Department of Physics
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Non-perturbative relativistic calculation of electronic quantum dynamics in low-energy ion-atom collisions

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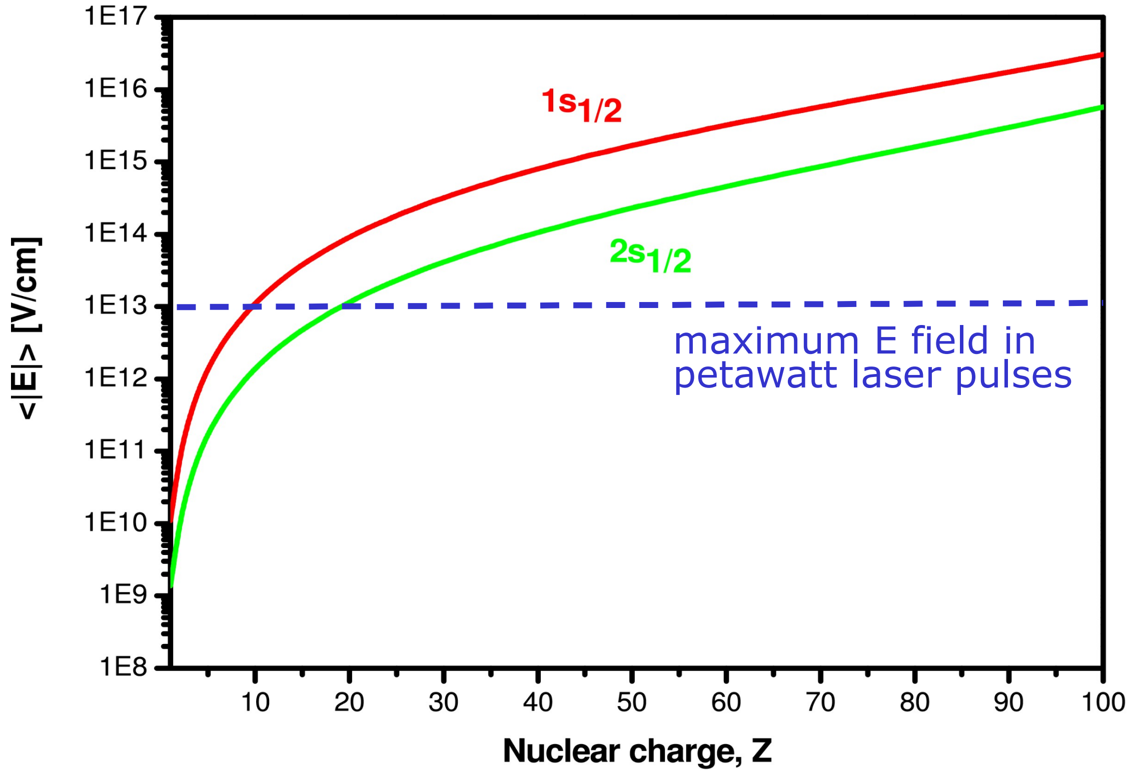
Outline

- Intoduction and Motivation
- Theoretical Description and Numerical Results
  - One-electron case
  - Many-electron case
- Summary and Outlook

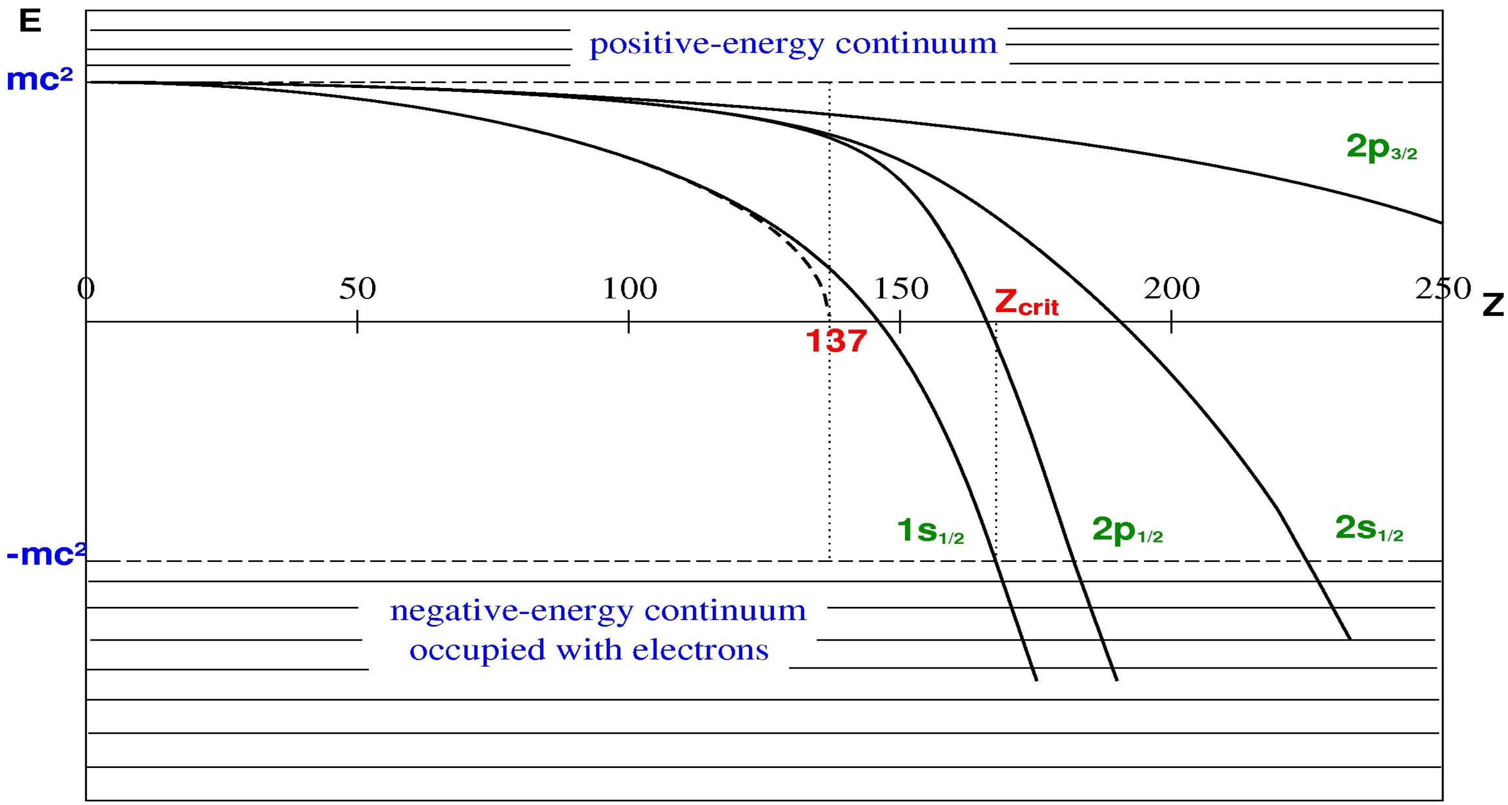
Introduction

Heavy few-electron ions provides possibility to test of QED at extremely strong electromagnetic fields



Introduction

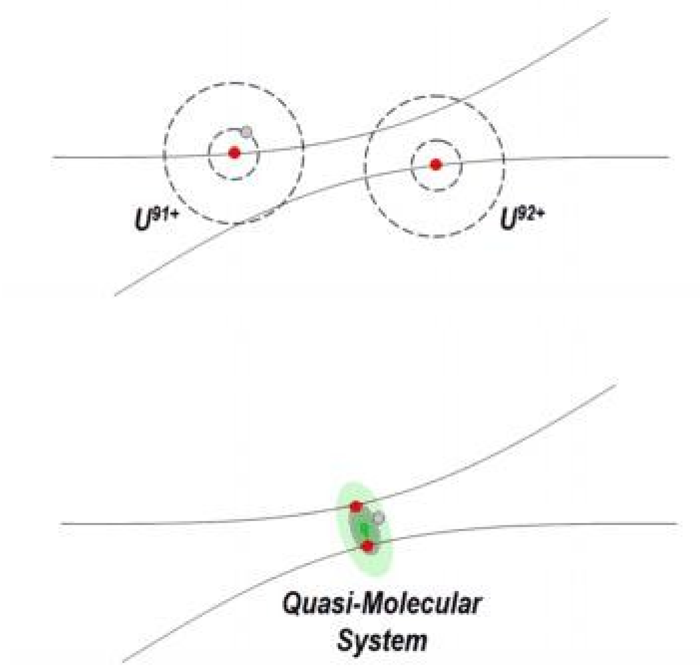
Point nucleus: $E_{1s} = mc^2\sqrt{1-(\alpha Z)^2}.$

