Department of Physics
St. Petersburg State University

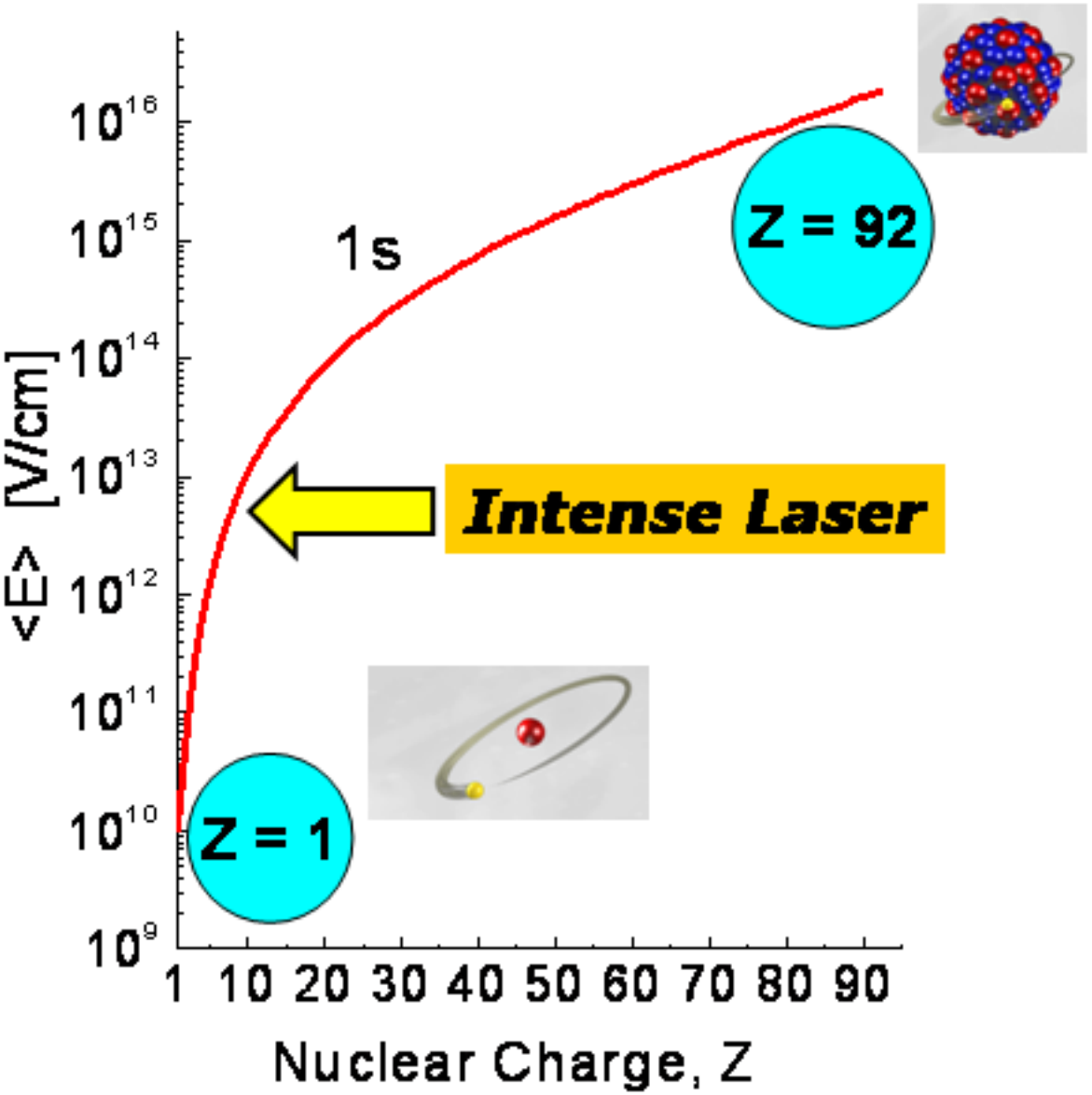
Relativistic Calculation of the Charge-Transfer Probabilities for Low-Energy Collisions of Heavy Ions

Yury Kozhedub

Outline

- Intoduction and Motivation
- Theoretical Description
- Numerical Results
- Summary and Outlook

