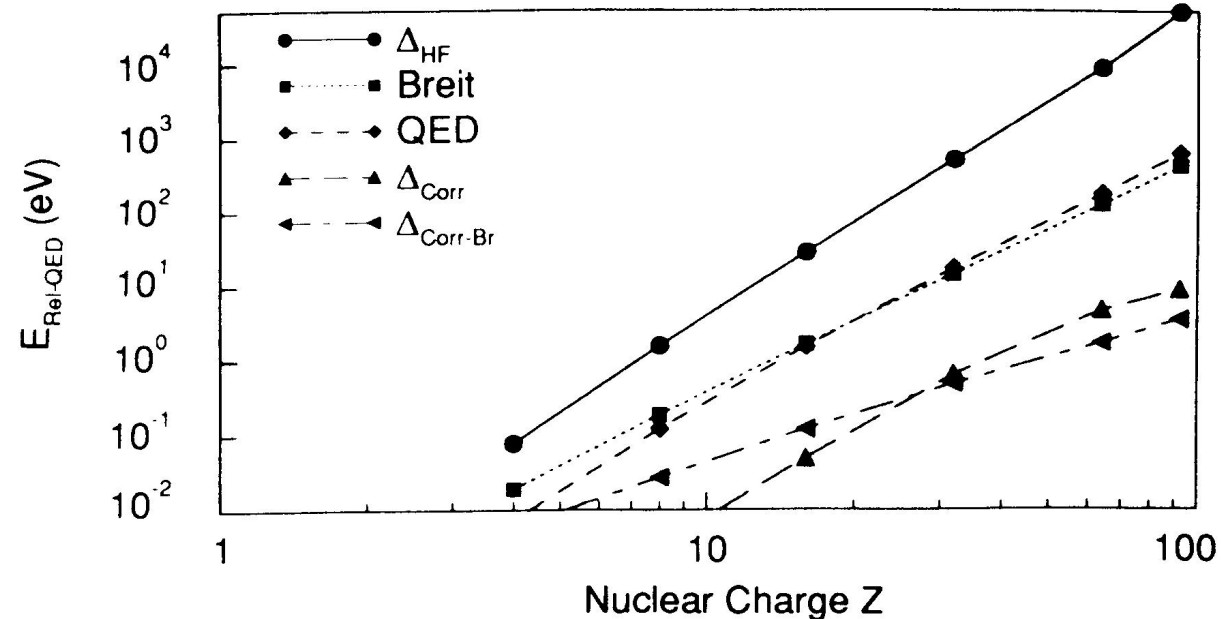
- energies
- transition probabilities (M1, ...)
- x-ray emission (angles & polarization)
- ...



Relativistic contraction  
of the wave functions

Relativistic and correlation contributions to  
the ground-state energy of Be-like ions

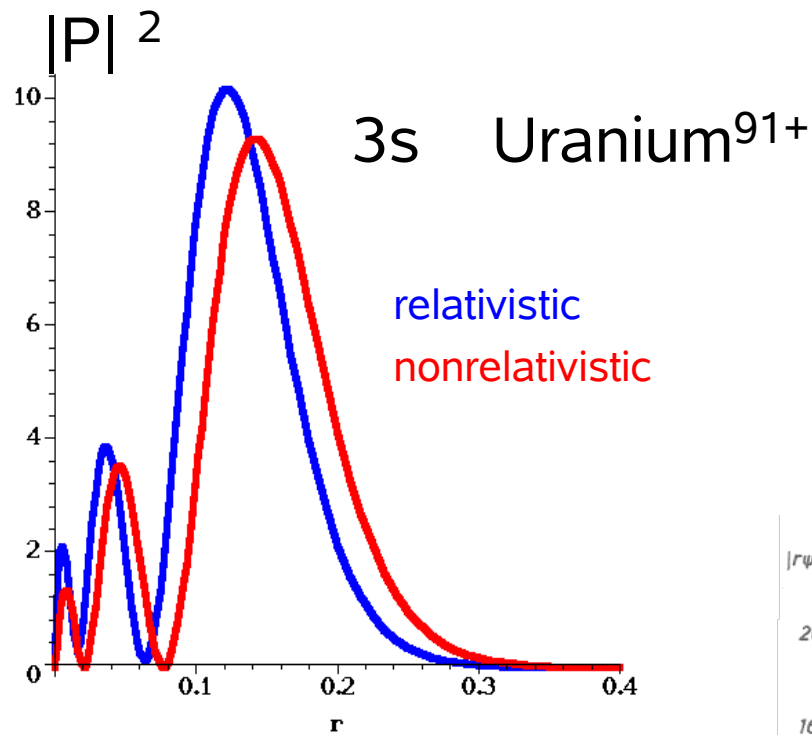
W. R. Johnson (1994)





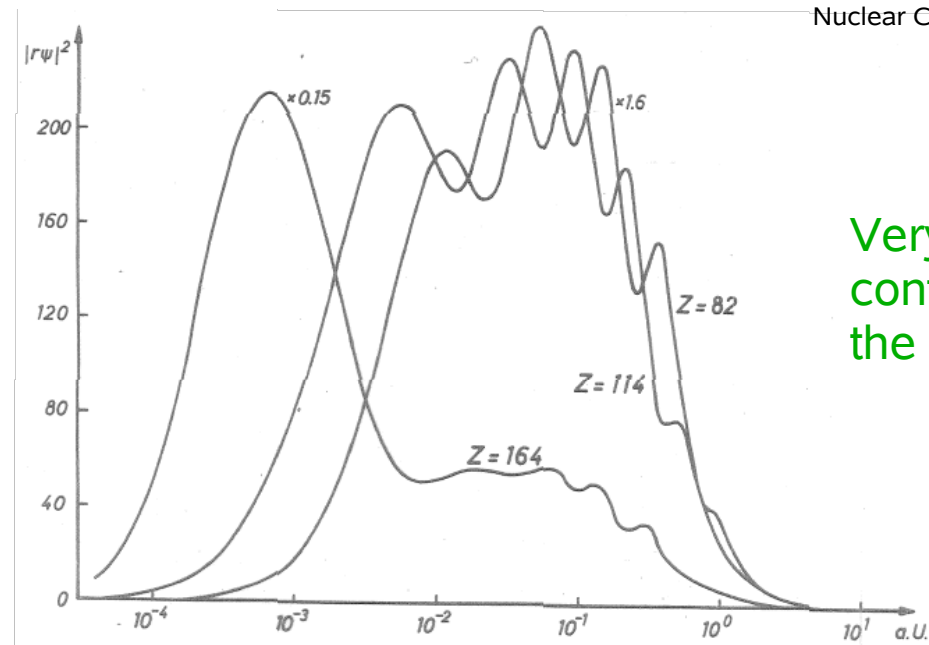
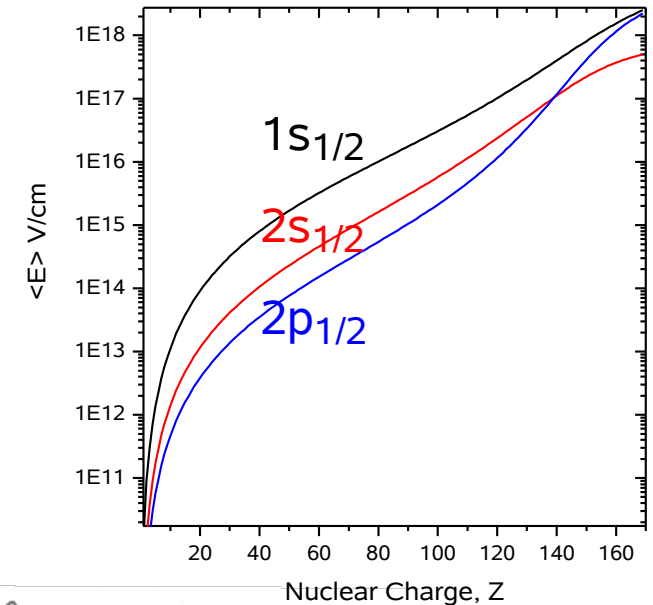
# Supercritical „static“ fields for atoms (II)

-- Relativistic motion and atomic notations



Relativistic contraction  
of the wave functions

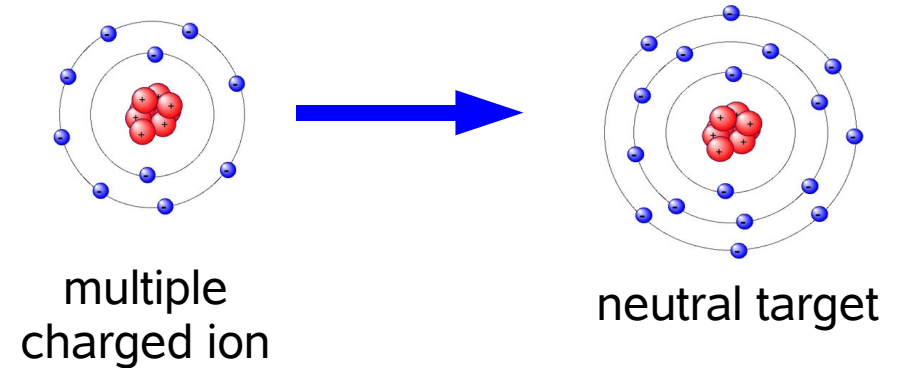
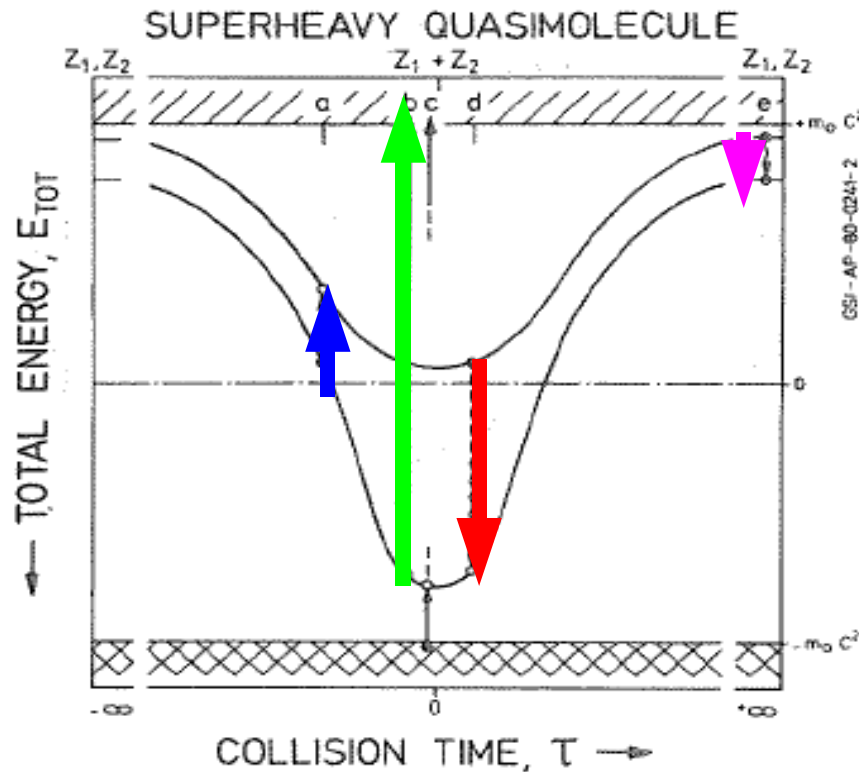
Shrinkage of the electron density due  
to the Dirac operator.