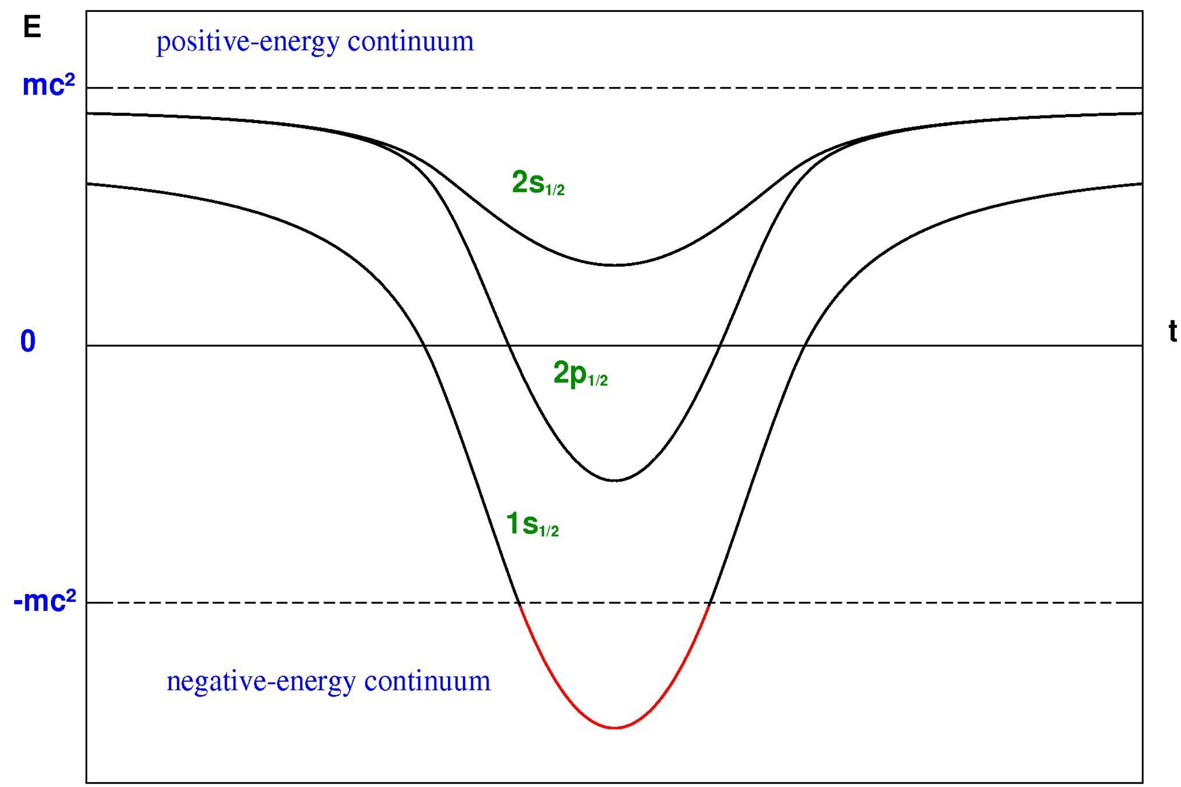


The 1s level dives into the negative-energy continuum at Z_{crit} ~173 *[S.S. Gershtein, Ya.B. Zeldovich, 1969; W. Pieper, W. Greiner, 1969]*.

Introduction: super-heavy quasi-molecules

Super-critical field could be achieved in collision of two heavy ions with $Z_1+Z_2>173$.





Diving time period is about 10^{-21} sec.

Spontaneous e^+e^- pair creation time is about 10^{-19} sec *[Müller et al., 1972]*.

Time-dependent equation

Features of the investigated process:

- Low-energy ions: ~ 6 MeV/u for U
- Relativistic electron: $v_e \sim (\alpha Z)c$
- $m_e \ll M_{nucl} \rightarrow$ Nuclei ($\boldsymbol{R}_A$, $\boldsymbol{R}_B$) move according to the Rutherford trajectory

The time-dependent many-electron two-center Dirac equation (in a.u.):

$$i\frac{d\Psi(x_1,x_2,\ldots,x_N,t)}{dt}=H(x_1,x_2,\ldots,x_N,t)\Psi(x_1,x_2,\ldots,x_N,t),$$

$$H=\sum_i h^{\mathrm{D}}(x_i)+\frac{1}{2}\sum_{i\neq j}V_{e-e}(x_i,x_j),$$

$$h^{\mathrm{D}}=c(\vec{\alpha}\cdot\vec{p})+\beta mc^2+V_{AB}(\vec{r}), \qquad V_{AB}(\vec{r})=V_{\mathrm{nucl}}^{(A)}(\vec{r}_A)+V_{\mathrm{nucl}}^{(B)}(\vec{r}_B),$$

where $\vec{\alpha},\beta$ are the Dirac matrices, and $\vec{r}_A=\vec{r}-\vec{R}_A$, $\vec{r}_B=\vec{r}-\vec{R}_B$.

One-electron case

The time-dependent one-electron two-center Dirac equations (in a.u.):

$$i\frac{d\psi}{dt}=h^{\mathrm{D}}\psi(\vec{r},t),\qquad h^{\mathrm{D}}=c(\vec{\alpha}\cdot\vec{p})+\beta mc^2+V_{\mathrm{nucl}}^{(A)}(\vec{r}_A)+V_{\mathrm{nucl}}^{(B)}(\vec{r}_B)$$

The coupled-channel approach: $\psi(\vec{r},t)=\sum_i C_i(t)\phi_i(\vec{r})$

$$\begin{cases} i\sum_j S_{ij}\dfrac{dC_j(t)}{dt}=\sum_j (H_{ij}-T_{ij})C_j(t) \\ \lim\limits_{t\to-\infty}\boldsymbol{C}(t)=\boldsymbol{C}^0 \end{cases}$$

$$H_{ij}=\langle\phi_i|h^D|\phi_j\rangle,\quad T_{ij}=i\langle\phi_i|\frac{\partial}{\partial t}|\phi_j\rangle,\quad S_{ij}=\langle\phi_i|\phi_j\rangle.$$

Central field Dirac and Dirac-Sturm orbitals

$\phi_{\alpha,\mu}(\vec{r}-\vec{R}_\alpha(t))$ - the Dirac and Dirac-Sturm orbitals, localized on each ion.

$$\phi_{nkm}(\vec{r},\sigma)=\begin{pmatrix} \frac{P_{nk}(r)}{r}\chi_{km}(\Omega,\sigma) \\ i\frac{Q_{nk}(r)}{r}\chi_{-km}(\Omega,\sigma) \end{pmatrix};$$

$$k=(-1)^{l+j+1/2}(j+1/2)$$

$$j=|k|-1/2,\ \ l=j+\frac{1}{2}\frac{k}{|k|}$$

The Dirac equation in the center field potential *V(r)*

$$\begin{cases} c\left(-\frac{d}{dr}+\frac{k}{r}\right)Q_{nk}(r)+(V(r)+c^2)P_{nk}(r)=\varepsilon_{nk}P_{nk}(r) \\ c\left(\frac{d}{dr}+\frac{k}{r}\right)P_{nk}(r)+(V(r)-c^2)Q_{nk}(r)=\varepsilon_{nk}Q_{nk}(r) \end{cases}$$

The Dirac-Sturm operator $h^S=h^D-\varepsilon_{0,}\quad h^S\phi_j=\lambda_j W(r)\phi_j,$