Introduction



H-like Uranium

$E_K = -132 \cdot 10^3$ eV

$\langle E \rangle = 1.8 \cdot 10^{16}$ V/cm

Hydrogen

$E_K = -13.6$ eV

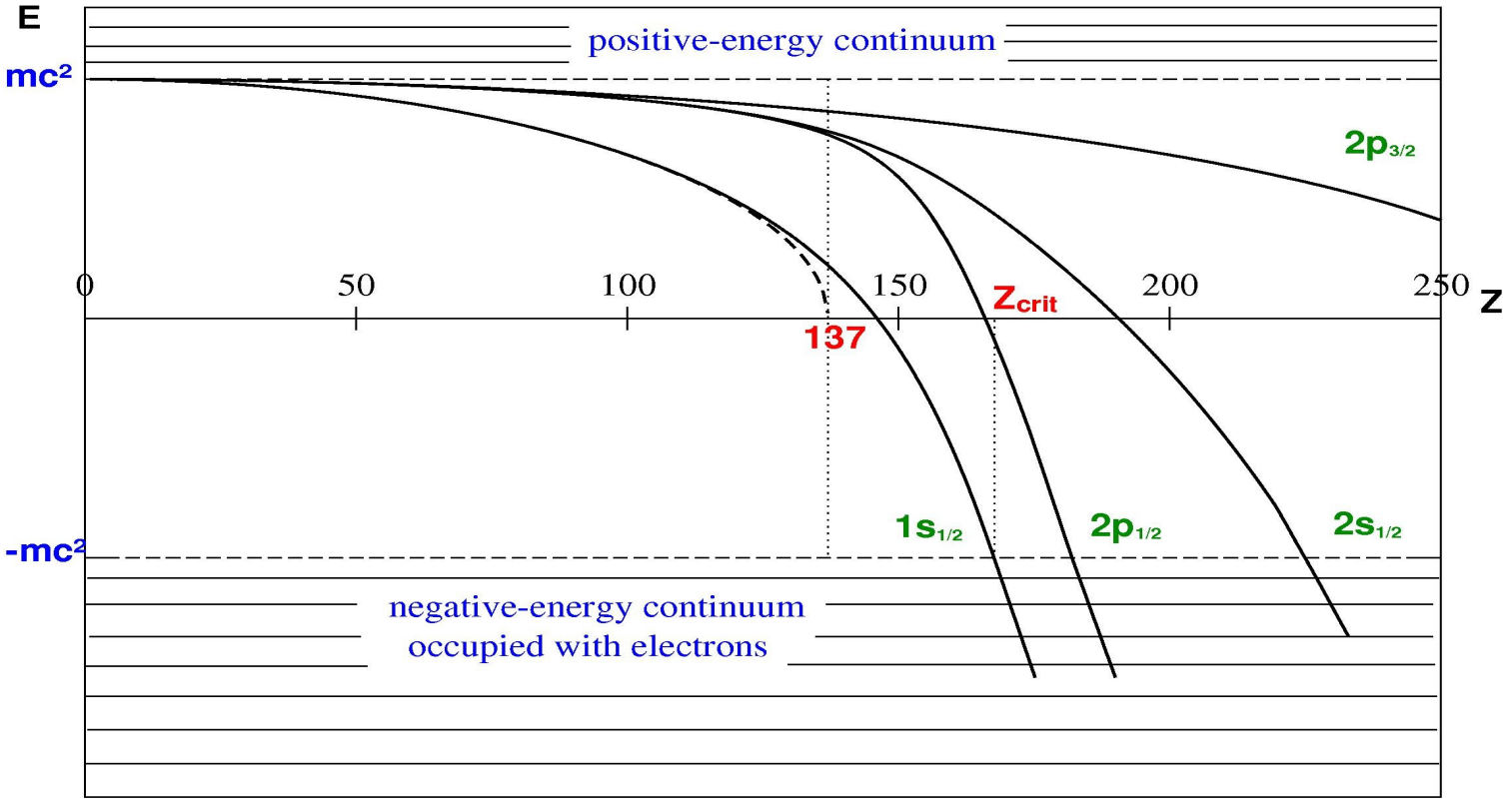
$\langle E \rangle = 1 \cdot 10^{10}$ V/cm

Introduction

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

Existence of point charge with value more then $\alpha Z > 1$ is forbidden

[Gätner et al., 1981].