Very strong  
contraction for  
the K-shell

# Origin of quasi-molecular radiation (I)

-- Elementary processes and notations



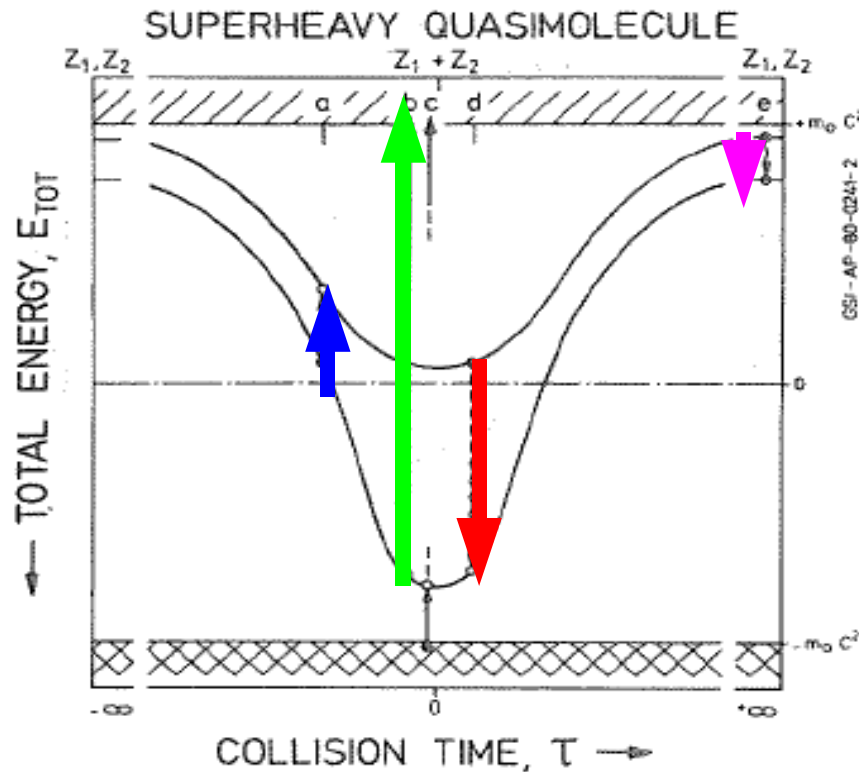
Mokler & Liesen (1982)

## Processes during the collision:

- excitation into higher shells
- ionization ( $\delta$ -electrons)
- MO radiation
- characteristic x-rays

# Origin of quasi-molecular radiation (I)

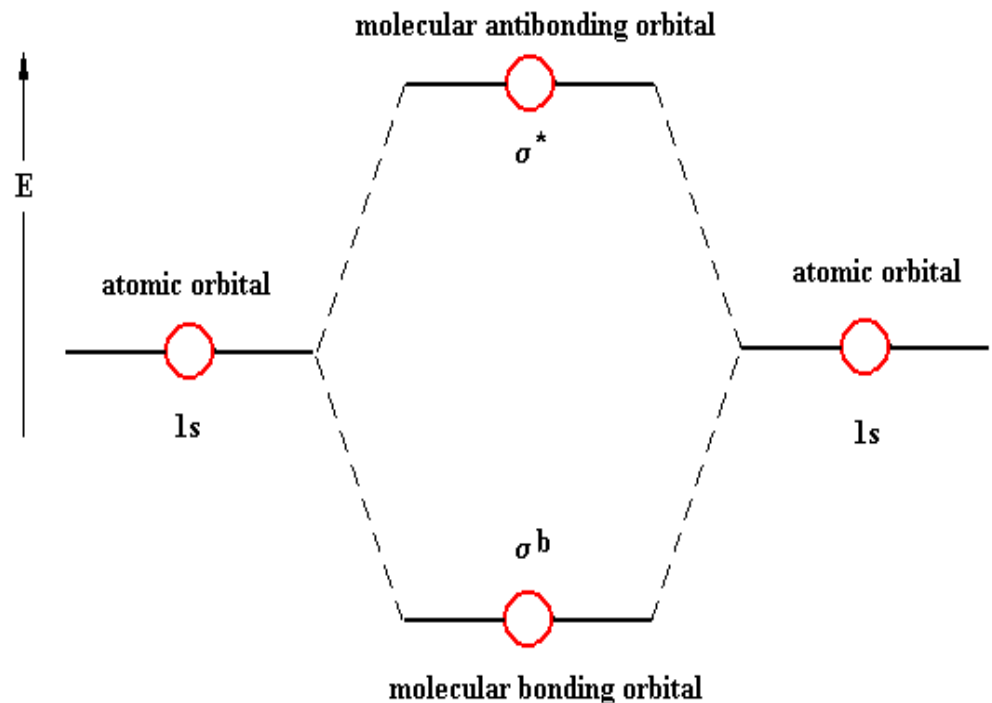
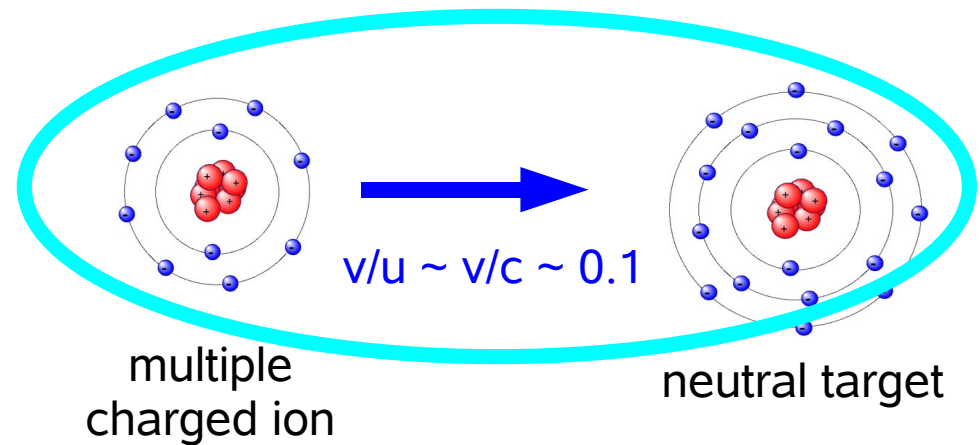
## -- Elementary processes and notations



Mokler & Liesen (1982)

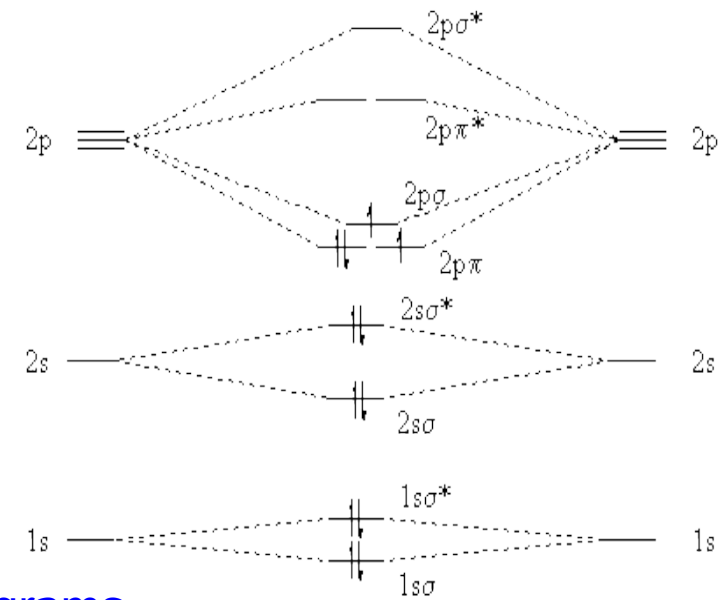
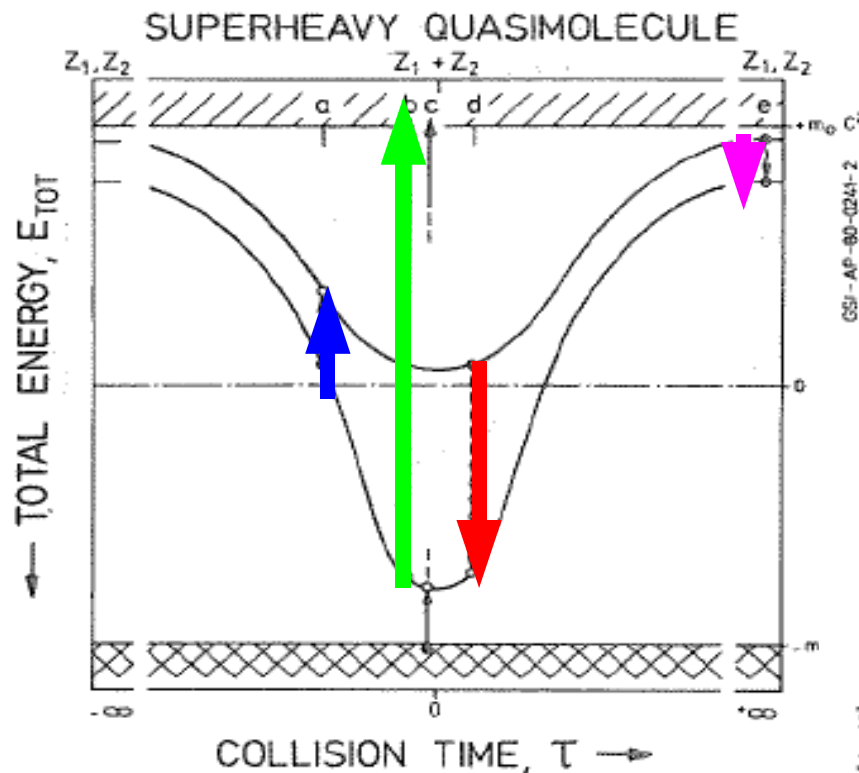
### Processes during the collision:

- excitation into higher shells
- ionization ( $\delta$ -electrons)
- MO radiation
- characteristic x-rays

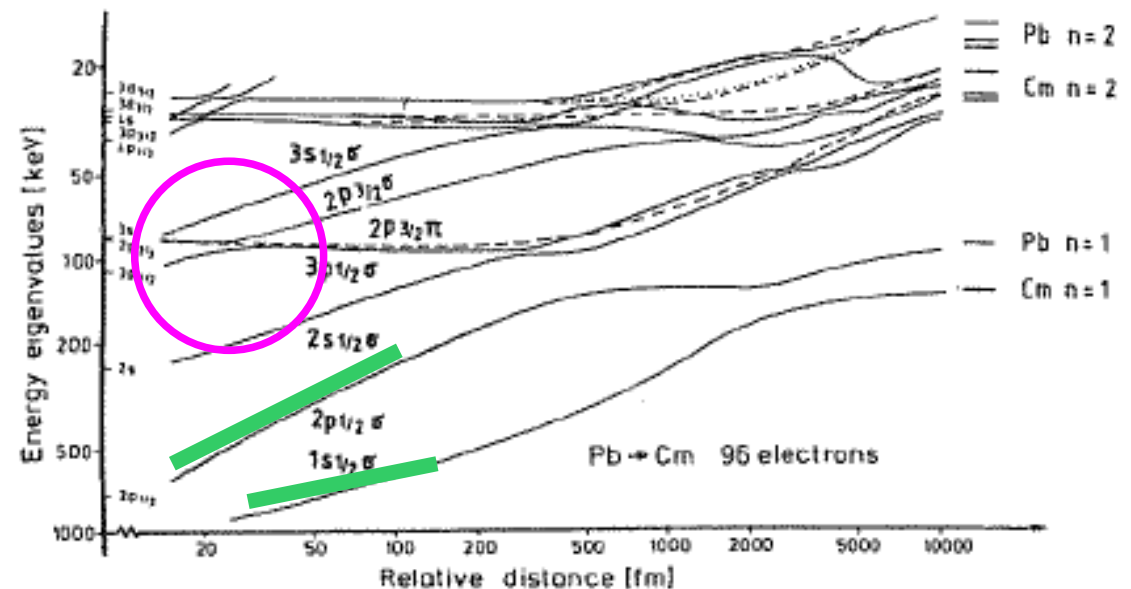


# Origin of quasi-molecular radiation (II)

-- Quasistationary approach



Correlation diagrams



Fricke et al. (1981)

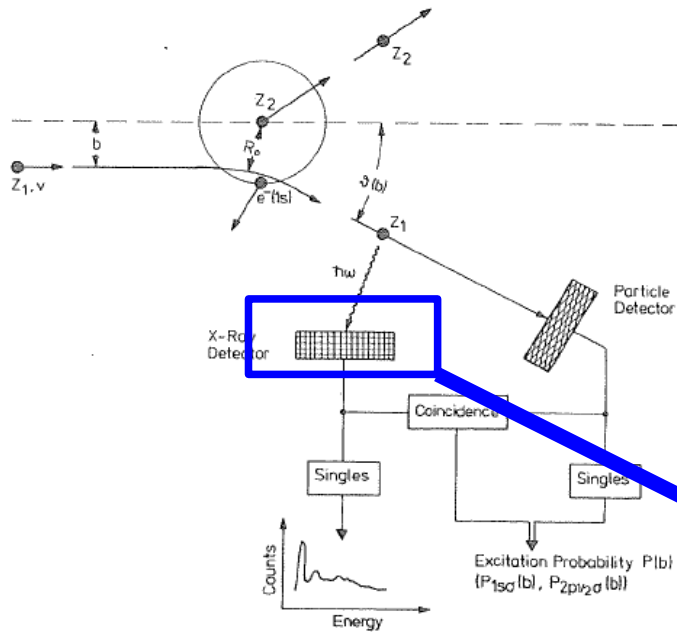
Mokler & Liesen (1982)

## Two further relativistic effects:

- Deepest bound levels ( $1s\sigma$ ,  $2p_{1/2}\sigma$ , ...) are not „flat“ at small R.
- Further levels crossings at small R that modify the inner-shell excitation.