$W(r)>0,\quad W(r)\to 0$ when $r\to\infty$

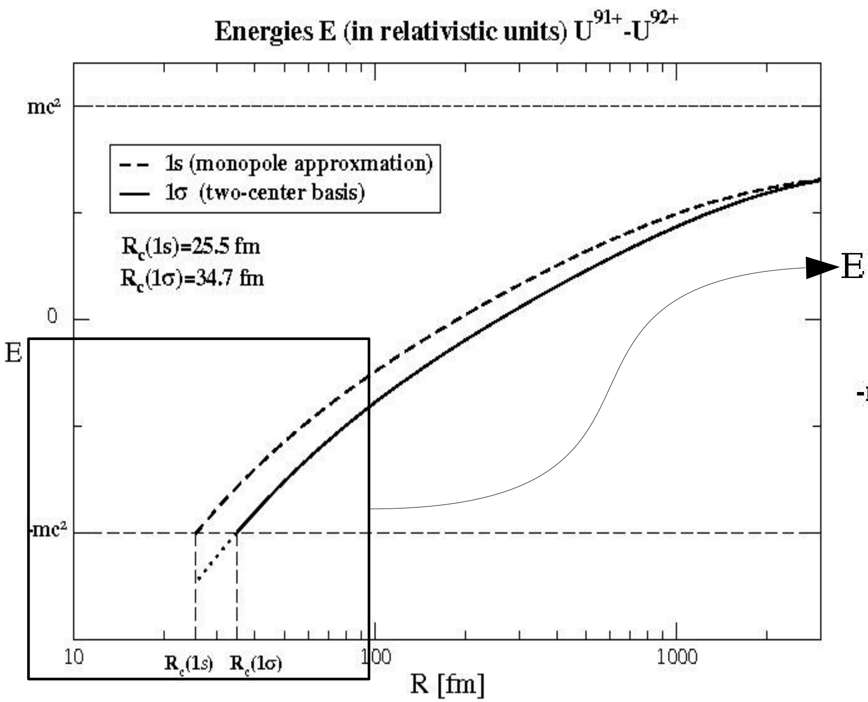
Energies of the $1\sigma_+$ ground state of quasimolecules

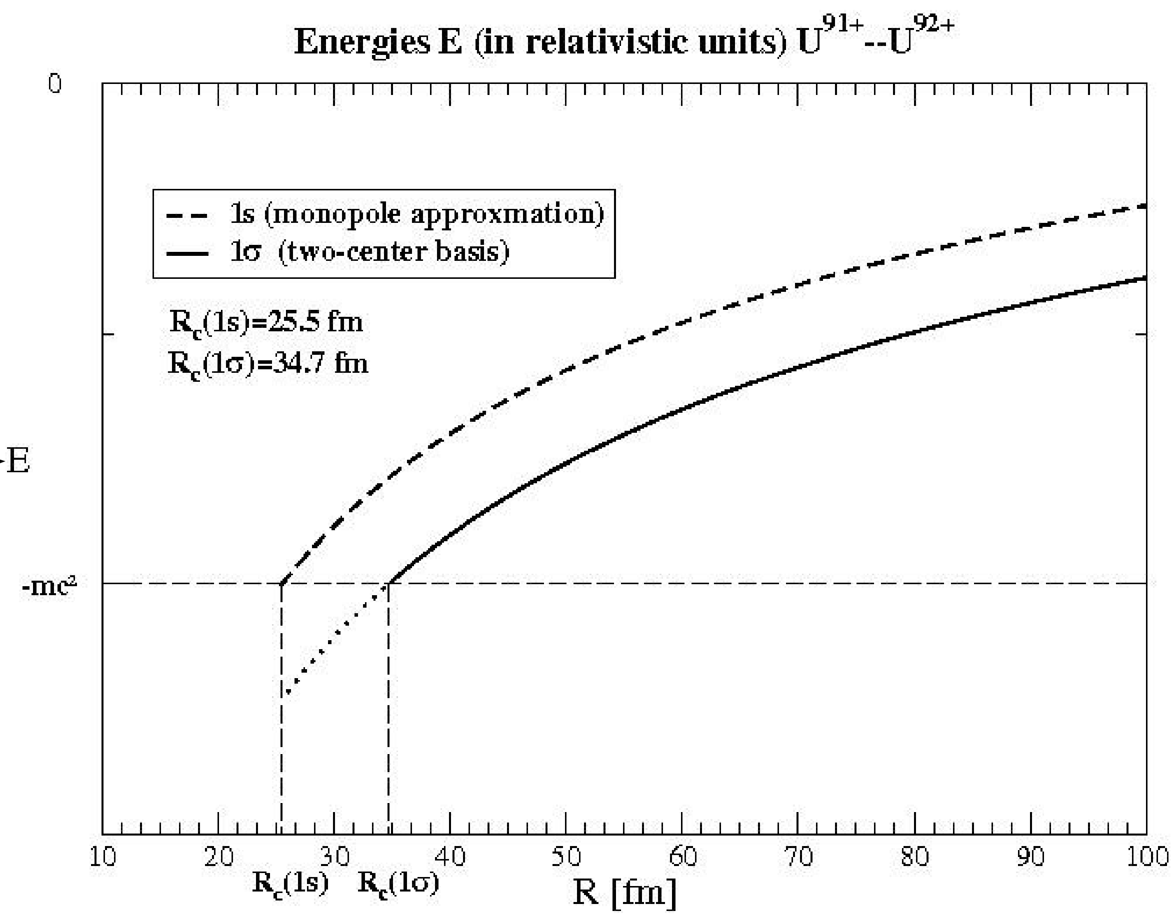
The $1\sigma_+$ state energy of the U_2^{183+} quasimolecule as a function of the internuclear distance R.

