Quasimolecular radiation in heavy-ion collisions
-- Two-center description

S. Fritzsche
FIAS Frankfurt & GSI Darmstadt
18\textsuperscript{th} July 2008

\begin{itemize}
\item Unique GSI/Unilac facility:
  \begin{itemize}
  \item (super-) strong em-fields
  \item \(Z_{\text{united}} = Z_1 + Z_2 \sim 170..180\), i.e. for \(Z\alpha > 1\)
  \item collision times \(10^{-19} .. 10^{-21}\) s
  \item extremly short-lived superheavy „quasimolecules“
  \item closest approach < 150 fm as typical for K-shell
  \end{itemize}
\end{itemize}
Quasimolecular radiation in heavy-ion collisions

-- Two-center description

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Creation of `positrons'

- spontaneous
- dynamical pairs (em field)
- induced by nuclear processes
Quasimolecular radiation in heavy-ion collisions

--- Two-center description

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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

Z~ 173

strong spin-orbit splitting; swapped ‘level order’

Fricke & Soff (1977)
Main QED contributions:

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

Fricke & Soff (1977)
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

|P|^2

3s  Uranium^{91+}

Relativistic contraction of the wave functions

„Dirac see“ visible in different properties
- energies
- transition probabilities (M1, ...)
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- ...

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

\[
|P|^2
\]

Relativistic contraction of the wave functions

Shrinkage of the electron density due to the Dirac operator.

Very strong contraction for the K-shell

Fricke (1972)
Origin of quasi-molecular radiation (I)

-- Elementary processes and notations

Processes during the collision:

- excitation into higher shells
- ionization (δ-electrons)
- MO radiation
- characteristic x-rays

Mokler & Liesen (1982)
Origin of quasi-molecular radiation (I)

-- Elementary processes and notations

**Processes during the collision:**
- excitation into higher shells
- ionization (δ-electrons)
- MO radiation
- characteristic x-rays

Mokler & Liesen (1982)
Origin of quasi-molecular radiation (II)

**-- Quasistationary approach**

Two further relativistic effects:

- Deepest bound levels (1s\(\sigma\), 2p\(\frac{1}{2}\)\(\sigma\), ...) are not "flat" at small R.
- Further levels crossings at small R that modify the inner-shell excitation.

**Correlation diagrams**

Mokler & Liesen (1982)

Fricke et al. (1981)
Formation of super-heavy quasimolecules

-- Previous ion-atom collisions

\[
\text{Pb} + \text{Pb} \quad \text{(subcritical, } Z = 164) \\
\text{Pb} + \text{Cm} \quad \text{(supercritical, } Z = 178) \\
\]

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

Calculated spectrum for the 1s\(\sigma\) MO radiation (Kirsch & Greiner, 1978)

Stoller et al. (1981)
Formation of super-heavy quasimolecules

-- Previous ion-atom collisions

**Pb + Pb**  
(sub-critical, Z = 164)

**Pb + Cm**  
(supercritical, Z = 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!
Difficulties and requests (~1980):

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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“

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

One-electron treatment in quasimolecular basis:

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

Fricke et al. (1981)
Adiabatic two-center description of ion-atom collisions

\[ i \hbar \frac{\partial}{\partial t} \Psi(\vec{r}_1, \ldots, \vec{r}_N, t) = \hat{H}_e \Psi(\vec{r}_1, \ldots, \vec{r}_N, t) \]

One-electron treatment in quasimolecular basis:

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

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

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

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

\[ \text{ih } S_{a'}(t) = H_{a}(t) \]

Two- vs. three-center description

\[ S_{l_j} = \langle \phi_l | \phi_j \rangle e^{-\frac{i}{\hbar} \int_{t}^{t'} (\varepsilon_j - \varepsilon_l) dt'} \]

\[ H_{l_j} = \langle \phi_l | i\hbar \frac{\partial}{\partial t} + \varepsilon_j - \hat{h}^{TDDF} | \phi_j \rangle e^{-\frac{i}{\hbar} \int_{t}^{t'} (\varepsilon_j - \varepsilon_l) dt'} \]
Adiabatic two-center description of ion-atom collisions

-- strongly dependent on the numerical basis

\[ \text{ih } S_a'(t) = H_a(t) \]

Two- vs. three-center description

Radial and rotational coupling of matrix elements.
Adiabatic two-center description of ion-atom collisions

-- strongly dependent on the numerical basis

\[ \text{ih } \text{Sa}(t) = \text{Ha}(t) \]