# Formation of super-heavy quasimolecules

-- Previous ion-atom collisions



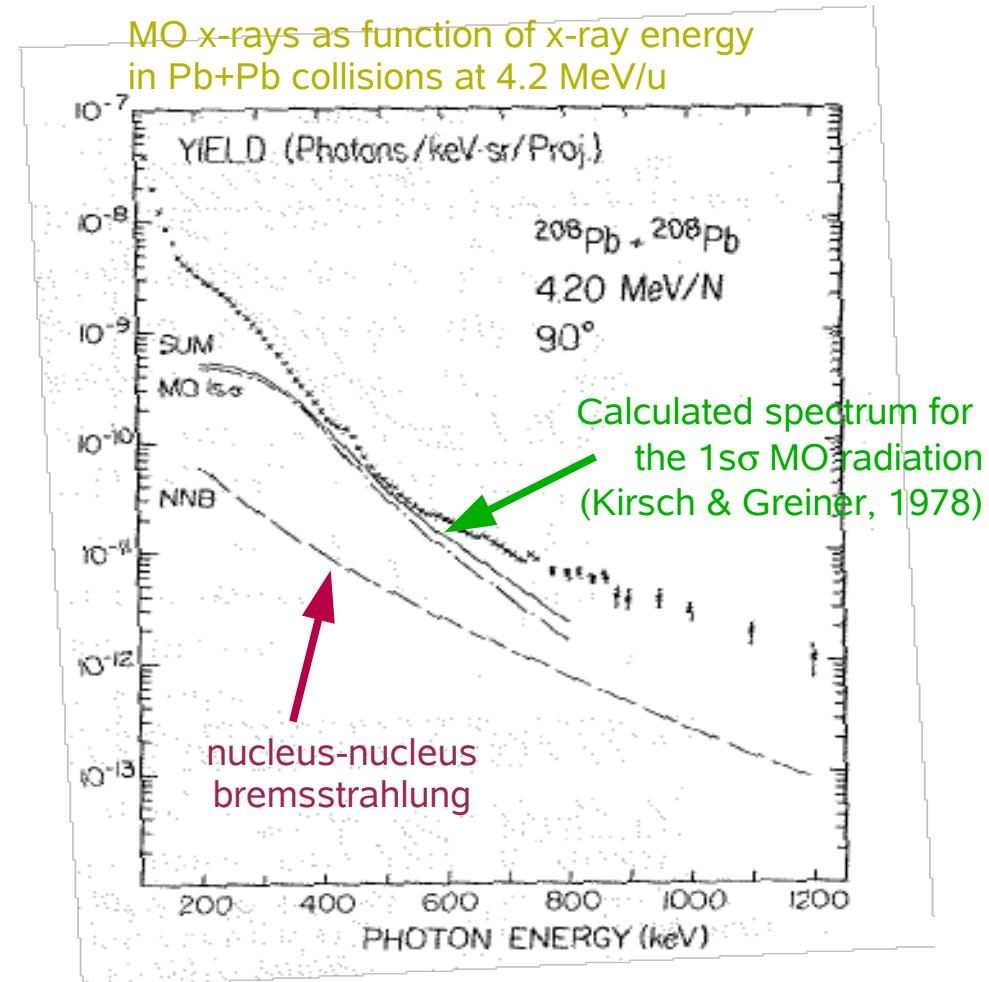
Pb + Pb

(subcritical,  $Z = 164$ )

Pb + Cm

(supercritical,  $Z = 178$ )

MO x-rays as function of x-ray energy  
in Pb+Pb collisions at 4.2 MeV/u



Stoller et al. (1981)

# Formation of super-heavy quasimolecules

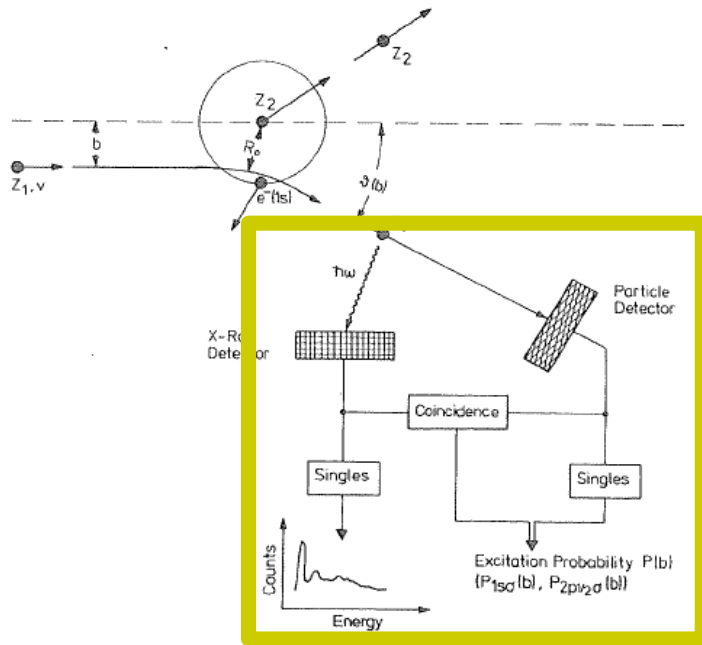
-- Previous ion-atom collisions

Pb + Pb

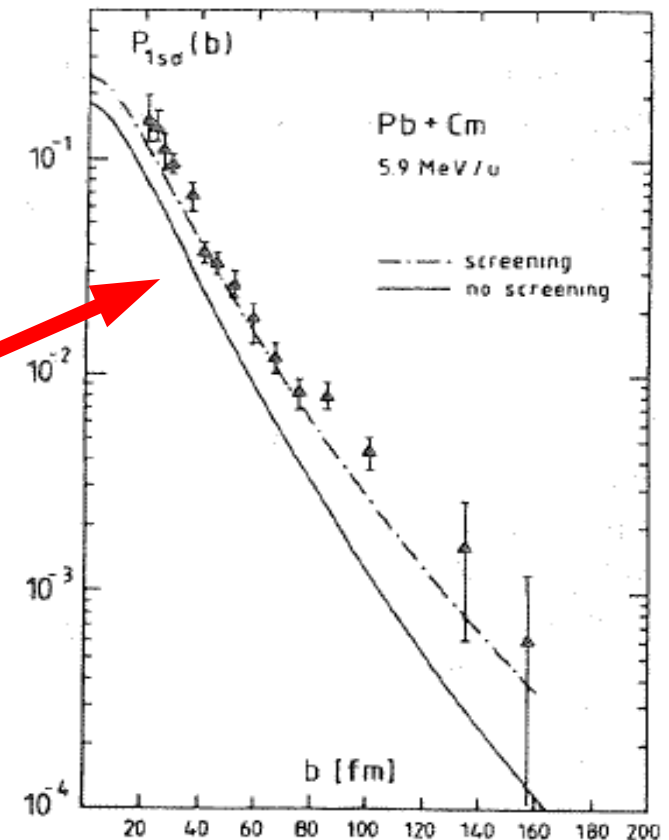
(sub-critical,  $Z = 164$ )

Pb + Cm

(supercritical,  $Z = 178$ )



Experimental vs. theoretical  $1s\sigma$  excitation probability in Pb+Cm collisions at 5.9 MeV/u

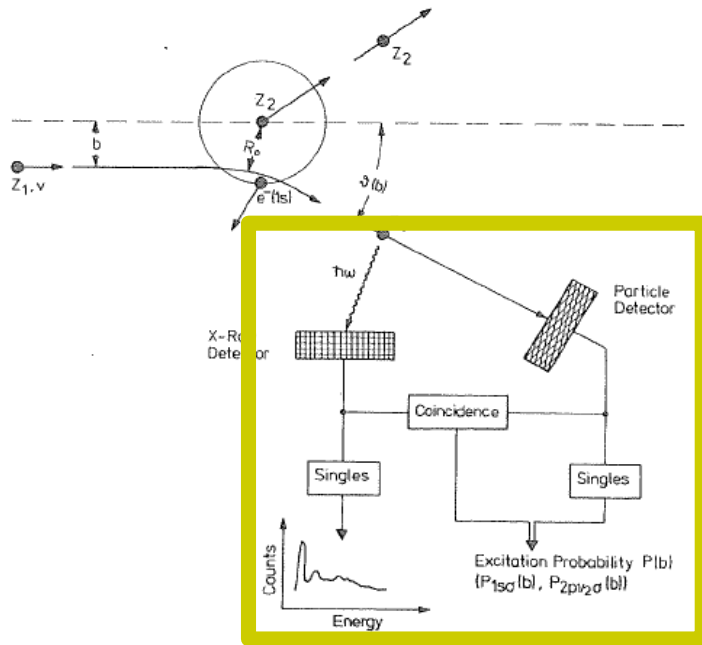


## Difficulties and requests (~1980):

- Creation of K-shell ( $1s\sigma$ ) holes
- Theoretical prediction confirmed:  
increased K-shell ionization probability
- Proper subtraction of background
- Selected coincidence experiments
- Detailed studies on the  $P(b)$  dependence
- However, no „clean“ collision system !

# Formation of super-heavy quasimolecules

-- Previous ion-atom collisions



Pb + Pb

(sub-critical,  $Z = 164$ )

Pb + Cm

(supercritical,  $Z = 178$ )

VOLUME 44, NUMBER 15

PHYSICAL REVIEW LETTERS

14 APRIL 1980

## Experimental Confirmation of a Scaling Law for the $1s\sigma$ Excitation Probability for $Z_1 + Z_2 > 120$ , and its Breakdown in Pb + Cm Collisions at Very Small Internuclear Distances

D. Liesen, P. Armbruster, F. Bosch, S. Hagmann, P. H. Mokler, and H. J. Wollersheim  
*Gesellschaft für Schwerionenforschung, D-6100 Darmstadt, Federal Republic of Germany*

and

H. Schmidt-Böcking  
*Institut für Kernphysik, D-6000 Frankfurt, Federal Republic of Germany*

and

R. Schuch  
*Physikalisches Institut, Universität Heidelberg, D-6900 Heidelberg, Federal Republic of Germany*

and

J. B. Wilhelmy  
*Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87545*  
(Received 9 November 1979)

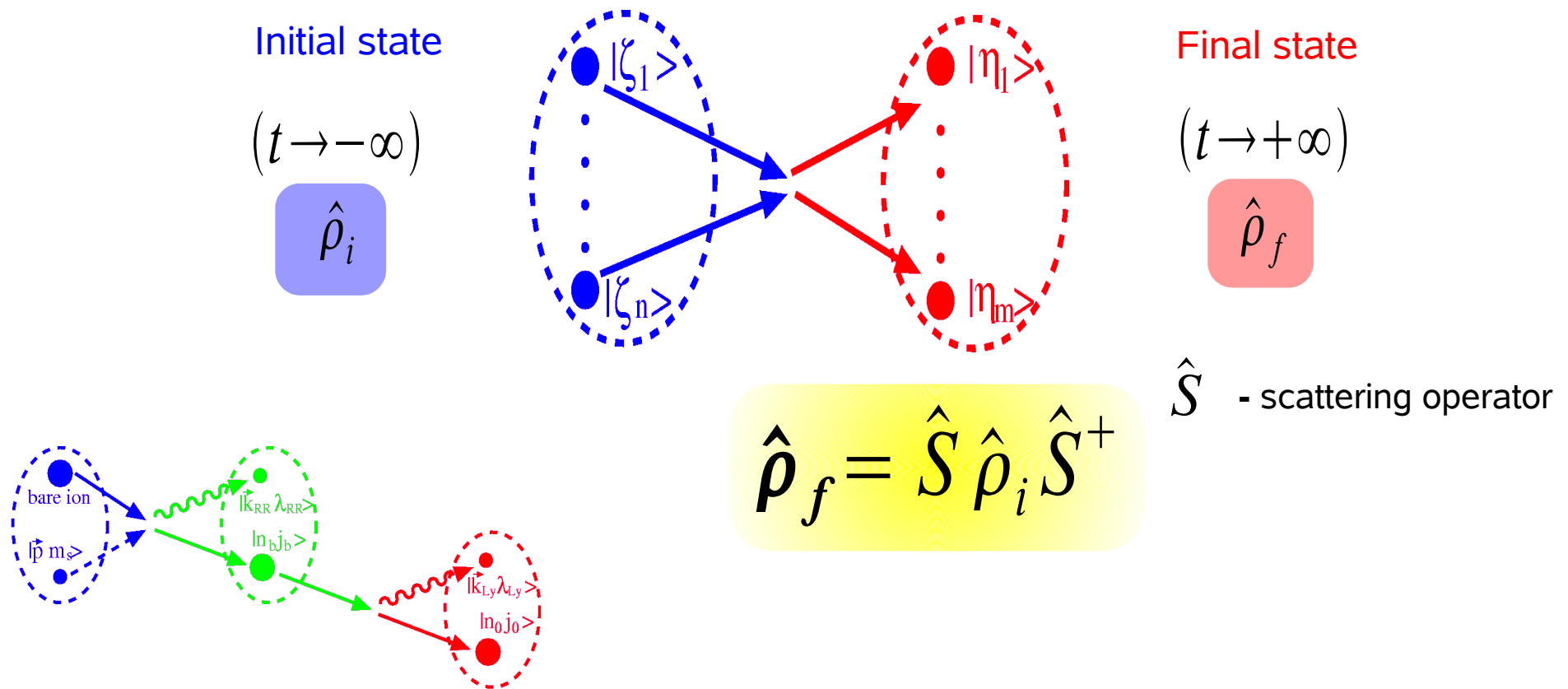
The excitation probability of the  $1s\sigma$ -molecular orbital has been measured as a function of the impact parameter  $b$  for several collision systems in the region  $129 \leq Z_1 + Z_2 \leq 178$  at the UNILAC. All published impact-parameter data agree with a simple scaling law except those for impact parameters  $b \leq 40$  fm in the Pb + Cm system ( $Z_1 + Z_2 = 178$ ).