$R_{crit}(1s)\ =25.5$ fm

$R_{crit}(1\sigma_+)=34.7$ fm

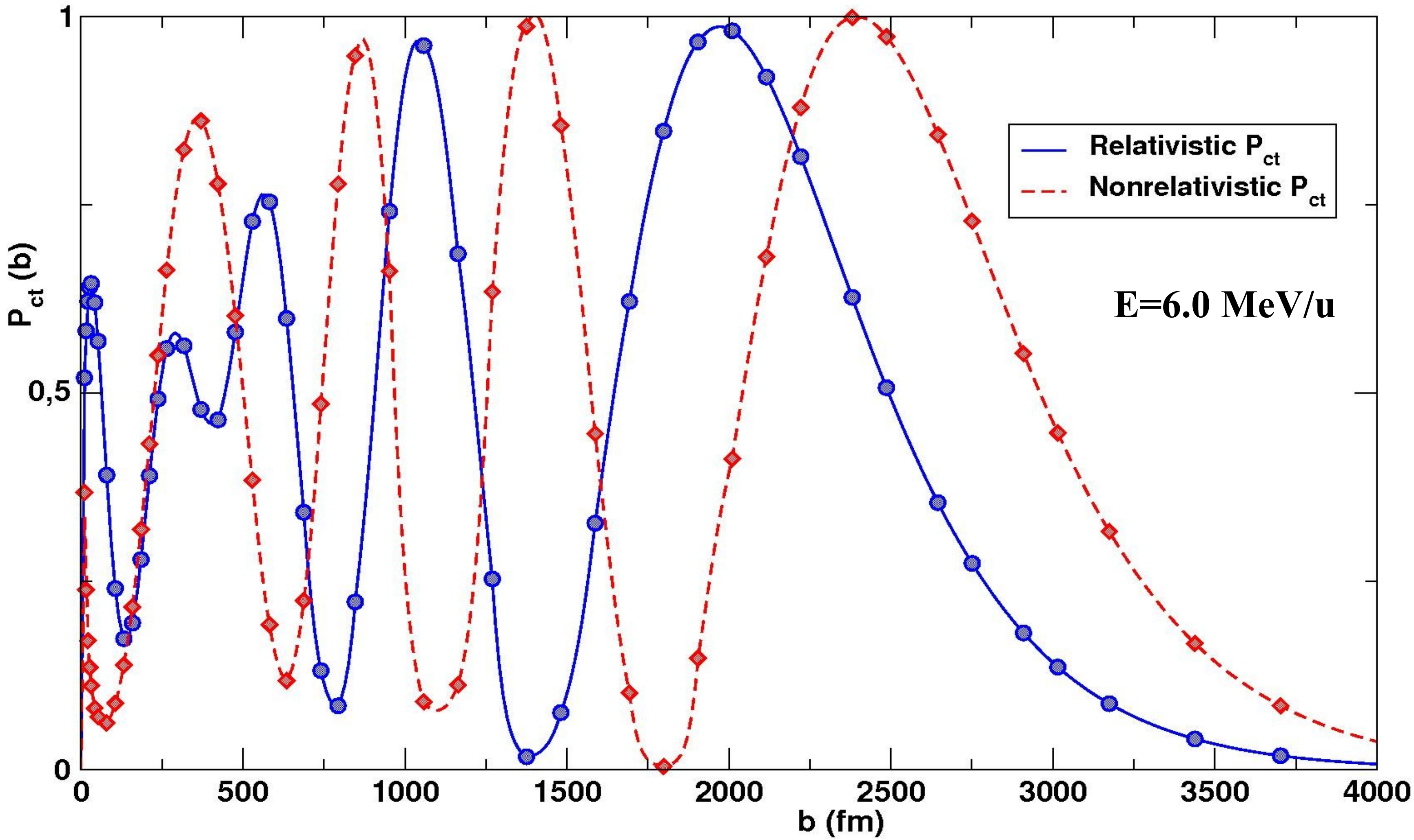
$R_{nucl}\ =\ 5.9$ fm





I.I. Tupitsyn, Y.S. Kozhedub et al., PRA 2010

$U^{91+}(1s)$-U^{92+}



Charge-transfer probability as a function of the impact parameter *b*

Tupitsyn, Kozhedub et al., PRA 2010; Maltsev et al., Phys. Scr. 2013

Many-electron case

$$i\frac{d\Psi(x_1,\ldots,x_N,t)}{dt}=H^{\mathrm{eff}}(x_1,\ldots,x_N,t)\Psi(x_1,\ldots,x_N,t)$$

Independent particle model: $H^{\mathrm{eff}}=\sum_i h_i^{\mathrm{eff}}$

$$\begin{cases} i\dfrac{d\psi_i(t)}{dt}=h_i^{\mathrm{eff}}\psi_i(t) \\ \lim\limits_{t\to-\infty}\left(\psi_i(t)-\psi_i^0(t)\right)=0 \end{cases}$$

$$\Psi(x_1,\ldots,x_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(x_1) & \cdots & \psi_N(x_1) \\ \vdots & & \vdots \\ \psi_1(x_N) & \cdots & \psi_N(x_N) \end{vmatrix}$$

Dirac-Kohn-Sham Hamiltonian

$$h^{\mathrm{DKS}}=c(\vec{\alpha}\cdot\vec{p})+\beta mc^2+V_{\mathrm{H}}[\rho]+V_{\mathrm{xc}}[\rho]$$

Evaluation of probabilities

$$P_{f_1,\dots,f_N} = \left| \langle \Psi_i(x_1,\dots,x_N,t=\infty) | \Psi_f(x_1,\dots,x_N) \rangle \right|^2$$

$$P_{f_1,\dots,f_q} = \sum_{f_{q+1}<\dots<f_N} P_{f_1,\dots,f_N} \qquad q<N$$

$$P_{f_1,\dots,f_q} = \det(\gamma_{nn'}) \quad n,n'=1,\dots,q \quad q<N$$ (Inclusive probability)

$$\gamma_{nn'} = \langle f_n | \rho | f_{n'} \rangle$$

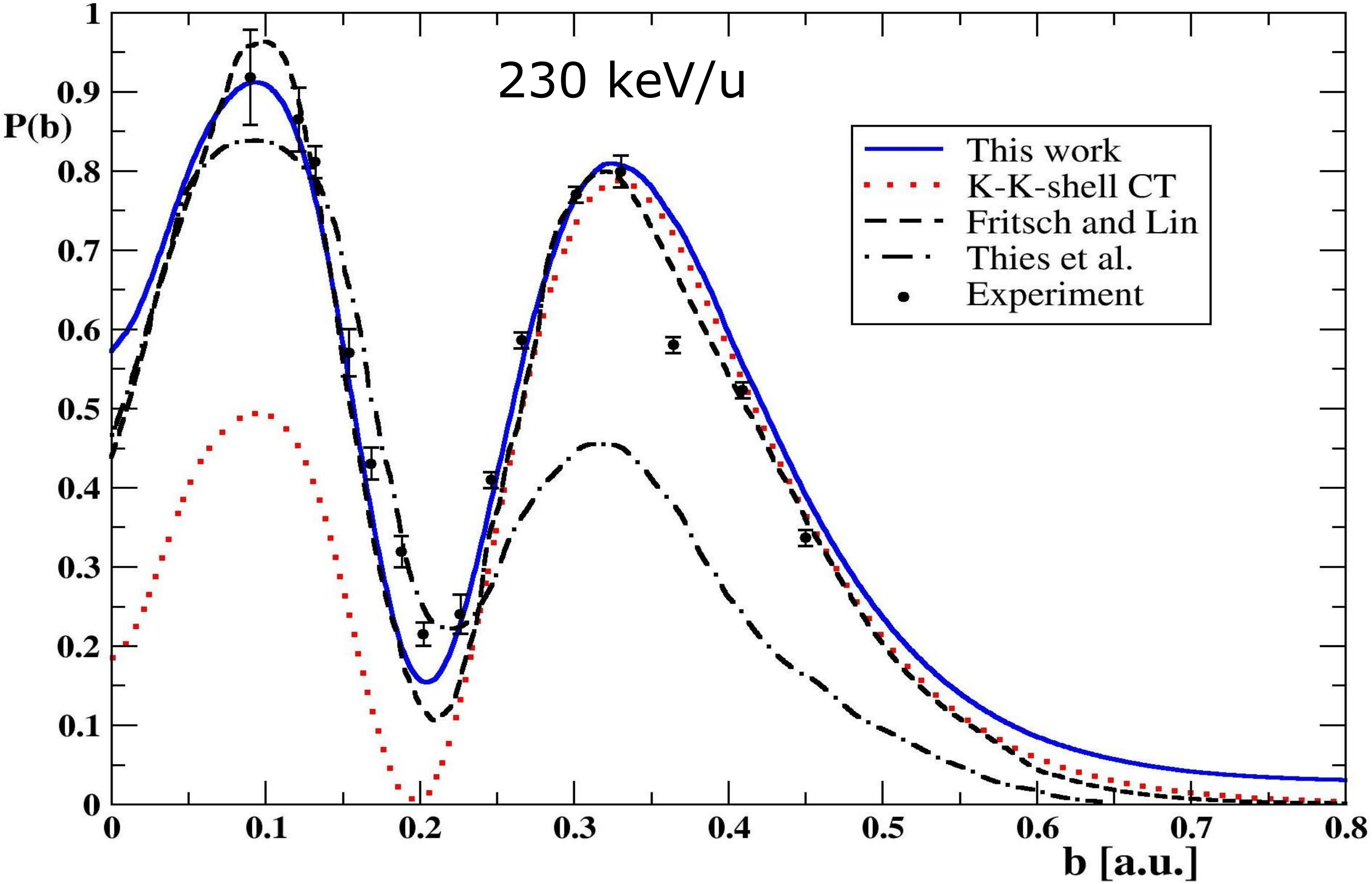
$$\rho(x,x') = \sum_i^N \left| \psi_i(x,t=\infty) \right\rangle \left\langle \psi_i(x',t=\infty) \right|$$

$$P_{f_1,\dots,f_q}^{f_{q+1},\dots,f_L} = P_{f_1,\dots,f_q} - \sum_{f_{q+1}} P_{f_1,\dots,f_q,f_{q+1}} + \sum_{f_{q+1}<f_{q+2}} P_{f_1,\dots,f_q,f_{q+1},f_{q+2}} + \dots$$