**Two- vs. three-center description**

\[
\phi_j(\vec{r}, \vec{R}) = \sum_{\nu=1}^{S} d_{j\nu}^{P}(\vec{R}) \psi_{\nu}^{P}(\xi(\vec{r}, \vec{R}), \vec{R}) \cdot \exp \left\{ \frac{i}{\hbar} m \vec{v}_P \cdot \vec{r} \right\} \\
+ \sum_{\nu=1}^{S} d_{j\nu}^{T}(\vec{R}) \psi_{\nu}^{T}(\xi(\vec{r}, \vec{R}), \vec{R}) \cdot \exp \left\{ \frac{i}{\hbar} m \vec{v}_T \cdot \vec{r} \right\} \\
+ \sum_{\nu=1}^{S} d_{j\nu}^{C}(\vec{R}) \psi_{\nu}^{C}(\xi(\vec{r}), \vec{R}) \\
\equiv \sum_{K',\nu} d_{j\nu}^{K'}(\vec{R}) \hat{S}_{K'} \left| \varphi_{\nu}^{K'} \right> \\
\]

\[
S_{lj} = \langle \phi_l | \phi_j \rangle e^{-i \int (\epsilon_j - \epsilon_l) dt} \\
H_{lj} = \langle \phi_l | i\hbar \frac{\partial}{\partial t} + \epsilon_j - \hat{H}_{\text{DDF}} | \phi_j \rangle e^{-i \int (\epsilon_j - \epsilon_l) dt} \\
\]

- **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

\[ \text{ih } S_a'(t) = H_a(t) \]

\[ S_{lj} = \langle \phi_l | \phi_j \rangle e^{-\frac{i}{\hbar} \int (\varepsilon_j - \varepsilon_l) dt'} \]

\[ H_{lj} = \langle \phi_l | i\hbar \frac{\partial}{\partial t} + \varepsilon_j - \hat{T}_{DDF} | \phi_j \rangle e^{-\frac{i}{\hbar} \int (\varepsilon_j - \varepsilon_l) dt'} \]

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

\[ \text{ih } Sa'(t) = Ha(t) \]

Two- vs. three-center description

\[ \phi_j(\vec{r}, \vec{R}) = \sum_{\nu=1}^{S} d_{j\nu}^{P}(\vec{r}) \]
\[ + \sum_{\nu=1}^{S} d_{j\nu}^{T}(\vec{R}) \]
\[ + \sum_{\nu=1}^{S} d_{j\nu}^{C}(\vec{R}) \]
\[ \equiv \sum_{K',\nu} d_{j\nu}^{K'}(\vec{R}) \]

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 ??
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- 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

\( \Phi_f(r) \) and \( \Phi_l(r) \) 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

\[ \psi_{\alpha}(PJM) = \sum_{r} c_r(\alpha) \chi_r PM > \]

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, ...

Many-body perturbation theory

\[ H = H_0 + V \]

Rest interaction to \( H_0 \) with known solutions

- order-by-order perturbation theory in \( V \) (MBPT)
- decomposition in classes of „virtual excitations“ (all-order methods)
Systematic „routes“ to atomic structure

Multiconfiguration expansions

\[ \psi_{\alpha}(PJM) = \sum_{r}^{n_{c}} c_{r}(\alpha) \chi_{r}PJM > \]

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, ...

Many-body perturbation theory

\[ H = H_{0} + V \]

Rest interaction to \( H_{0} \)

- 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

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

<table>
<thead>
<tr>
<th>Shell Structure</th>
<th>Dimension of the Hilbert Space</th>
<th>Level and Transition Energies</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p^4 )</td>
<td>5</td>
<td>(~ 1 \ldots 3 %)</td>
</tr>
<tr>
<td>( p^3 s )</td>
<td>10</td>
<td>(~ 10 \ldots 500 %)</td>
</tr>
<tr>
<td>( d^8 )</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td>( d^7 p )</td>
<td>110</td>
<td></td>
</tr>
<tr>
<td>( f^7 s^2 )</td>
<td>327</td>
<td></td>
</tr>
<tr>
<td>( f^7 sp )</td>
<td>3808</td>
<td></td>
</tr>
<tr>
<td>( f^7 p^2 )</td>
<td>4724</td>
<td></td>
</tr>
<tr>
<td>( f^6 spd )</td>
<td>31804</td>
<td></td>
</tr>
</tbody>
</table>

Concept of electron configurations gets lost!
Optical spectroscopy at Fermium (Z = 100)
-- first observation and classification of atomic levels

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 sukzessive Neutroneinfang und Betazerfall hergestellt werden kann. Jetzt ließ sich erstmals die atomare Struktur spektroskopisch studieren. Dafür wurde eine 2 ng leichte Probe von $^{255}$Fm (Halbwertszeit 20,1 Stunden) am Hochfluss-Kernreaktor des Oak Ridge National Laboratory, USA, produziert und nach Deutschland versandt [1].