## Difficulties and requests (~1980):

- Creation of K-shell ( $1s\sigma$ ) holes
- Theoretical prediction confirmed:  
increased K-shell ionization probability
- Proper subtraction of background
- Selected coincidence experiments
- Detailed studies on the  $P(b)$  dependence
- However, no „clean“ collision system !

# Perturbative description of ion-atom collisions

-- for instance, by means of the density matrix

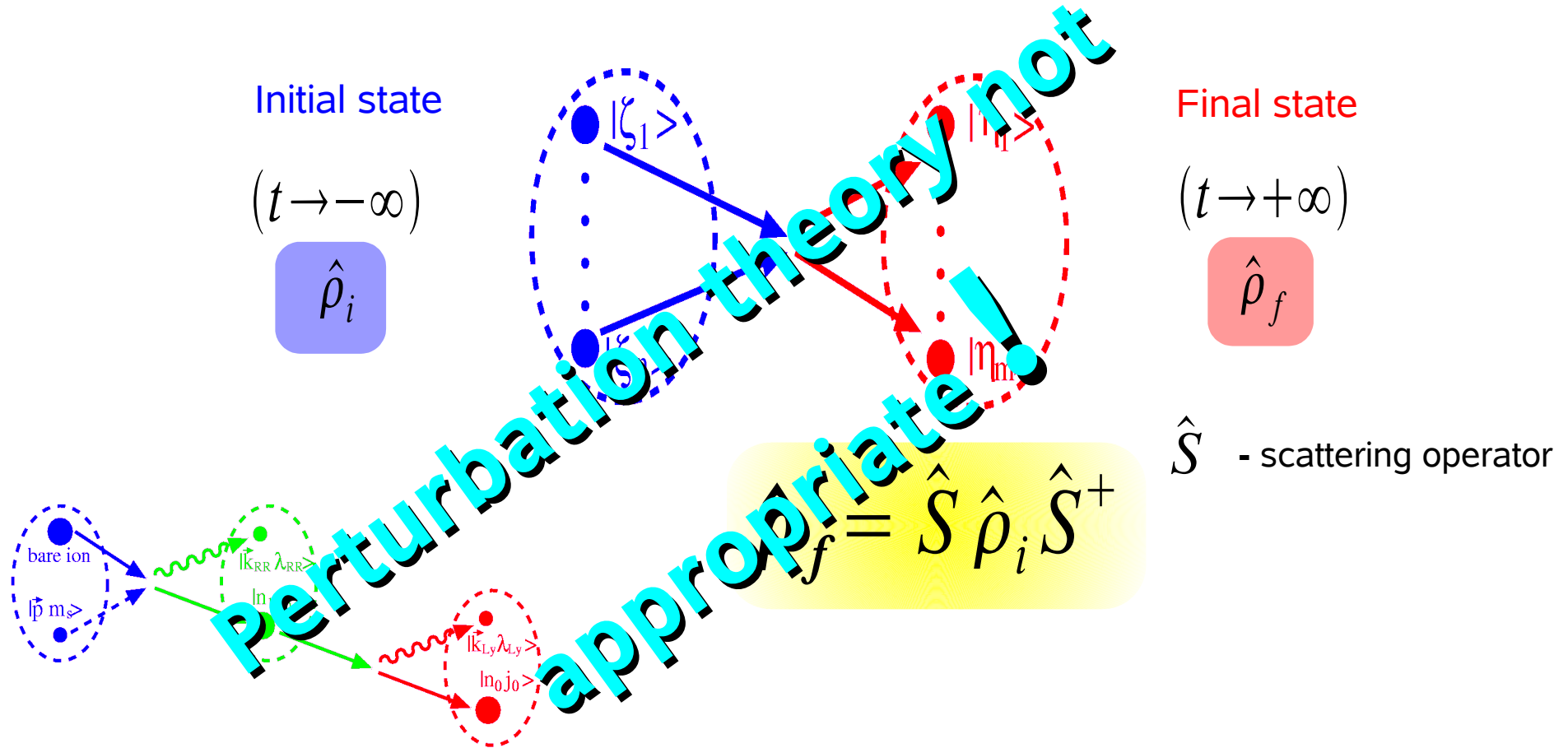


Using the density matrix, a quantum system can be conveniently accompanied through several individual steps of the interaction but not for (quasi-) adiabatic processes !



# Perturbative description of ion-atom collisions

-- for instance, by means of the density matrix



Using the density matrix, a quantum system can be conveniently accompanied through several individual steps of the interaction but not for (quasi-) adiabatic processes !

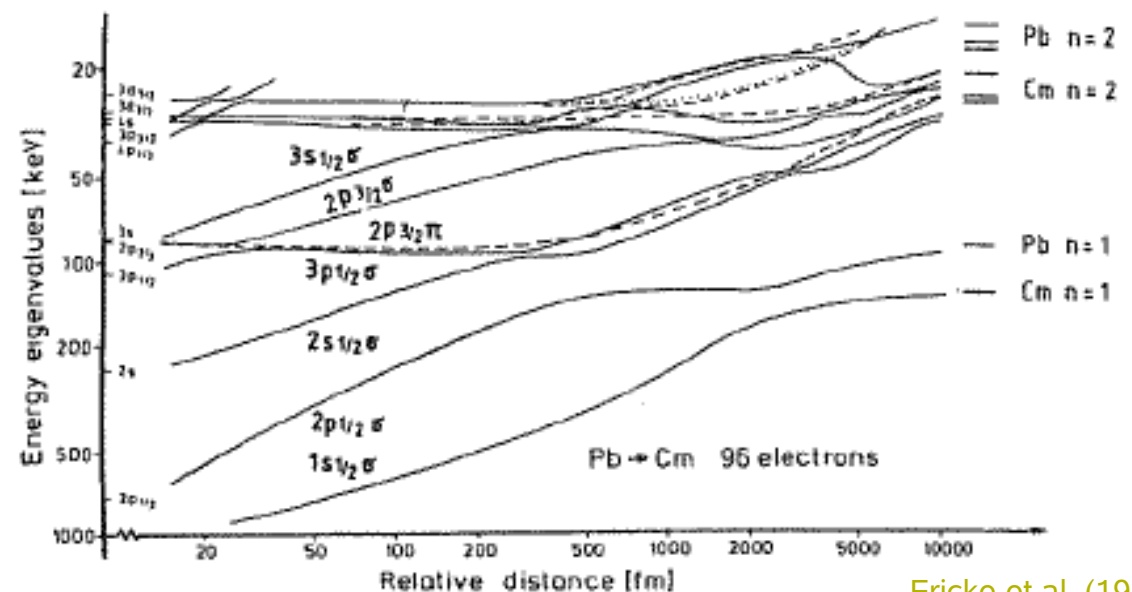
# Adiabatic two-center description of ion-atom collisions

-- dynamics „along the diatomic correlation diagram“

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}_1, \dots, \vec{r}_N, t) = \hat{H}_{el} \Psi(\vec{r}_1, \dots, \vec{r}_N, t)$$

One-electron treatment in quasimolecular basis:

(Müller ~ 1975: discrete  
Rumrich, Soff ~ 80er: continuum)



# Adiabatic two-center description of ion-atom collisions

-- dynamics „along the diatomic correlation diagram“

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}_1, \dots, \vec{r}_N, t) = \hat{H}_{el} \Psi(\vec{r}_1, \dots, \vec{r}_N, t)$$

One-electron treatment in quasimolecular basis:

(Müller ~ 1975: discrete  
Rumrich, Soff ~ 80er: continuum)

$$\Psi(\vec{r}_1, \dots, \vec{r}_N, t) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\vec{r}_1, t) & \dots & \psi_1(\vec{r}_N, t) \\ \dots & \dots & \dots \\ \psi_N(\vec{r}_1, t) & \dots & \psi_N(\vec{r}_N, t) \end{vmatrix}$$

$$\psi_i(\vec{r}, t) = \sum_{j=1}^M a_{ji}(t) \phi_j(\vec{r}, R(t)) e^{-\frac{i}{\hbar} \int^t \epsilon_j dt'}$$

Coupled-channel equations

$$\dot{a}_{nk}(t) = - \sum_{j \neq k} a_{nj}(t) \langle \phi_k | \partial / \partial t | \phi_j \rangle e^{i(\chi_k - \chi_j)}$$

time-dependent  
molecular orbitals

fast oscillating translation factors

# Adiabatic two-center description of ion-atom collisions

-- strongly dependent on the numerical basis

$$i\hbar S a'(t) = H a(t)$$

$$S_{lj} = \langle \phi_l | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$
$$H_{lj} = \langle \phi_l | i\hbar \frac{\partial}{\partial t} + \epsilon_j - \hat{h}^{TDDF} | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$

Two- vs. three-center description



# Adiabatic two-center description of ion-atom collisions

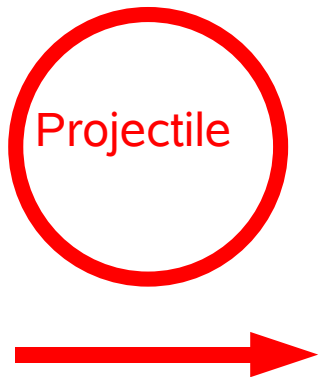
-- strongly dependent on the numerical basis

$$i\hbar S a'(t) = H a(t)$$

$$S_{lj} = \langle \phi_l | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$
$$H_{lj} = \langle \phi_l | i\hbar \frac{\partial}{\partial t} + \epsilon_j - \hat{h}^{TDDF} | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$

Radial and rotational coupling  
of matrix elements.

Two- vs. three-center description



# Adiabatic two-center description of ion-atom collisions

-- strongly dependent on the numerical basis

$$i\hbar S a'(t) = H a(t)$$

$$S_{lj} = \langle \phi_l | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$

$$H_{lj} = \langle \phi_l | i\hbar \frac{\partial}{\partial t} + \epsilon_j - \hat{h}^{TDDF} | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$

## Two- vs. three-center description

$$\begin{aligned} \phi_j(\vec{r}, \vec{R}) &= \sum_{\nu=1}^S d_{j\nu}^P(\vec{R}) \varphi_{\nu}^P(\vec{\xi}(\vec{r}, \vec{R}), \vec{R}) \cdot \exp \left\{ \frac{i}{\hbar} m \vec{V}_P \cdot \vec{r} \right\} \\ &+ \sum_{\nu=1}^S d_{j\nu}^T(\vec{R}) \varphi_{\nu}^T(\vec{\xi}(\vec{r}, \vec{R}), \vec{R}) \cdot \exp \left\{ \frac{i}{\hbar} m \vec{V}_T \cdot \vec{r} \right\} \\ &+ \sum_{\nu=1}^S d_{j\nu}^C(\vec{R}) \varphi_{\nu}^C(\vec{\xi}(\vec{r}), \vec{R}) \\ &\equiv \sum_{K', \nu} d_{j\nu}^{K'}(\vec{R}) \hat{S}_{K'} \left| \varphi_{\nu}^{K'} \right\rangle \end{aligned}$$



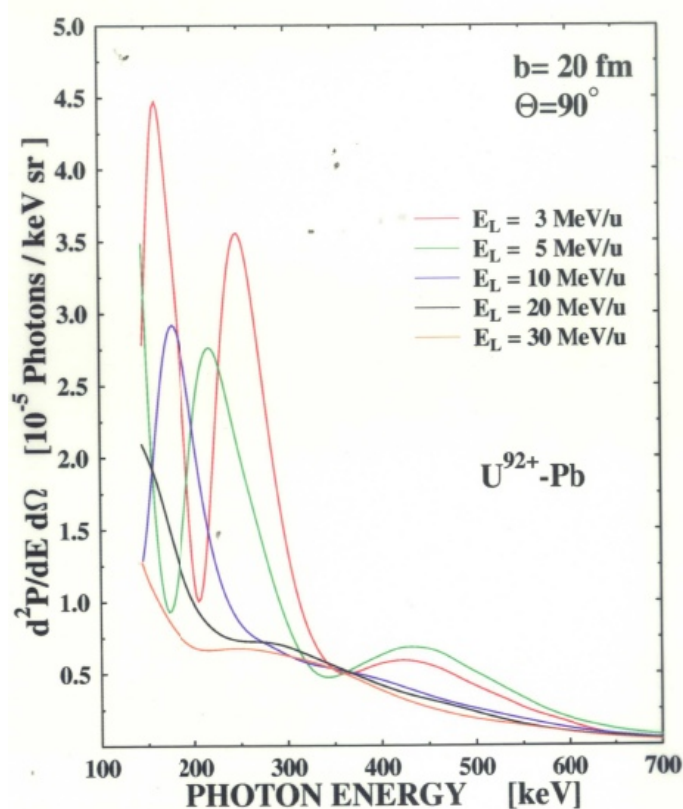
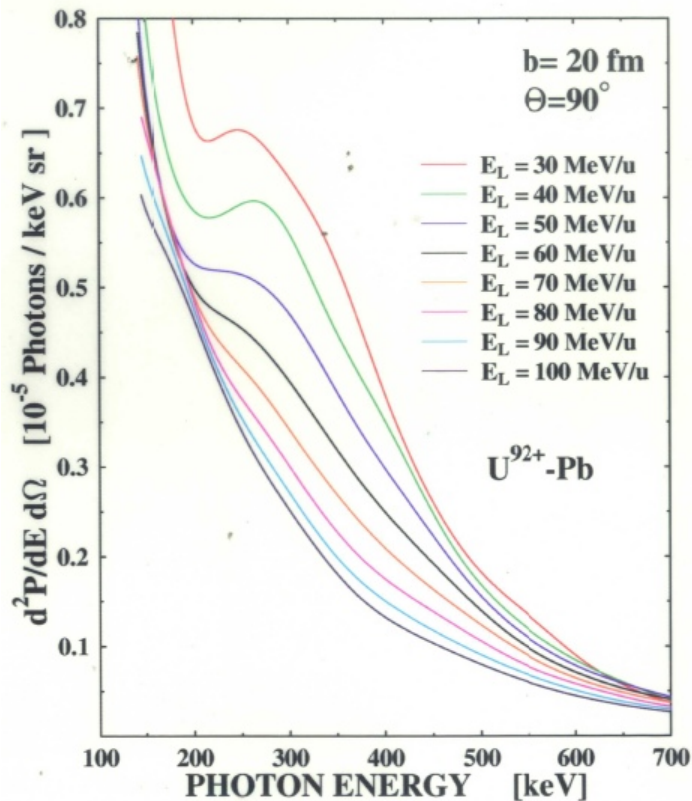
- Ansatz for the molecular orbitals at a given time  
--> **optimized basis** (due to the molecular, i.e. diatomic treatment).
- Problem-adapted basis due to the explicit use of the electronic translation factors.
- For fast collisions ( $v_{\text{orbit}} \ll v_{\text{nuc}}$ ), the Fock matrix is diagonal in atomic basis.
- Center-of-mass basis help describe 'saddle-point' electrons.