$$\dots + (-1)^{L-q} P_{f_1,\dots,f_q,f_{q+1},\dots,f_L}$$

H. J. Lüdde and R. M. Dreizler, JPB, 1985
P. Kürpick and H. J. Lüdde, Comp Phys. Comm., 1993

$Ne(1s^2 2s^2 2p^6)$-$F^{8+}(1s)$

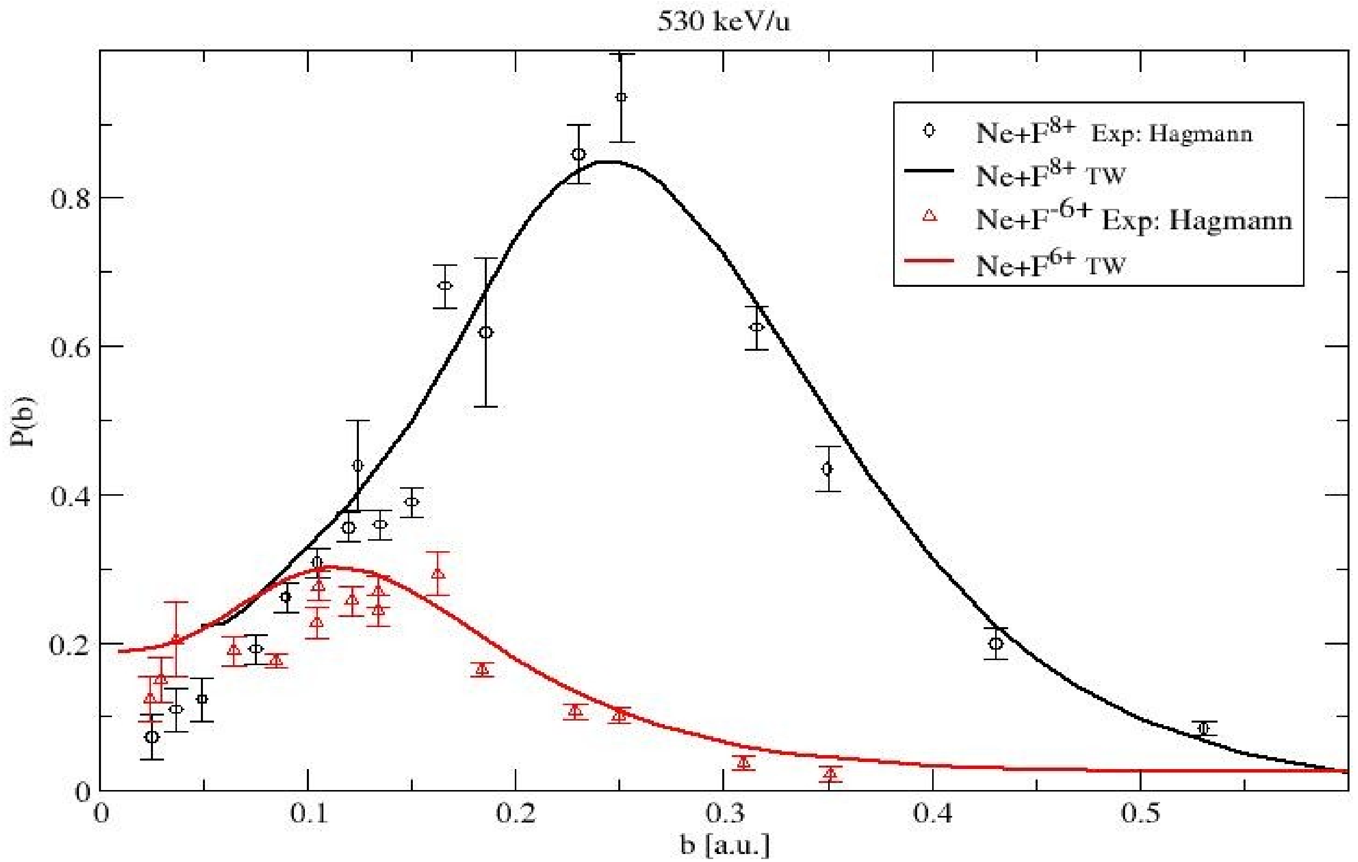


The probability of Ne K-shell-vacancy production as a function of the impact parameter *b*

Experiment: S. Hagmann et al., PRA 1982; 1986; 1987

I.I. Tupitsyn, Y.S. Kozhedub et al., PRA 2012

Ne($1s^2 2s^2 2p^6$)–F^{8+}($1s$); -F^{6+}($1s^2 2s$)



The probability of Ne K-shell-vacancy production as a function of the impact parameter *b*

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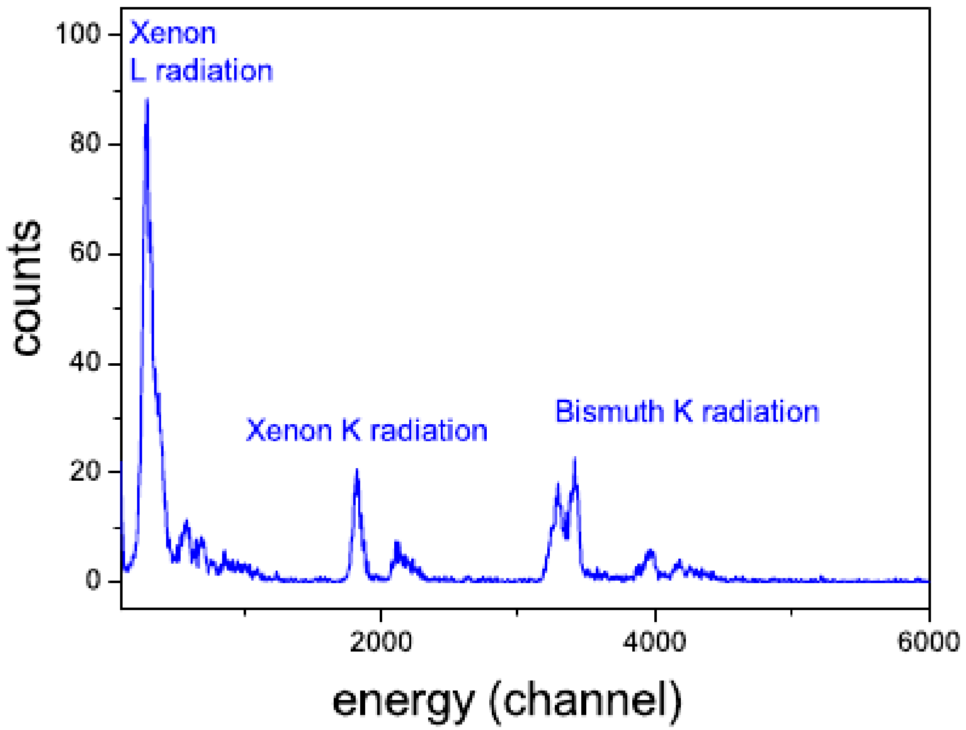
Y.S. Kozhedub et al., Phys. Scr. 2013

Xe-Bi^{83+} 70 MeV/u: the x-ray emission

X-ray emission following the Xe-Bi^{83+} collisions. [A. Gumberidze *et al*, GSI Scientific Report (2011)]