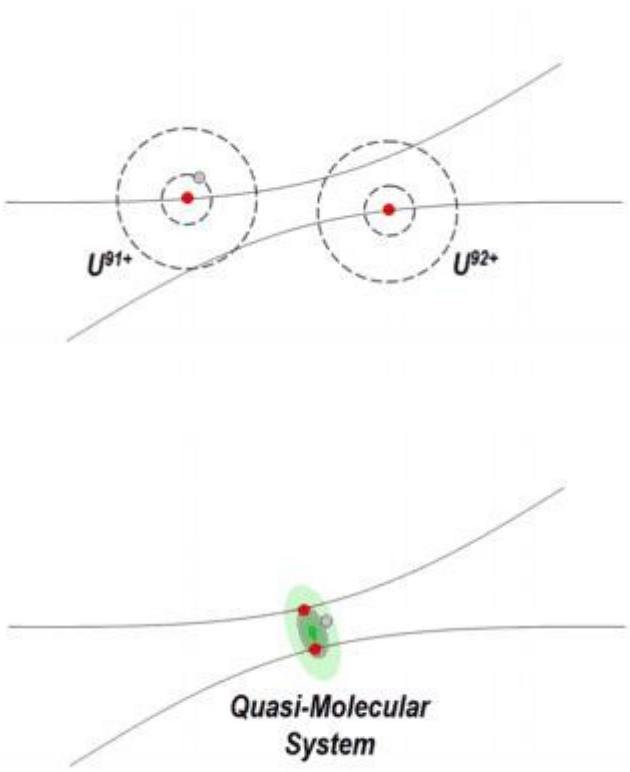


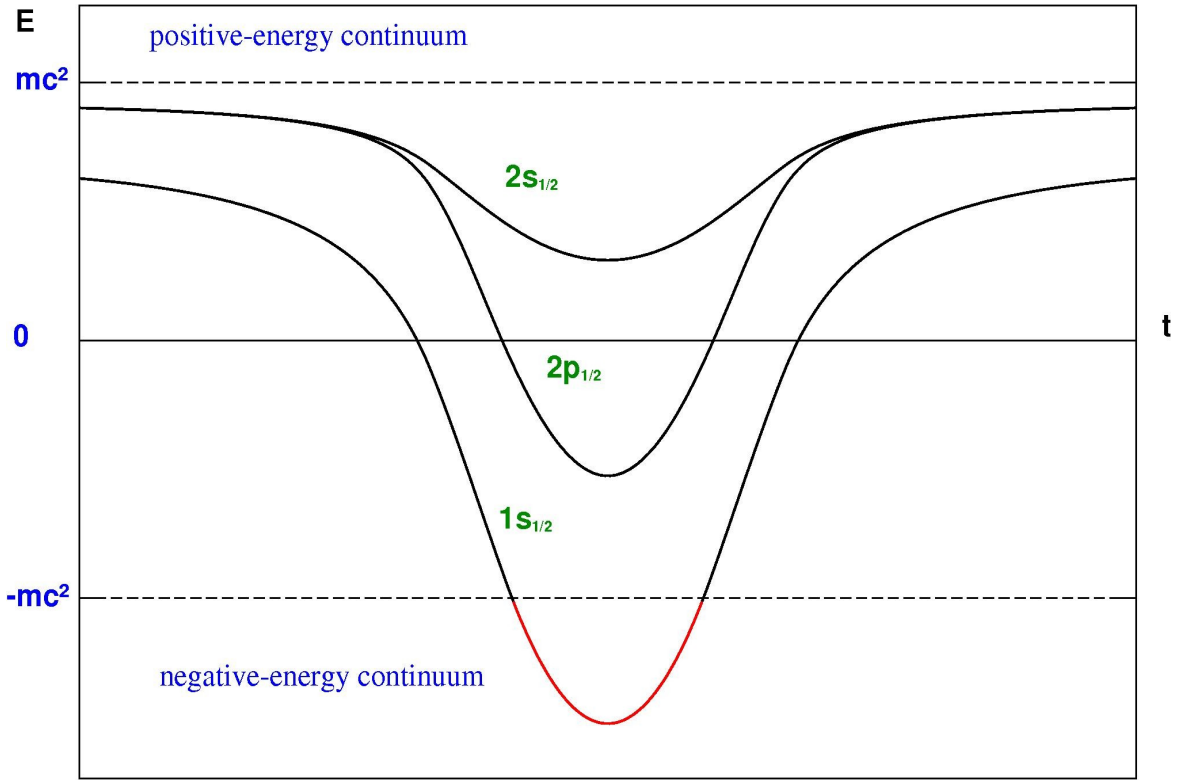
The 1s level dives into the negative-energy continuum at Z_{crit} ~173

[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 $Z_1+Z_2>173$.