# Adiabatic two-center description of ion-atom collisions

-- strongly dependent on the numerical basis

$$i\hbar S a'(t) = H a(t)$$

$$S_{lj} = \langle \phi_l | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$
$$H_{lj} = \langle \phi_l | i\hbar \frac{\partial}{\partial t} + \epsilon_j - \hat{h}^{TDDF} | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$



Initially filled K and L-shell of Pb and U.

Schulze, Anton & Fricke (1990ies)

# Adiabatic two-center description of ion-atom collisions

-- strongly dependent on the numerical basis

$$i\hbar S a'(t) = H a(t)$$

$$S_{lj} = \langle \phi_l | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$
$$H_{lj} = \langle \phi_l | i\hbar \frac{\partial}{\partial t} + \epsilon_j - \hat{h}^{TDDF} | \phi_j \rangle e^{-\frac{i}{\hbar} \int^t (\epsilon_j - \epsilon_l) dt'}$$

Two- vs. three-

$$\begin{aligned} \phi_j(\vec{r}, \vec{R}) &= \sum_{\nu=1}^S d_{j\nu}^P(\vec{R}) \phi_{\nu}^P(\vec{r}) \\ &+ \sum_{\nu=1}^S d_{j\nu}^T(\vec{R}) \phi_{\nu}^T(\vec{r}) \\ &+ \sum_{\nu=1}^S d_{j\nu}^C(\vec{R}) \phi_{\nu}^C(\vec{r}) \\ &\equiv \sum_{K', \nu} d_{j\nu}^{K'}(\vec{R}) \phi_{\nu}^{K'}(\vec{r}) \end{aligned}$$

## Previous successes (AG Fricke, Kassel, until 1990ies)

- ◆ Solution of the time-dependent Dirac (HFS) equation for ion-atom collisions in sub- and supercritical fields.
- ◆ Unified description of excitation, transfer and ionization, including combined processes; incorporates the AO and MO picture as limit (sizeable programs; available ?)
- ◆ No correlation, so far, but expected to be small for inner-shell processes.
- ◆ Method of inclusive probabilities to find the proper orbital occupation after the collisions.
- ◆ Can be done but sophisticated and very time-consuming.

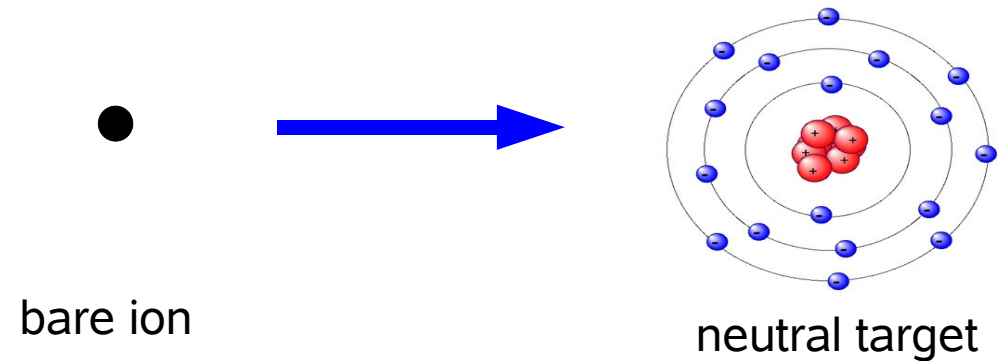


# Formation and observation of super-heavy quasimolecules

-- Future studies

## Suggestions for the future:

- Naked projectiles ( $U^{92+}$ )
- No creation of K-shell holes required  
--> 10..100 x larger cross sections at small  $b$
- Gas-jet target to ensure „clean system“
- Storage ring or „off-line“ at the Unilac ??
- Coincidence experiments with charge state ??
- Impact-parameter dependence ??

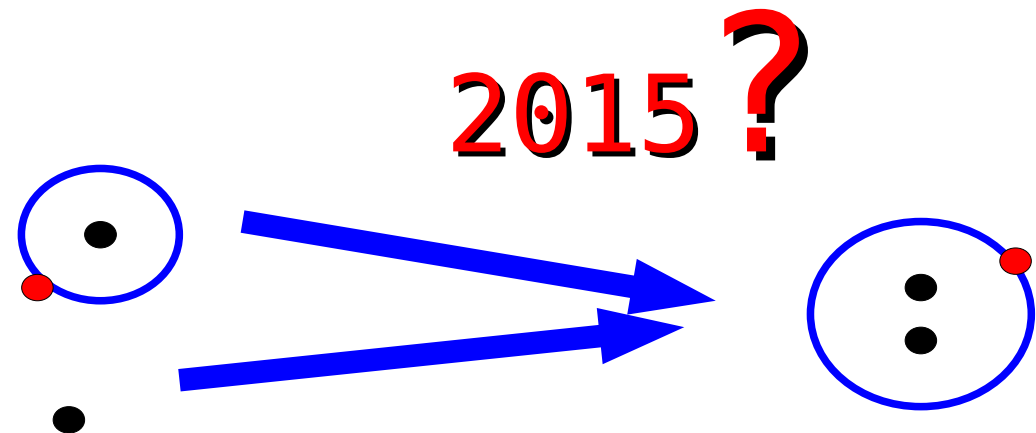
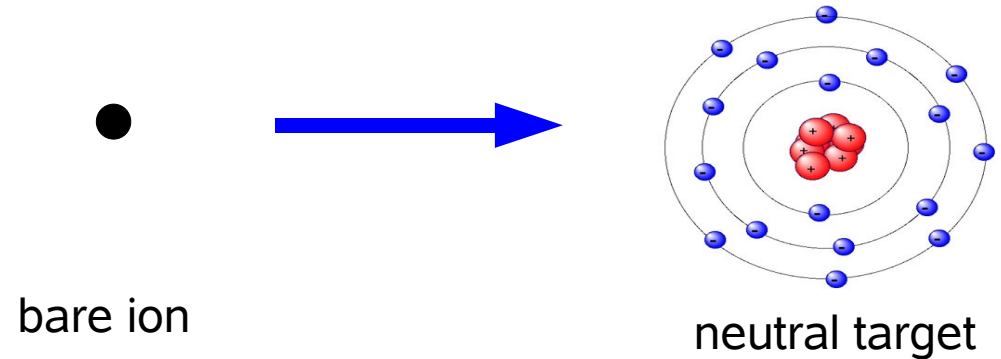


# Formation and observation of super-heavy quasimolecules

-- Future studies

## Suggestions for the future:

- Naked projectiles ( $U^{92+}$ )
- No creation of K-shell holes required  
--> 10..100 x larger cross sections at small  $b$
- Gas-jet target to ensure „clean system“
- Storage ring or „off-line“ at the Unilac ??
- Coincidence experiments with charge state ??
- Impact-parameter dependence ??
- Co-linear collisions with just a single electron involved !







# Radiative potential for QED

$$\Phi_{\text{rad}}(r) = \Phi_U(r) + \Phi_g(r) + \Phi_f(r) + \Phi_l(r) + \frac{2}{3} \Phi_{\text{WC}}^{\text{simple}}(r)$$

$$\Phi_g(r) + \Phi_f(r) + \Phi_l(r) =$$



$$\Phi_U(r) + \frac{2}{3} \Phi_{\text{WC}}^{\text{simple}}(r) =$$

$\Phi_g(r)$  – magnetic formfactor

$\Phi_f(r)$  – electric formfactor

$\Phi_l(r)$  – low energy electric formfactor

$\Phi_U(r)$  – Uehling potential

$\Phi_{\text{WC}}(r)$  – Wichmann-Kroll potential

$\Phi_g(r)$  and  $\Phi_f(r)$  have free parameters which are chosen to fit QED corrections to the energies (Mohr, et al) and weak matrix elements (Kuchiev, Flambaum; Milstein, Sushkov, Terekhov; Sapirstein et al)



# Systematic „routes“ to atomic structure

## Multiconfiguration expansions

$$\psi_{\alpha}(P J M) = \sum_r^{n_c} c_r(\alpha) \gamma_r P J M >$$

Construct a basis in the  
N-electron Hilbert space

### Shell-model

all CSF including virtual single-, double-, ... excitations  
from occupied into the **unoccupied(sub-) shells**  $n, n+1, \dots$

## Many-body perturbation theory

$$H = H_0 + V$$

Rest interaction to  $H_0$  with known solutions

- order-by-order perturbation theory in **V** (MBPT) or
- decomposition in classes of „virtual excitations“ (all-order methods)

# Systematic „routes“ to atomic structure

## Multiconfiguration expansions

$$\psi_{\alpha}(P J M) = \sum_r^{n_c} c_r(\alpha) \gamma_r P J M >$$

Construct a basis in the N-electron Hilbert space

### Shell-model

all CSF including virtual single-, double-, ... excitations from occupied into the **unoccupied(sub-) shells**  $n, n+1, \dots$

## Many-body perturbation theory

$$H = H_0 + V$$

Rest interaction to H

- order-by-order perturbation theory in **V**
- decomposition in classes of „virtual excitations“

### Energies & Wave functions

- GRASP(-92)
- „Desclaux“
- Coupled-Cluster



# „Electronic correlations“

-- Fine-structure of open-shell configurations

Dimension of the  
Hilbert space

$p^4$   
 $p^3 s$

5  
10

$p^3 s$

$p^4$

Computational requirements depend  
very critically on the shell structure  
of the atoms and ions !