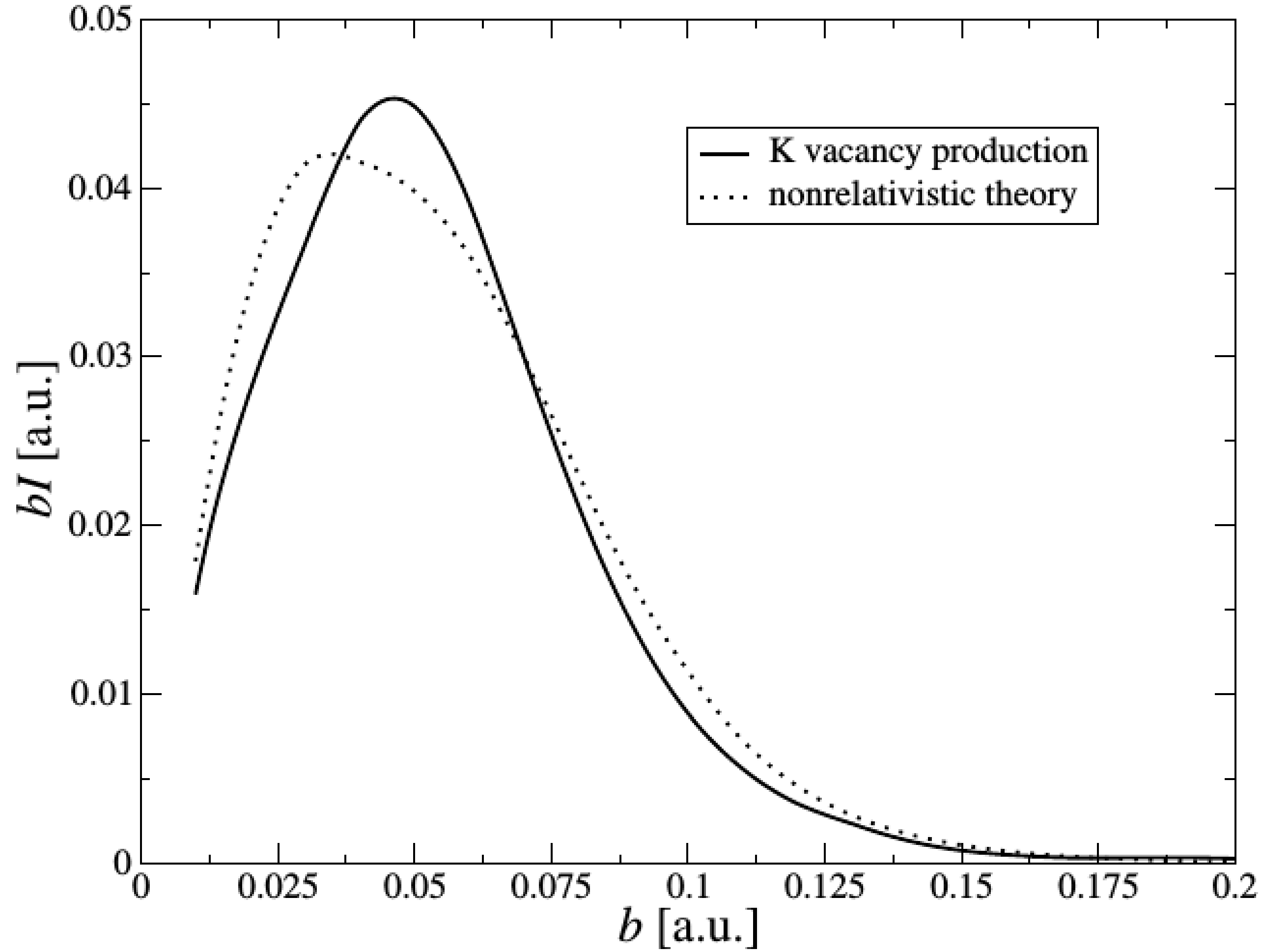
- Looking for states *f* of the ions which can de-excite via the considered x-ray emission
- Calculating the probabilities P_f to find the system in the states *f* after the collision
- Determination the radiative de-excitation probabilities with *m* emitted x-ray photons for the states *f* under consideration $P_m^{\mathrm{rad}}(f)$
- Evaluation the "relative" x-ray radiation intensities (the number of the emitted photons per collision) as $I = \sum_{f,m} m P_m^{\mathrm{rad}}(f) P_f$

Xe-Bi^{83+} 70 MeV/u: (Xe, K) radiation

P_1 and P_2 are the probabilities to find one and two K-shell vacancies.

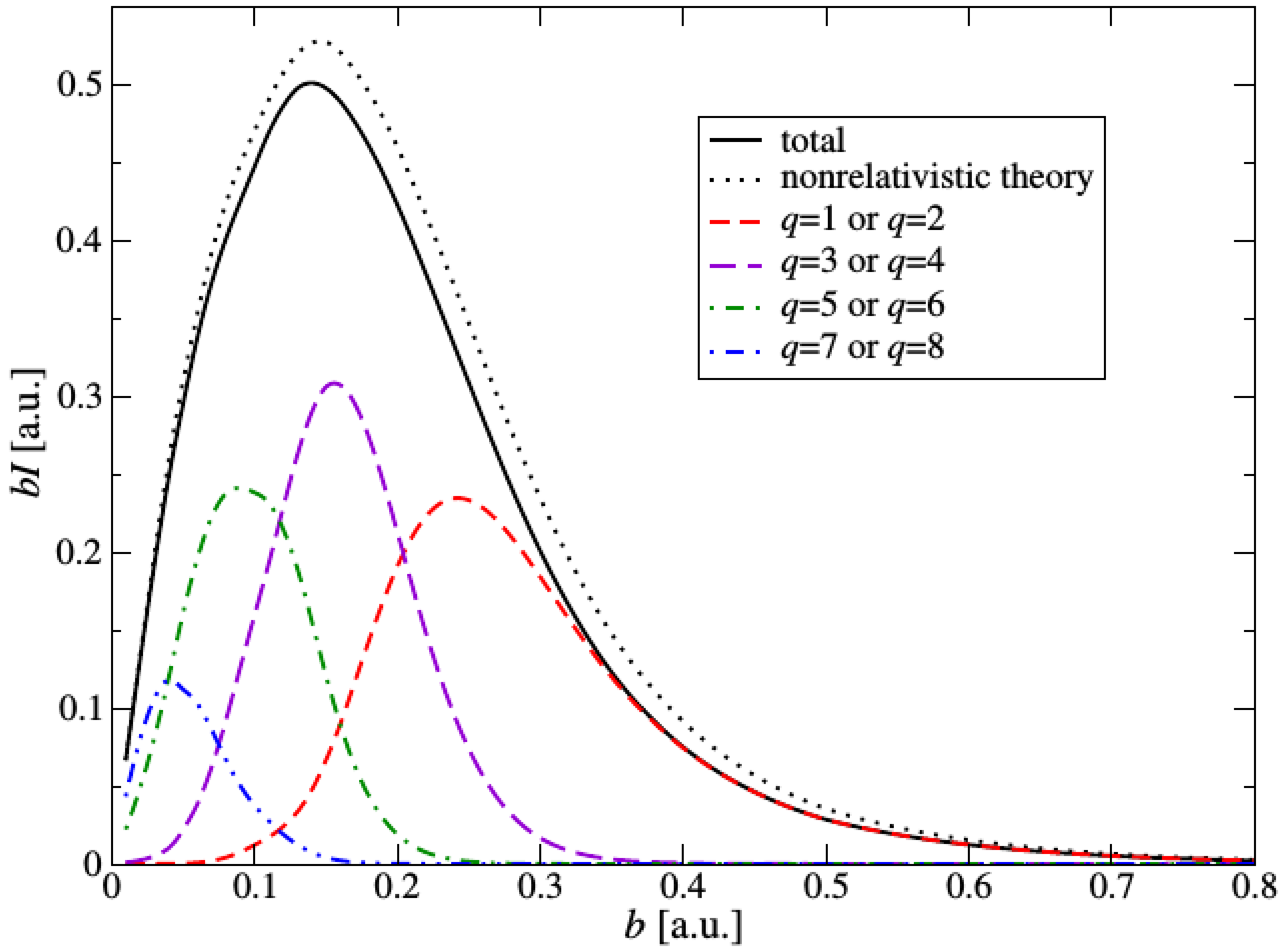
$P^{\text{rad}}(\text{K})$ is the fluorescence yield coefficient for the xenon K shell.

$$I_{\text{K}} = P^{\text{rad}}(\text{K})(P_1 + 2P_2)$$



The intensity I of the Xe K-shell-vacancy production weighted by the impact parameter b.

Xe-Bi^{83+} 70 MeV/u: (Xe, L) radiation



The total- and q-intensities I of the Xe L-shell-vacancy production weighted by the impact parameter b.

Kozhedub *et. al.*, PRA (2014)

Xe-Bi^{83+} 70 MeV/u

Cross sections σ (10^{-14} cm^2) of the x-ray radiation processes.

Process	(Xe, K)	(Xe, L)	(Bi, K_{α_1}) $(2p_{3/2}$-$1s)$	(Bi, K'_{α_2}) $(2p_{1/2}$-$1s)$	(Bi, K''_{α_2}) $(2s$-$1s)$
σ of the x-ray radiation	47(3)	200(25)	20(6)	13(4)	26(10)
Nonrelativistic theory	50	218	31	20	24

Relative intensities of the x-ray radiation.