Two center Dirac equation

Features of the investigated process:

- Low-energy ions: ~ 6 MeV/u for U^{91+}-U^{92+}
- Relativistic electron: $v_e \sim (\alpha Z)c$
- $m_e \ll M_{nucl}$ → Nuclei ($\boldsymbol{R}_A$, $\boldsymbol{R}_B$) move according to the Rutherford trajectory

The time-dependent and stationary (for fixed R_{AB}) Dirac equations (in a.u.):

$$h^D \Psi(\vec{r},t) = i\frac{d\Psi}{dt}, \qquad h^D \psi_n(\vec{r}) = \varepsilon_n \psi_n(\vec{r}),$$

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

where $\vec{\alpha}, \beta$ are the Dirac matrices, and $V_{AB}(\vec{r}) = V^{(A)}_{nucl}(\vec{r}_A) + V^{(B)}_{nucl}(\vec{r}_B)$,

$$\vec{r}_A = \vec{r} - \vec{R}_A, \quad \vec{r}_B = \vec{r} - \vec{R}_B.$$

Finite Basis Expansion

$$\Psi(\vec{r}) = \sum_i c_i \varphi_i(\vec{r}), \qquad \Psi(\vec{r}, t) = \sum_i C_i(t) \varphi_i(\vec{r}).$$

Stationary case:

$$\sum_j S_{ij} c_j = \sum_j H_{ij} c_j$$

Time-dependent case:

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

where $H_{ij} = \langle \varphi_i | h_D | \varphi_j \rangle$, $T_{ij} = i \langle \varphi_i | \dfrac{\partial}{\partial t} | \varphi_j \rangle$, $S_{ij} = \langle \varphi_i | \varphi_j \rangle$.

$$\Psi(\vec{r}, t) = \sum_{\alpha = A, B} \sum_{\mu} C_{\alpha, \mu}(t) \varphi_{\alpha, \mu}(\vec{r} - \vec{R}_\alpha(t))$$

$\varphi_{\alpha, \mu}$ - the Dirac and Dirac-Sturm orbitals, localized on each ion.

Central field Dirac orbitals

Center field Dirac bispinors:

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

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

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

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 $V(r)$

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

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

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

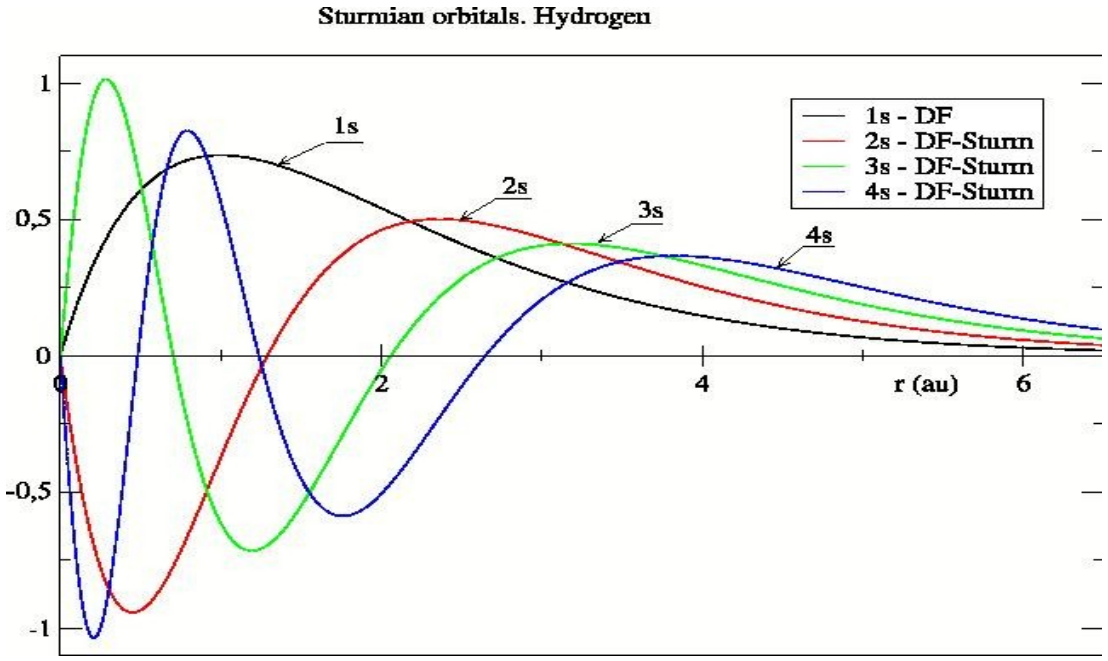
$$\begin{cases} c\left(-\dfrac{d}{dr}+\dfrac{k}{r}\right)\bar{Q}_{nk}(r)+\left(V(r)+c^2-\varepsilon_{n_0 k}\right)\bar{P}_{nk}(r)=\lambda_{nk} W(r)\bar{P}_{nk}(r) \\ c\left(\dfrac{d}{dr}+\dfrac{k}{r}\right)\bar{P}_{nk}(r)+\left(V(r)-c^2-\varepsilon_{n_0 k}\right)\bar{Q}_{nk}(r)=\lambda_{nk} W(r)\bar{Q}_{nk}(r)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