$d^8$   
 $d^7 p$

9  
110

$\sim 1 \dots 3 \%$

level and  
transition  
energies

$f^7 s^2$

327

$f^7 sp$

3808

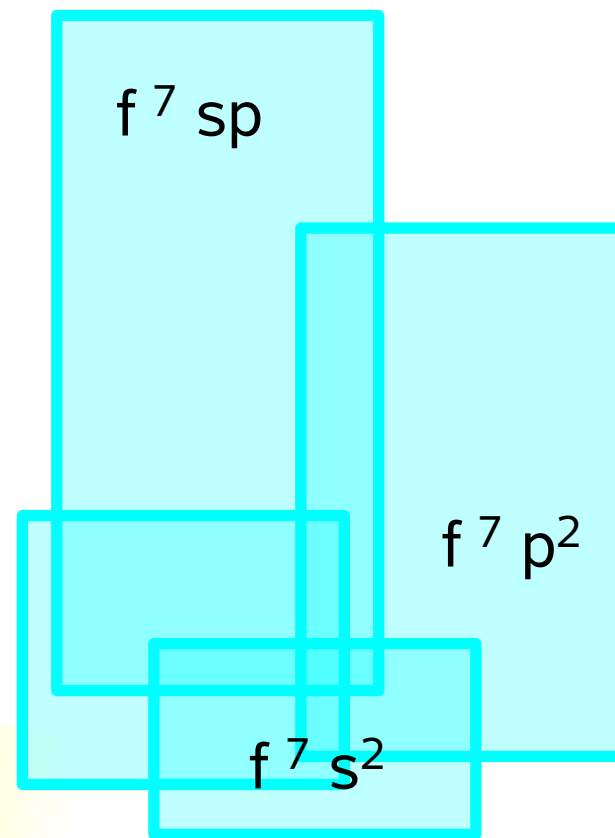
$f^7 p^2$

4724

$f^6 spd$

31804

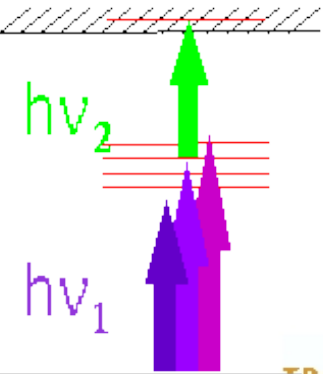
$\sim 10 \dots 500 \%$



**Concept of electron configurations gets lost !**

# Optical spectroscopy at Fermium ( $Z = 100$ )

-- first observation and classification of atomic levels

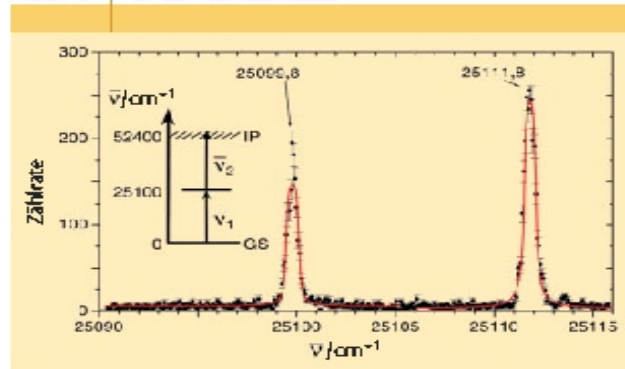


TRANSURANE

## Erstmalige Spektroskopie des Elements Fermium

Das Element Fermium ( $Z=100$ ) wurde 1952 in den Überresten einer thermonuklearen Explosion entdeckt. Es ist das schwerste Element, das über sukzessiven Neutroneneinfang und Betazerfall hergestellt werden kann. Jetzt ließ sich erstmals die atomare Struktur spektroskopisch studieren. Dafür wurde eine 2 ng leichte Probe von  $^{255}\text{Fm}$  (Halbwertszeit 20,1 Stunden) am Hochfluss-Kernreaktor des Oak Ridge National Laboratory, USA, produziert und nach Deutschland versandt [1].

ABB. 1 SPEKTRALLINIEN



Beobachtete Spektrallinien von Fermium und das zweistufige Anregungsschema. Die rot eingezeichneten Kurven stellen theoretische Berechnungen der Spektrallinien dar.

relativistische Massenzunahme. Die Orbitale schrumpfen, was eine verstärkte Abschirmung des Coulomb-Potentials für die äußeren Leuchtelektronen zur Folge hat. Dadurch könnten sich die chemischen Eigenschaften der schweren Elemente so verändern, dass sie unerwartete, nicht mehr im Einklang mit der Extrapolation innerhalb einer Gruppe stehende Eigenschaften bekommen. Solche relativistischen Effekte äußern sich neben Änderungen in den chemischen Eigenschaften auch im Anregungsspektrum des Atoms und damit in seinen Spektrallinien.

Bei der Spektroskopie des Isotops  $^{255}\text{Fm}$  treten zwei Probleme auf: Zum

Physical Review  
**Focus**

Focus Archive PNU Index Image Index Focus Search

Previous Story / Next Story / January - June 2003 Archive

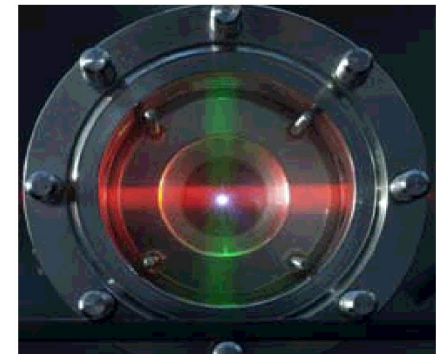
Phys. Rev. Lett. **90**, 163002  
(issue of 25 April 2003)  
Title and Authors

25 April 2003

## Fermium Wins Heavyweight Title

In the 1952 detonation of the first nuclear bomb, the element fermium has since sat in a corner of the periodic table where few tools of chemistry could reach. Now a team has measured a piece of its spectrum--the wavelengths of light it absorbs--making the heaviest element ever to be so studied. The researchers rushed their samples of the short-lived element from a nuclear reactor in the US to New York, where they probed it with just atoms at a time. Appearing in April *PRL*, their findings shed light on the energies of fermium's orbitals and provide a way for theorists to test their calculations for even heavier, more elusive elements.

Available energy levels for electrons can now determine both what kind of element it forms and what other elements it reacts with. Fermium is element 100, just doors past plutonium in the periodic table--and calculating the energies of its orbitals is a tricky business. Einstein's relativity comes into play for the moving electrons of such an atom, changing the rules that usually indicate which orbitals are most stable.

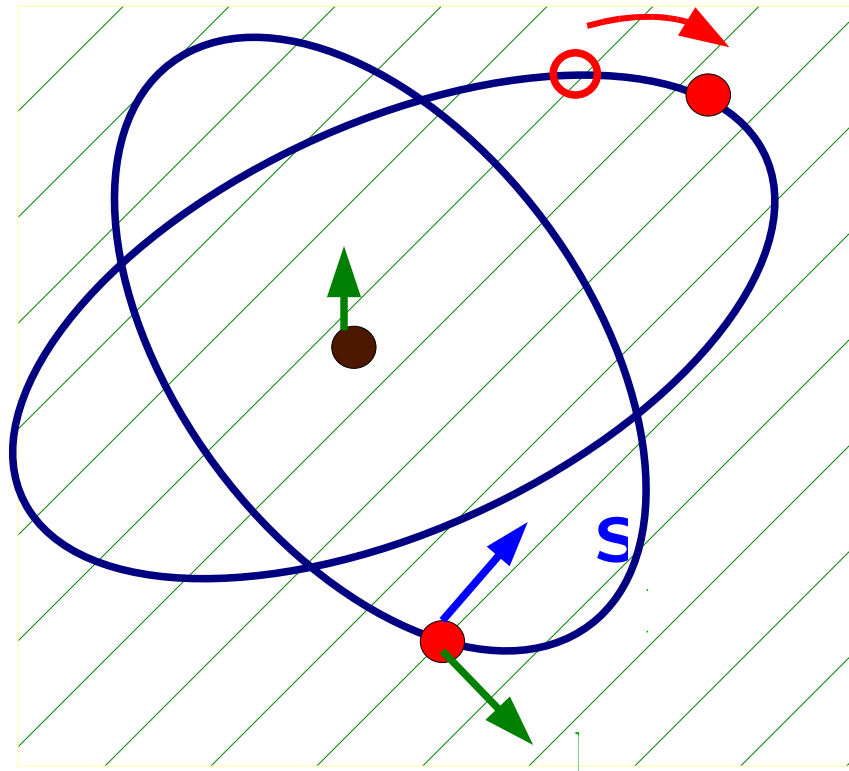


A. Zschau

**Fermium, revealed.** Lasers probed the spectrum of light absorbed by fermium atoms using this chamber, in which ionized atoms are drawn toward the exit hole (white) in back. The experiment makes fermium the heaviest element whose atomic spectrum has been measured.

# Hierarchy of inner-atomic interactions

-- Self-consistent field calculations



*External  
fields*

- Nuclear potential
- Instantaneous Coulomb repulsion between all pairs of electrons
- Spin-orbit interaction
- Relativistic electron velocities; magnetic contributions and retardation

- QED: radiative corrections
- Hyperfine structure
- Electric and magnetic nuclear moments (isotopes)

Perturbation theory

- ★ Motion of the nucleus: Reduced mass and mass polarization



Methods of solution:

- Direct numerical integration of PDE
- Expansion w.r.t. atomic basis
- Expansion w.r.t. adiabatic basis

Expansion of the wavefunction:

$$\psi_n^{(+)}(\vec{r}, t) = \sum_k a_{nk}(t) \phi_n(\vec{r}, \vec{R}(t)) e^{-i\chi_k(t)} \quad \text{with the phase} \quad \chi_k(t) = \int^t dt' E_k(R(t'))$$

Coupled channel equations

$$\dot{a}_{nk}(t) = - \sum_{j \neq k} a_{nj}(t) \langle \phi_k | \partial / \partial t | \phi_j \rangle e^{i(\chi_k - \chi_j)}$$

to be integrated with the initial condition  $a_{ik}(t \rightarrow -\infty) = \delta_{ik}$

Coupling operator:  $\frac{\partial}{\partial t} = \dot{R} \frac{\partial}{\partial R} - i \vec{\omega} \cdot \vec{J}$

Strong radial couplings between  $s_{1/2}$  or  $p_{1/2}$  states in the limit  $R \rightarrow 0$ .

*Multi-step processes* are important. 1st order perturbation theory not sufficient.

$$\dot{a}_{nk}(t) = - \sum_{j \neq k} a_{nj}(t) \langle \phi_k | \partial / \partial t | \phi_j \rangle e^{i(\chi_k - \chi_j)}$$

# Field theoretical description

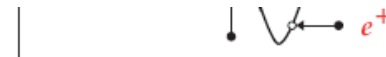
Field operator: 
$$\hat{\psi}(x) = \sum_{n>F} \hat{b}_n^{\text{in}} \psi_n^{(+)} + \sum_{n<F} \hat{d}_n^{\text{in}\dagger} \psi_n^{(+)}$$

The state vector  $|F\rangle$  is prepared as 
$$\begin{cases} \hat{b}_n^{\text{in}}|F\rangle = 0 & , \quad n > F \\ \hat{d}_n^{\text{in}}|F\rangle = 0 & , \quad n < F \end{cases}$$

Expansion in terms of out-operators: 
$$\hat{\psi}(x) = \sum_{n>F} \hat{b}_n^{\text{out}} \psi_n^{(-)} + \sum_{n<F} \hat{d}_n^{\text{out}\dagger} \psi_n^{(-)}$$

Canonical transformation: 
$$\hat{b}_n^{\text{out}} = \sum_{k>F} \hat{b}_k^{\text{in}} a_{kn} + \sum_{k<F} \hat{d}_k^{\text{in}\dagger} a_{kn}$$

## • K-hole production



High ionisation rates:  $P_{1s\sigma} \simeq 10\%$  .

Approximate scaling behaviour:

$$P_{1s\sigma}(b) \simeq D(Z) e^{-2R_{\text{min}}q_{\text{min}}} \quad \text{where} \quad q_{\text{min}} = \frac{E_{1s\sigma}^B(R_{\text{min}})}{\hbar v_{\text{ion}}} \quad (\text{minimum momentum transfer})$$

→ "Spectroscopy" of superheavy quasimolecules.

## • $\delta$ -electron production

The high-energy tail (up to  $E_e > 2 \text{ MeV}$ ) probes the high-momentum components of the the quasimolecular wave functions.

## • Quasimolecular X rays (MOX)

Broad photon spectra. No "end point", quasistatic picture not applicable.

## • Positron creation

- Drastic increase of positron yield with nuclear charge  $Z$  :

$$P_{e^+} \propto Z^{20}$$

- *No qualitative signal* for level diving expected. (Collisional broadening)
- Good quantitative agreement with experiments:  $P(b)$ ,  $P(Z)$ ,  $dP/dE_{e^+}$  .

## Summary

- This method allows an ab-initio solution of the time-dependent Dirac equation for the ion-atom collision process.
- It allows to calculate excitation, transfer and ionization or any combined process for many electrons in a unified way. What is needed is just the electron-electron and electron-nucleus  $1/r$ -interaction.

Personally I would not speak of correlated processes because this correlation depends on the simple Pauli correlation and a relatively good treatment of the  $1/r$ -interaction between the electrons.

- Because one needs separate calculations

- at all internuclear distances
- for all energies
- and all impact parameters

an actual calculation is very time-consuming and complicated.