	(Xe, L)/(Xe, K)	(Bi, K_{α_1})/(Xe, K)	(Bi, K_{α_2})/(Xe, K)
Theory	4.2(6)	0.43(14)	0.83(30)
Experiment	3.6(2)	0.59(3)	0.69(3)

Theory: Kozhedub *et. al.*, PRA (2014)
Experiment: Gumberidze *et. al.*, GSI SR (2011)

Summary

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- A new method employing the Dirac-Sturm (Dirac-Fock-Sturm) basis functions for evaluation of electronic quantum dynamics in low-energy heavy-ion collisions has been developed
- Systematic calculations of inner-shell atomic processes in low-energy ion-atom collisions have been carried out
- Relativistic and many-particle effects have been studied

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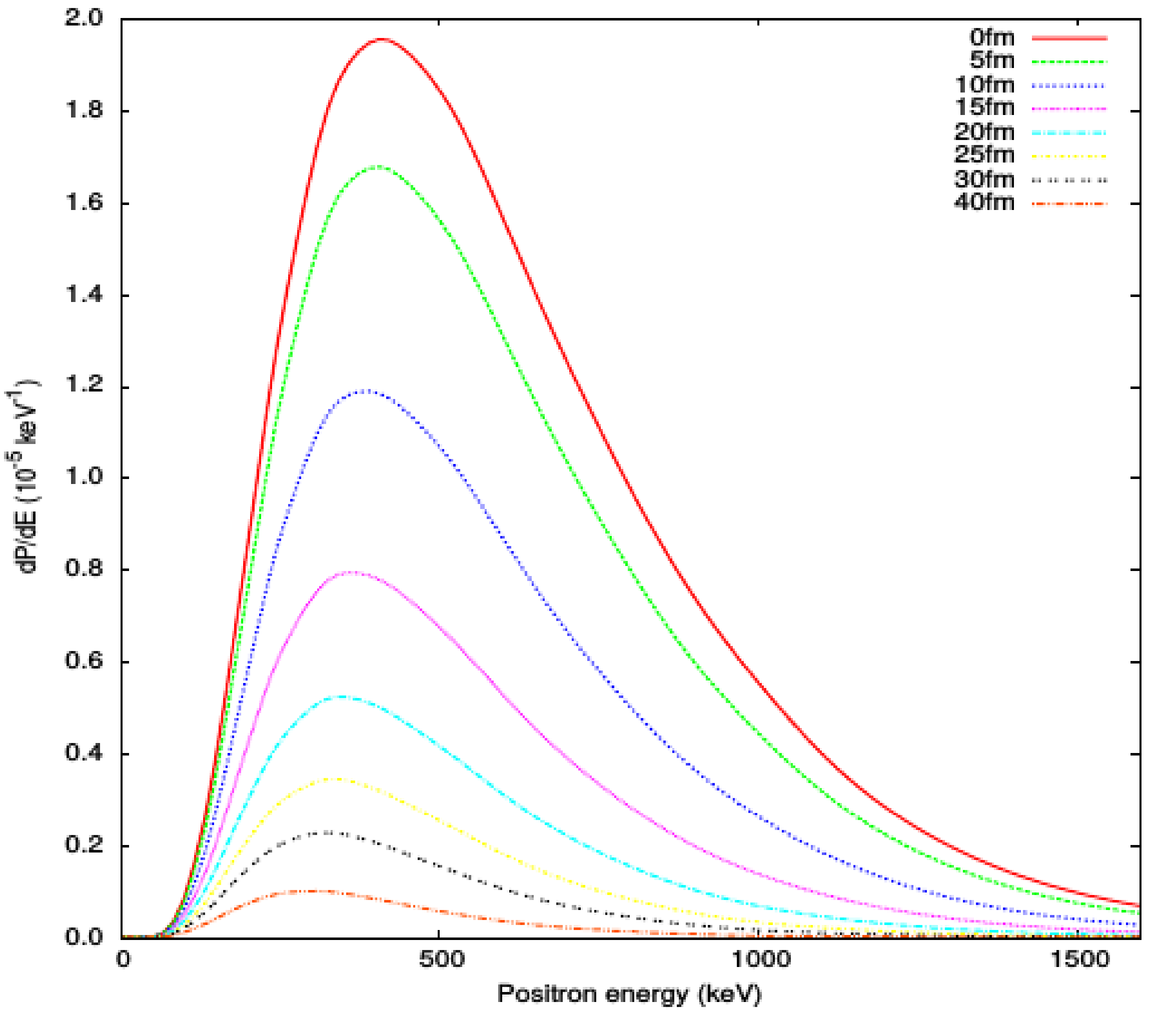
- A new method employing the Dirac-Sturm (Dirac-Fock-Sturm) basis functions for evaluation of electronic quantum dynamics in low-energy heavy-ion collisions has been developed
- Systematic calculations of inner-shell atomic processes in low-energy ion-atom collisions have been carried out
- Relativistic and many-particle effects have been studied

Thank you!

Summary and Outlook

Electron-positron pair production in low-energy U-U collisions



Central field Dirac orbitals

Center field Dirac bispinors: $\phi_{\alpha,\mu}(\vec{r}-\vec{R}_\alpha(t))$

$$\phi_{nkm}(\vec{r},\sigma)=\begin{pmatrix} \dfrac{P_{nk}(r)}{r}\chi_{km}(\Omega,\sigma) \\ i\dfrac{Q_{nk}(r)}{r}\chi_{-km}(\Omega,\sigma) \end{pmatrix};$$

$$k=(-1)^{l+j+1/2}(j+1/2)$$

$$j=|k|-1/2,\ \ l=j+\frac{1}{2}\frac{k}{|k|}$$

where P_{nk} and Q_{nk} are the large and small components, respectively.

The large and small radial components are obtained by solving numerically the Dirac equation in the center field potential *V(r)*

$$\begin{cases} c\left(-\dfrac{d}{dr}+\dfrac{k}{r}\right)Q_{nk}(r)+(V(r)+c^2)P_{nk}(r)=\varepsilon_{nk}P_{nk}(r) \\ c\left(\dfrac{d}{dr}+\dfrac{k}{r}\right)P_{nk}(r)+(V(r)-c^2)Q_{nk}(r)=\varepsilon_{nk}Q_{nk}(r) \end{cases}$$

Monopole approximation

Monopole approximation enables partly accounting for the potential of the second ion in constructing the basis functions. For example, the potential of the center A is given by

$$V^{(A)}(r) = V^{(A)}_{nucl}(r) + V^{(B)}_{mon}(r),$$

where (for the point nucleus case)

$$V^{(B)}_{mon}(r) = -\frac{1}{4\pi}\int d\Omega \frac{Z_B}{|\vec{r}-\vec{R}_{AB}|} = \begin{cases} -\dfrac{Z_B}{r} & r \geq R_{AB} \\ -\dfrac{Z_B}{R_{AB}} & r < R_{AB} \end{cases}$$

Central field Dirac-Sturm orbitals

Dirac orbitals

- The set of the Dirac wave functions of the discrete spectrum without the continuum spectrum does not form a complete basis set
- The contribution of the continuum spectrum may be more than 50%
- The radius of the Dirac orbitals rapidly increases with increasing the principal quantum number *n*