In the 1952 detonation of the first nuclear bomb, the element m has since sat in a corner of the c table where few tools of try reach. Now a team has a piece of its spectrum—the ngths of light it absorbs—making easiest element ever to be so ed. The researchers rushed their ample of the short-lived element nuclear reactor in the US to ny, where they probed it with just atoms at a time. Appearing in April PRL, their findings shed the energies of fermium’s ns and provide a way for theorists their calculations for even heavier r elusive elements.

A. Zachau

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 spectrum has been measured.

Available energy levels for electrons $^m$o determine both what kind of $^n$ forms and what other elements it reacts with. Fermium is element x doors past plutonium in the periodic table—and calculating the energies of electrons is a tricky business. Einstein’s relativity comes into play for the wing electrons of such an atom, changing the rules that usually indicate orbitals are most stable.
Hierarchy of inner-atomic interactions
-- Self-consistent field calculations

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

External fields

Perturbation theory
Methods of solution:

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

Expansion of the wavefunction:

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

Coupled channel equations

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

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

Coupling operator:

\[
\frac{\partial}{\partial t} = \hat{R} \frac{\partial}{\partial R} - i \vec{\omega} \cdot \vec{J}
\]

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

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

\[
\dot{a}_{nk}(t) = - \sum_{j \neq k} a_{nj}(t) \left\langle \phi_k | \partial / \partial t | \phi_j \right\rangle e^{i(\chi_k - \chi_j)}
\]
Field theoretical description

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

The state vector \( |F\rangle \) is prepared as:
\[
\begin{align*}
\hat{b}^\text{in}\,|F\rangle &= 0 \quad , \quad n > F \\
\hat{d}^\text{in}\,|F\rangle &= 0 \quad , \quad n < F
\end{align*}
\]

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

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

- **K-hole production**
  High ionisation rates: \( P_{1\sigma} \approx 10\% \).
  Approximate scaling behaviour:
  \[
  P_{1\sigma}(b) \approx D(Z) e^{-2R_{\text{min}}q_{\text{min}}} \quad \text{where} \quad q_{\text{min}} = \frac{E_{1\sigma}R_{\text{min}}}{\hbar v_{\text{ion}}} \quad \text{(minimum momentum transfer)}
  \]
  "Spectroscopy" of superheavy quasimolecules.

- **\( \delta \)-electron production**
  The high-energy tail (up to \( E_c > 2 \text{ MeV} \)) probes the high-momentum components of 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 DF-GL
2. Auswahl der Basisfunktionen für die Molekülläufe
3. Molekülechnungen für alle internuklearen Abstände
   - dabei auch Berechnung der Matrixelemente
4. Abspeichern aller notwendigen Ergebnisse auf Diskette
5. Test auf relative Vorgabe für alle Mo's für verschiedene R
6. Auswahl der Mo's oder Konfigurationen
7. Erzeugung der Input für die gekoppelten Kanal-Rechnungen
8. Gekoppelte Kanal Rechnungen für alle Energien und Stoßparameter (nur beteiligte Elektronen)
9. Vielschichtinterpretation mit der gefundenen Satz aus entsprechend der physikalischen Erkenntnis

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

\[
\begin{align*}
A^{n+} + B & \quad \rightarrow \quad A^{n+} + B^* \\
A^{n-} + (n-1)^+ + B^+ & \\
A^* (n-m)^+ + B^* k^+ + (k-m) e^- &
\end{align*}
\]
Reactions of relativistic projectiles in extreme dynamical fields

\[
\gamma = \frac{1}{\sqrt{1 - \beta^2}}
\]

\[U^{92+}\]

\[t \leq 0.1 \text{ as } I \approx 10^{21} \text{ W/cm}^2\]

intense fields
ultra-short electromagnetic pulses
pair production
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.

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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

* Z = 92
* Z = 1

$g = 1$

$g = 5$
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/cm²), 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 $\langle J, |j \parallel D \parallel J'\rangle$

$$\psi_\alpha(PJM) = \sum_{r}^{n_c} c_r(\alpha) |\gamma_r PJM\rangle$$

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
Spontaneous pair creation
Charged vacuum
Heavy ion collisions

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

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 $\hat{\vec{R}}$ 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 $R_{cr} = 37$ fm (point nuclei, unscreened)
$R_{cr} = 26$ fm (extended nuclei, HFS screening)