**But it can be done!**

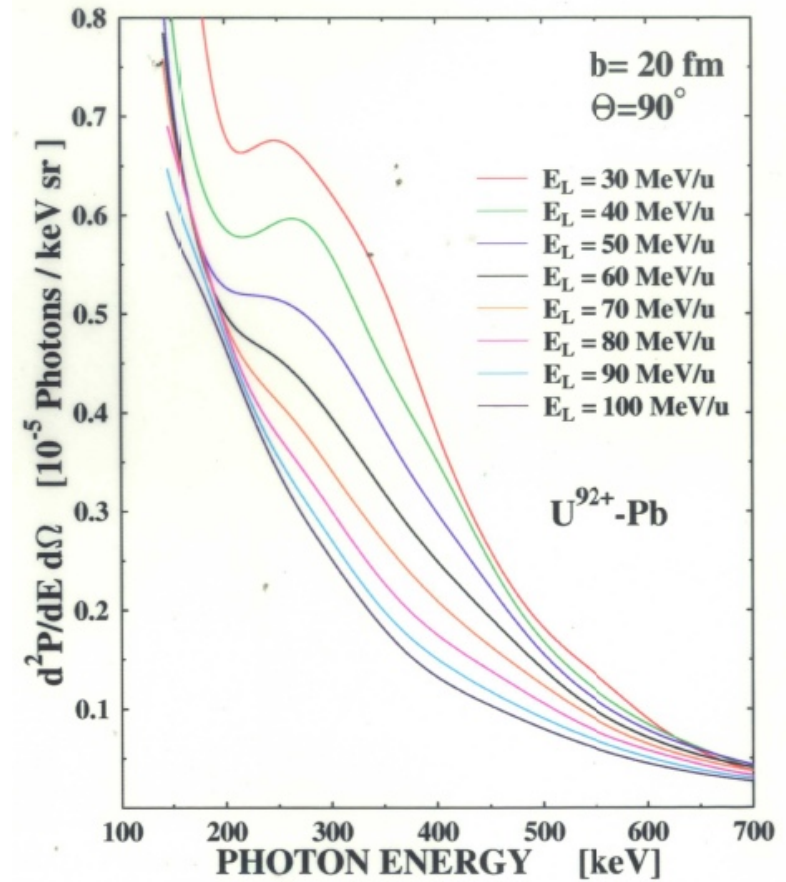
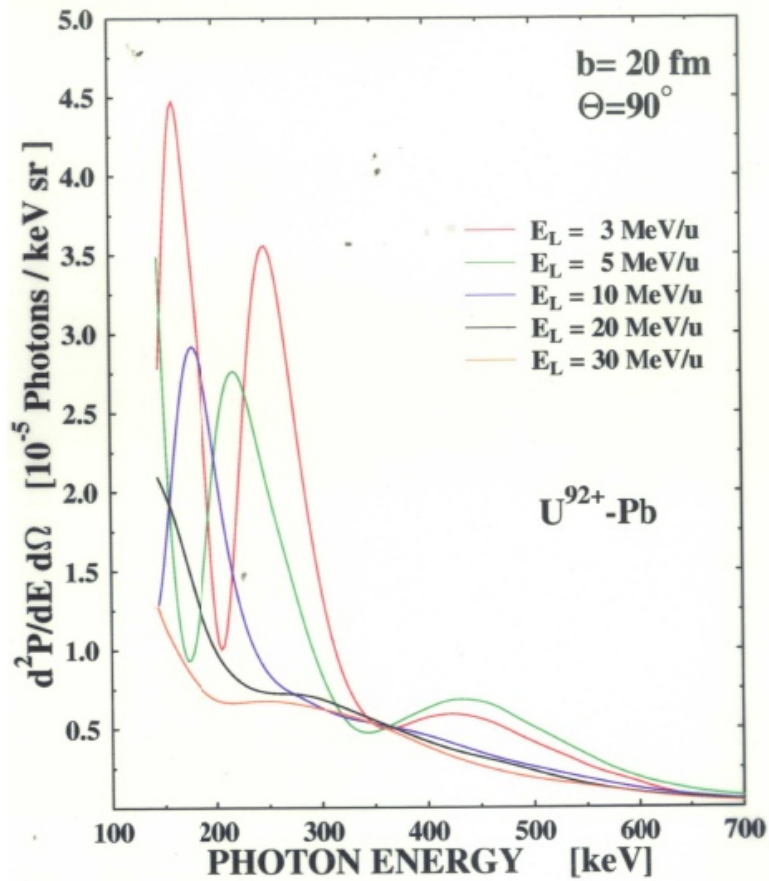
## Vorgehen:

1. Lösung der atomaren DFS Gleichungen
2. Auswahl der Basisfunktionen für die Molekülläufe
3. Molekülberechnungen für alle internuklearen Abstände – dabei auch Berechnung aller Matrixelemente
4. Ausschreiben aller notwendigen Ergebnisse auf File
5. Test auf relatives Vorzeichen für alle MO's für verschiedene R.
6. Auswahl der MO's oder Konfigurationen
7. Erzeugung des Input für die gekoppelten Kanäle Rechnungen
8. Gekoppelte Kanäle Rechnungen für alle Energien und Stoßparameter (und beteiligte Elektronen)
9. Vultüchcheninterpretation mit der gefundenen Satz als entsprechend der physikalischen Freigestellung

Folgende Fortschritte sind in den letzten Jahren erzielt worden:

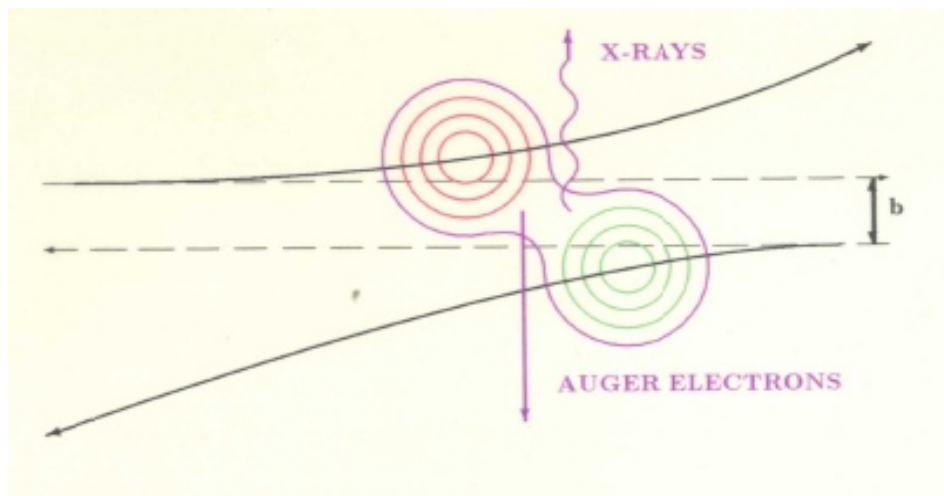
1. Konstruktion einer auch qualitativ neuen zeitabhängigen 3-Zentren Basis zur Beschreibung eines Ion-Atom Stoßes
2. Einbau expliziter zeitabhängiger Translationsfaktoren
3. Universelle Beschreibung des Ion-Atom Stoßes für alle Stoßenergien mit dem AO- und MO-Bild als Grenzfälle
4. Erstmalige direkte nicht-störungstheoretische Berechnung einer Ionisation für einfache Mehr-Elektronen Stoßsysteme