Dirac-Sturm orbitals

$$h^S = h^D - \varepsilon_{0,} \quad h^S \phi_j = \lambda_j W(r) \phi_j,$$

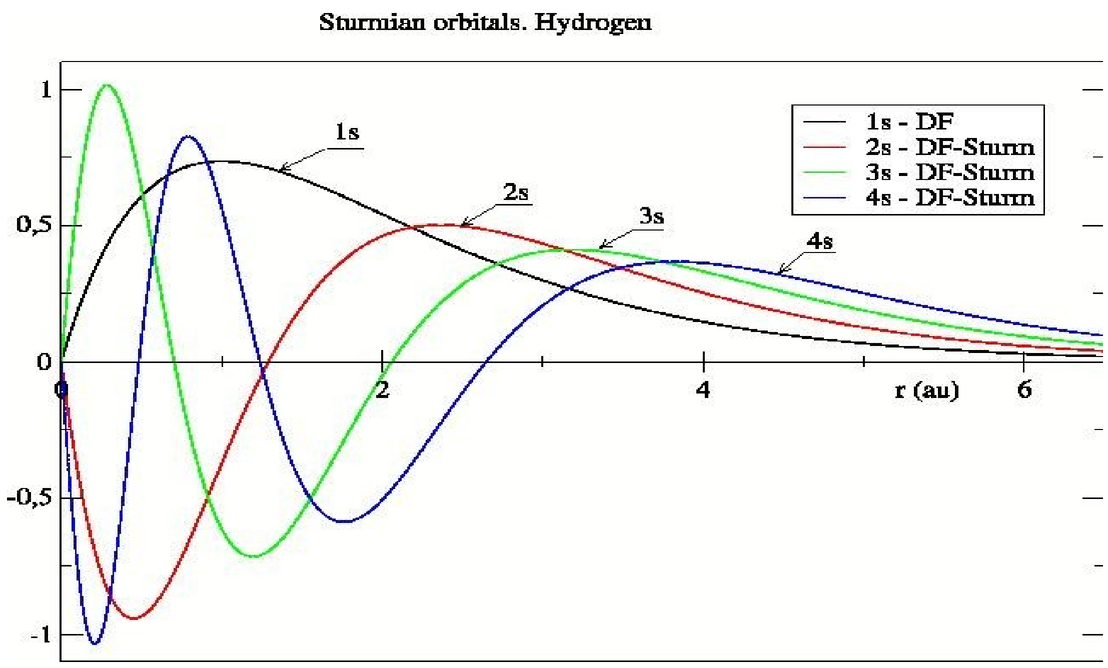
$$\begin{cases} c\left(-\dfrac{d}{dr}+\dfrac{k}{r}\right)\bar{Q}_{nk}(r)+\left(V(r)+c^2-\varepsilon_{n_0 k}\right)\bar{P}_{nk}(r)=\lambda_{nk}W(r)\bar{P}_{nk}(r) \\ c\left(\dfrac{d}{dr}+\dfrac{k}{r}\right)\bar{P}_{nk}(r)+\left(V(r)-c^2-\varepsilon_{n_0 k}\right)\bar{Q}_{nk}(r)=\lambda_{nk}W(r)\bar{Q}_{nk}(r) \end{cases}$$

$W(r)>0, \quad W(r)\to 0$ when $r\to\infty;$

$$W(r)=\left[\frac{1-\exp(-(\alpha r)^2)}{(\alpha r)^2}\right].$$

Central field Dirac-Sturm orbitals

- The Dirac-Sturm operator does not have continuum spectrum
- The set of the Dirac-Sturm orbitals forms a complete basis set
- The Dirac-Sturm orbitals have the correct asymptotic behavior for $r \to 0$ and for $r \to \infty$
- All Dirac-Sturm orbitals have approximately the same size, which does not depend on the principal quantum number n



Basis set properties

- Spectrum of the Dirac-Sturm operator is discrete and complete (including functions of the negative Dirac spectrum)
- DSO have correct asymptotic behavior when $r \to 0$ and $r \to \infty$
- All DSO have approximately the same space scale, which does not depend on the principal quantum number n
- Monopole approximation enables partly accounting for the potential of the second ion in constructing of the basis functions

- Posseses fast basis convergence, that significantly reduces the size of matrix problem and calculation time
- Provides the natural satisfaction of the initial conditions
- Allows one to evaluate the ionization processes
- Is perfect for describing the quasi-molecular states at small inter-nuclear distance. This is especially important for investigation of the diving effect

Dirac-Kohn-Sham equation

Dirac-Kohn-Sham equation $$i\frac{d\psi}{dt}=h^{\mathrm{DKS}}\psi(\vec{r},t)$$

$$h^{\mathrm{DKS}}=c(\vec{\alpha}\cdot\vec{p})+\beta mc^2+V_{AB}(\vec{r})$$

$$V_{AB}(\vec{r})=V_{\mathrm{H}}[\rho]+V_{\mathrm{xc}}[\rho]$$

$$V_{\mathrm{H}}[\rho]=V_{\mathrm{nucl}}^{A}(\vec{r}_A)+V_{\mathrm{nucl}}^{B}(\vec{r}_B)+V_{\mathrm{C}}[\rho]$$

$$V_{\mathrm{nucl}}(\vec{r})=\int d^3\vec{r}\,'\frac{\rho_{\mathrm{nucl}}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\qquad V_{\mathrm{C}}[\rho]=\int d^3\vec{r}\,'\frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}$$

$V_{\mathrm{xc}}[\rho]$ is the exchange-correlation potential
in the Perdew-Zunger parametrization
Perdew and Zunger, PRB 23, 5048 (1981)

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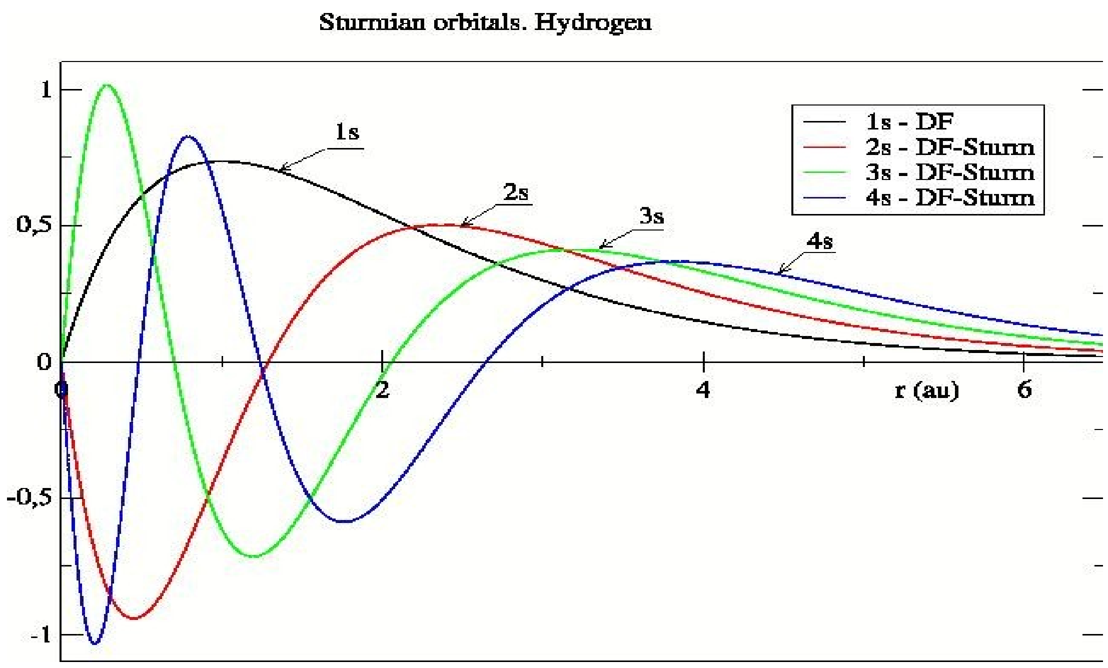

Critical Distances

Critical Distances R_c (fm)

	Point nucleus		Extended nucleus	
Z	This work	Others	This work	Others
88	24.27	24.24[a]	19.91	19.4[d]
90	30.96	30.96[a]	27.06	26.5[d]
92	38.43	38.4[b]	34.74	34.7[b]
		38.42[a]		34.3[d]
		36.8[c]		34.7[f]
94	46.58	46.57[a]	43.13	42.6[d]
96	55.38	55.37[a]	52.10	
98	64.79	64.79[a]	61.61	61.0[d]
				61.1[f]

[a]*V. Lisin et al., PRL 1977*

[b]*A. Artemyev et al., JPB 2010*

[c]*J. Rafelski and B. Müller, PL 1976*

[d]*V. Lisin et al., PL 1980*

[f]*B. Müller and W. Greiner, ZN 1975*

I.I. Tupitsyn, Y.S. Kozhedub et al., PRA 2010

$U^{91+}(1s)$-U^{92+}

The population probability of the 1s target state P_{1s} one-electron and $\bar{P}_{1s}$ many-electron pictures.

b (fm)	$\bar{P}_{1s}$	$(\bar{P}_{1s} - P_{1s}) \times 10^{-4}$
15	0.550244	8.09
20	0.669606	3.25
30	0.811627	0.61
40	0.886144	0.13
50	0.909947	0.03

G. Deyneka et al., Eur. Phys. J. D 67, 258 (2013)