10 electrons in the K and L-shell of Pb

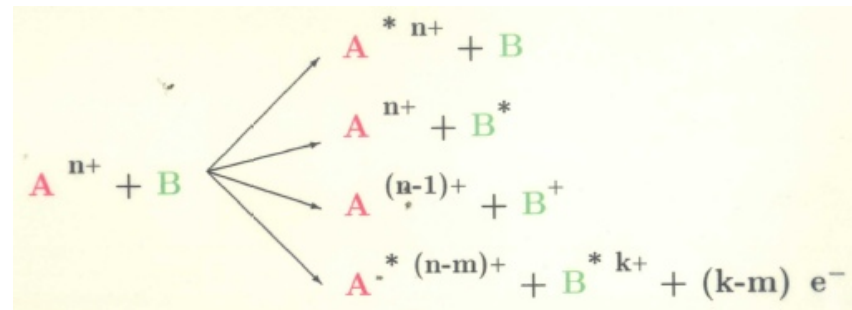




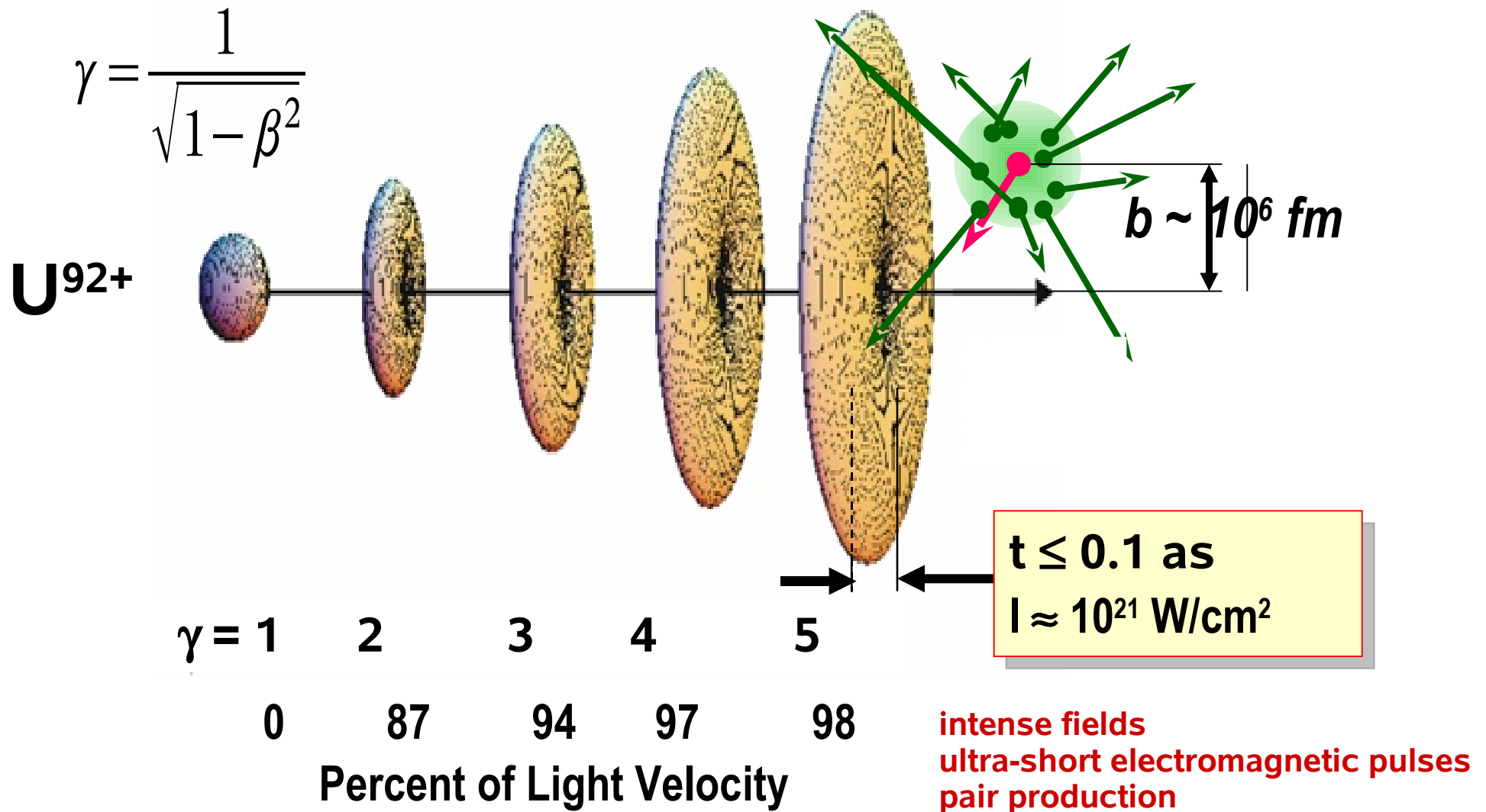
Energy

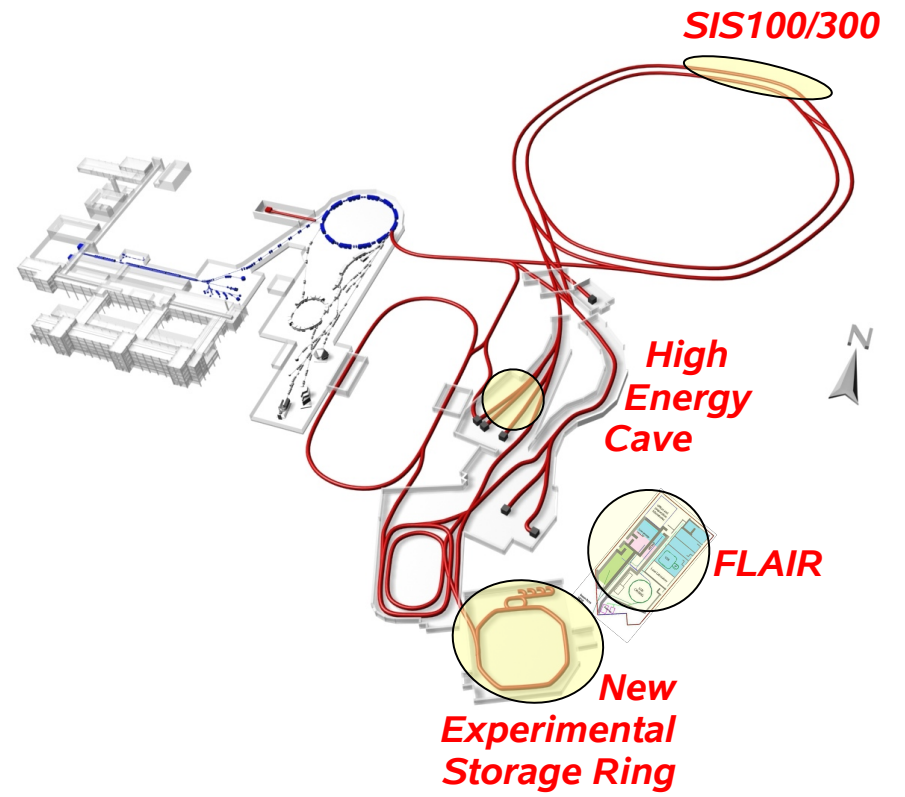
Scattering angle resp. impact parameter

State selective

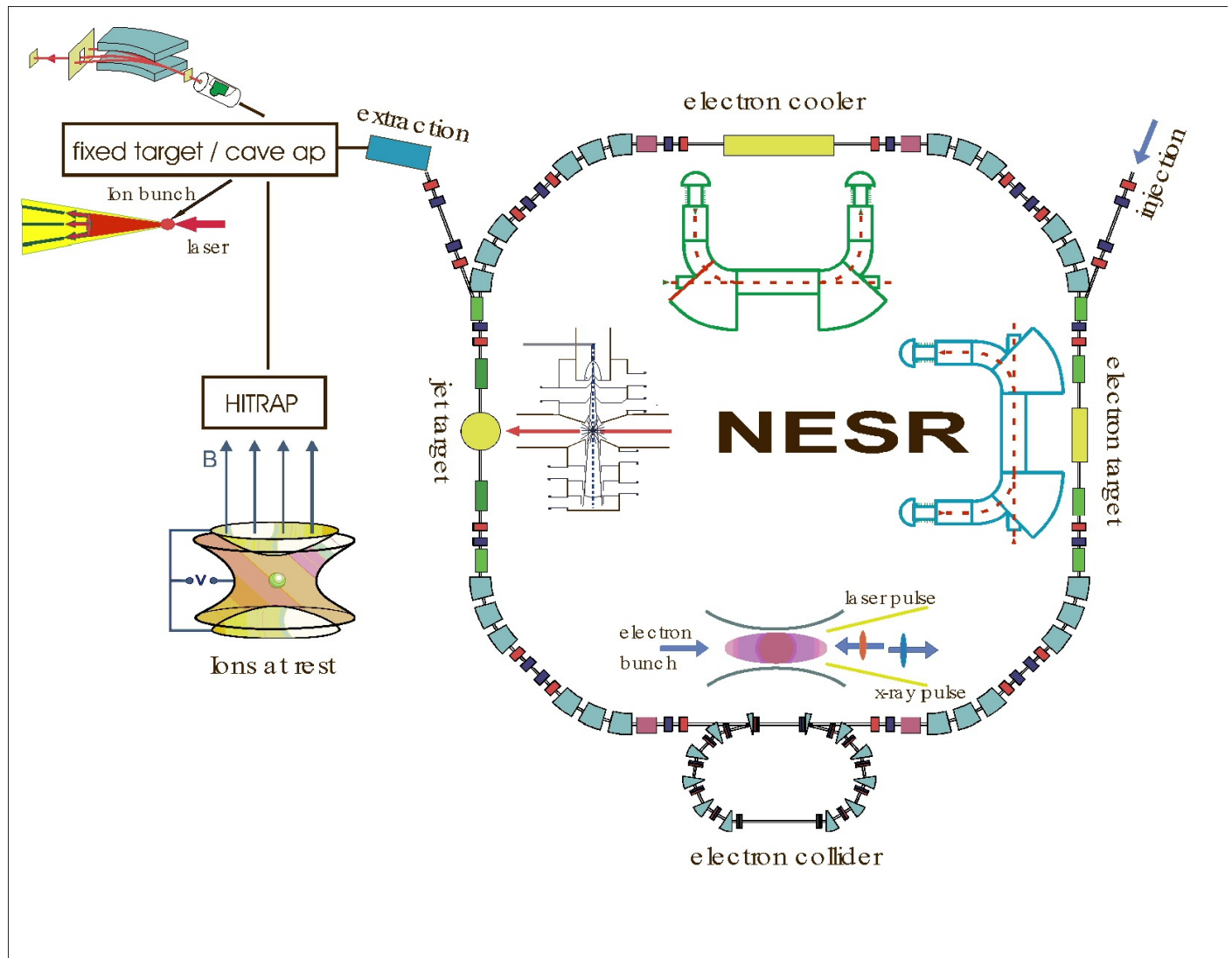


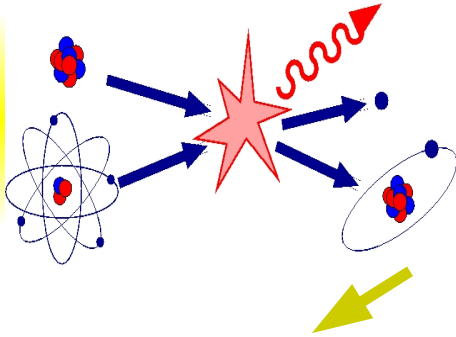
# Reactions of relativistic projectiles in extreme dynamical fields





## Novel Instrumentation



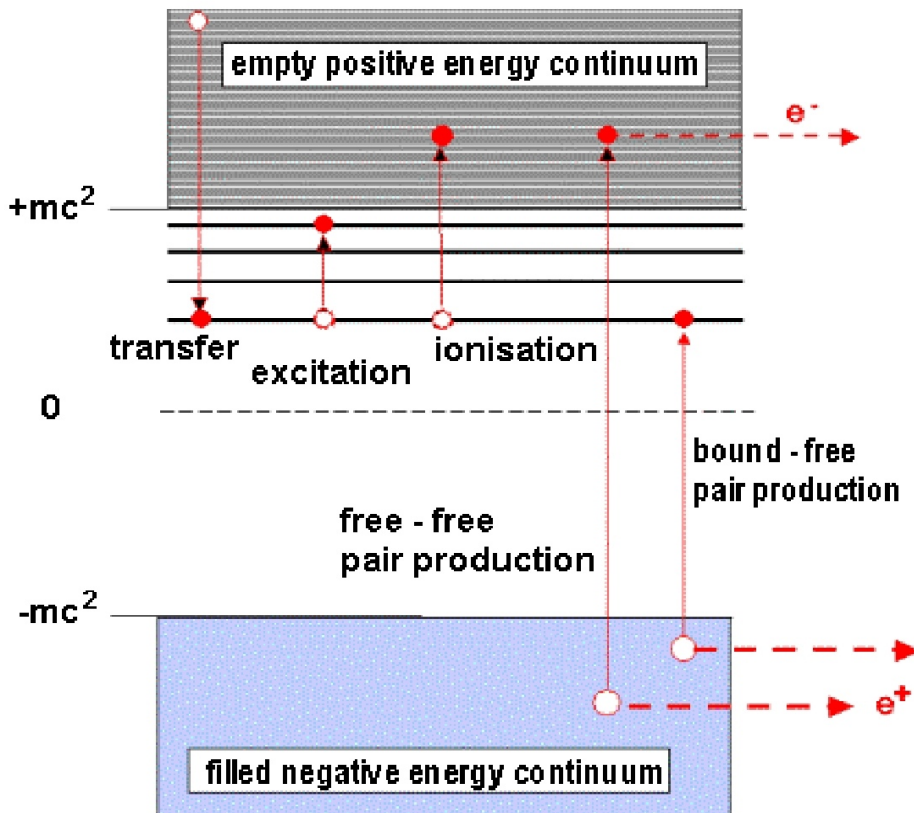


# Ion-Atom Stöße

schnelle Stöße

„Einteilchenbild“

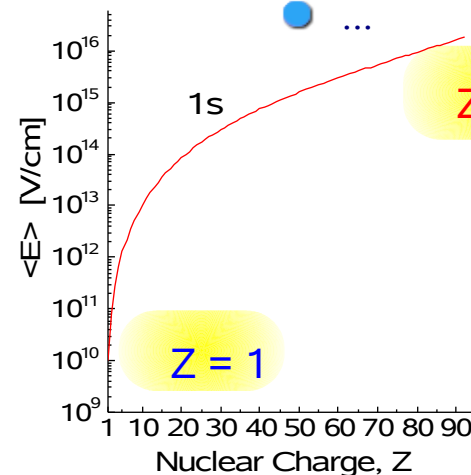
- ▶ Hochgeladene Ionen sind sehr gut geeignet, um die elementaren Prozesse in (extrem) starken Feldern zu verstehen.



langsame Stöße

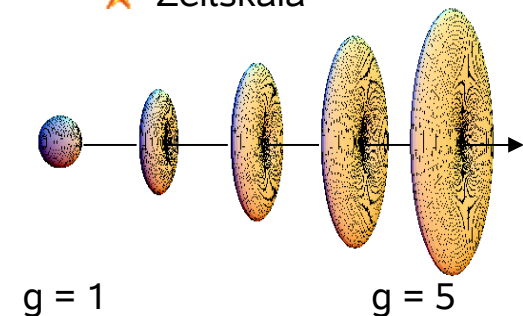
„Vielteilchenbild“

- ▶ Besseres Verständnis der Vielteilchendynamik erforderlich.
- Verstärkung des REC bei langsamen Ionen (!)
- Resonante (dielektronische) Rekombination.
- Abbremsen und Einfang in Fallen.
- Wichtig für Ionen-Oberflächen Prozesse.
- ...



Ionen sind variabel:

- ★ Feldstärke
- ★ Zahl der Elektronen
- ★ Zeitskala

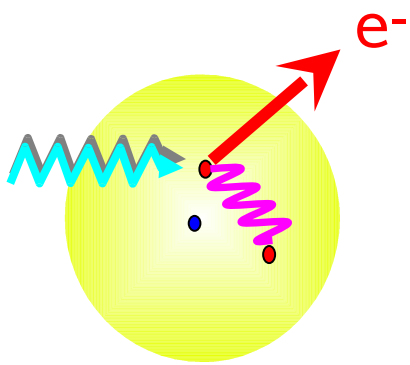


## Summary

- ◆ There has been great progress in the multiple ionization of noble gases due to FEL radiation and high-resolution electron spectroscopy.
- ◆ For present-day intensities ( $< 10^{16}$  W/cm<sup>2</sup>), ionization can be well described by **perturbation theory**; if appropriate for the **'first'** electron, than also suitable for all subsequent steps (since IP increases).
- ◆ Parametrization of the sequential photoionization enables one to understand the **ionization dynamics of the individual steps** and to help reveal **dynamical correlations in the electron-photon interaction**.

## Weak radiation fields: Perturbative approaches

- cross sections
- angular distributions
- „complete“ experiments
- spin polarization
- entanglement



No information about the second electron  
but the knowledge of the state of the final  
photoion !

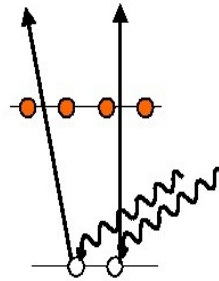
# Two-photon double ionization (TPDI) of atomic neon

-- with resolved electron-momentum distributions



Many-particle photoionization  
amplitudes  $\langle J, l_j || D || J' \rangle$

$$\psi_{\alpha}(P J M) = \sum_r^{n_c} c_r(\alpha) |\gamma_r P J M\rangle$$



## Wave function expansions:

- Construction and classification of N-particle Hilbert spaces
- Shell model:** Systematically enlarged CSF basis

## RATIP

Relativistic Atomic Transition  
and Ionization Properties

(CPC library)

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

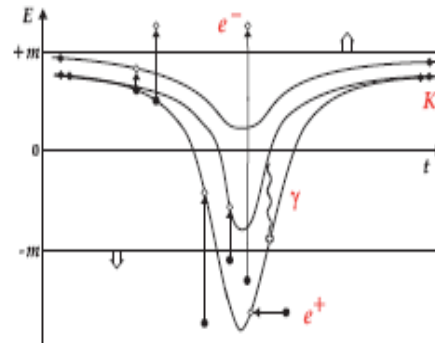


Spontaneous pair creation

Charged vacuum

Heavy ion collisions

Dynamics of  $e^+e^-$  creation, ...



Frankfurt group

Greiner, Müller, Soff, Reinhardt, Müller-Nehler, ...

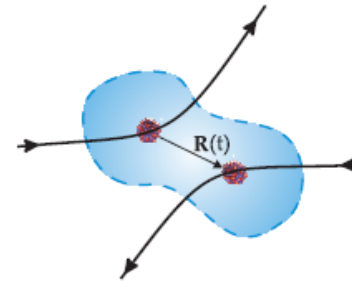
Two Center Dirac Hamiltonian:

$$H_{\text{TCD}}(\vec{R}) = -i\vec{\alpha} \cdot \vec{\nabla} + \beta m + V_1(\vec{r}, \vec{R}) + V_2(\vec{r}, \vec{R})$$

Semiclassical approximation:  $\vec{R}(t)$  = Rutherford trajectory.

If the velocity  $\dot{\vec{R}}$  is "small" the electrons follow the  
**adiabatic quasimolecular basis**

$$H_{\text{TCD}}(\vec{R}) \phi_n = E_n(R) \phi_n$$



TCD solutions:	Discrete states:	B. Müller	~ 1975
	Continuum:	Wietschorke, Rumrich, Soff	~ 1985

Critical distance for U+U	$R_{\text{cr}} = 37 \text{ fm}$	(point nuclei, unscreened)
	$R_{\text{cr}} = 26 \text{ fm}$	(extended nuclei, HFS screening)