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

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

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



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)

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

Basis set

Basis of DO and DSO, localized on each ion:

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

---

Basis 1:	Positive: 1s-3s, 2p, 3p, 3d, $\overline{4s}$-$\overline{6s}$, $\overline{4p}$-$\overline{6p}$, $\overline{4d}$-$\overline{6d}$, $\overline{4f}$-$\overline{6f}$:	220 functions
	Negative: -$\overline{1s}$-(-$\overline{6s}$), -$\overline{2p}$-(-$\overline{6p}$) … :	220 functions
Basis 2:	Positive: 1s, $\overline{2s}$-$\overline{8s}$, $\overline{2p}$-$\overline{8p}$, $\overline{3d}$-$\overline{8d}$, $\overline{4f}$-$\overline{6f}$, $\overline{5g}$-$\overline{6g}$:	392 functions
	Negative: -$\overline{1s}$-(-$\overline{8s}$), -$\overline{2p}$-(-$\overline{8p}$) … :	392 functions

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

The "chemical" inter-nuclear distance R_{AB} =2.0/Z (a.u.).
Calculations are performed for the Point Nuclear case.

	$H_2^+(Z=1)$		$Th_2^{179+}(Z=90)$	
	Energy	Relative Error	Energy	Relative Error
Basis 1	-1.1026248	$1.5\cdot10^{-5}$	-9504.573	$1.9\cdot10^{-5}$
Basis 2	-1.1026405	$1.0\cdot10^{-6}$	-9504.732	$2.5\cdot10^{-6}$
”Exact”	-1.1026416[a]		-9504.756[b]	

[a] *[L. Yang, D. Heinemann, D. Kolb, Chem. Phys. Lett., 178, 213 (1991)];*
[b] *[O. Kullie, D. Kolb, Eur. Phys. J. D, 17, 167 (2001)]*

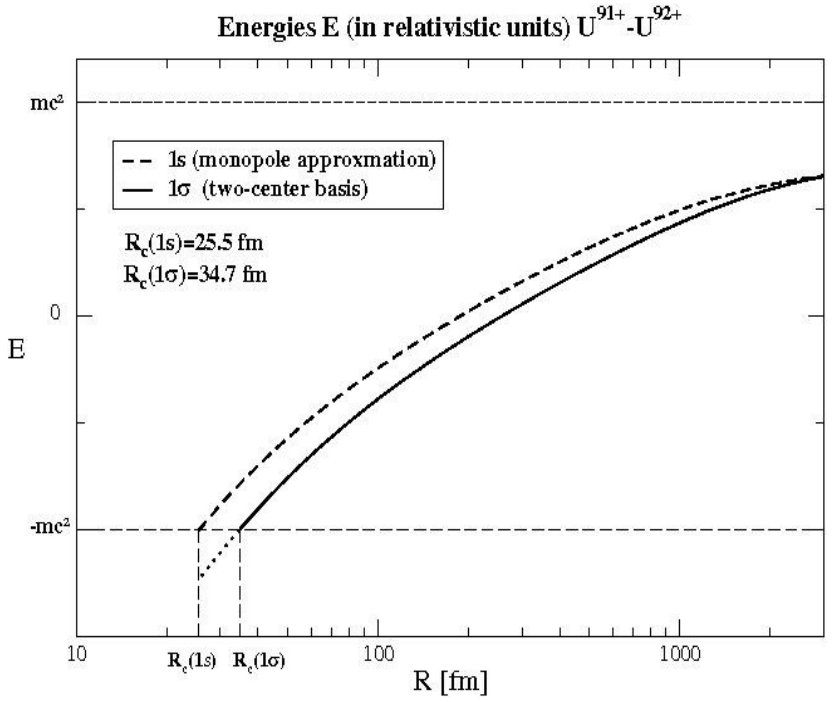
Energies of the $1\sigma_+$ ground state of quasimolecules

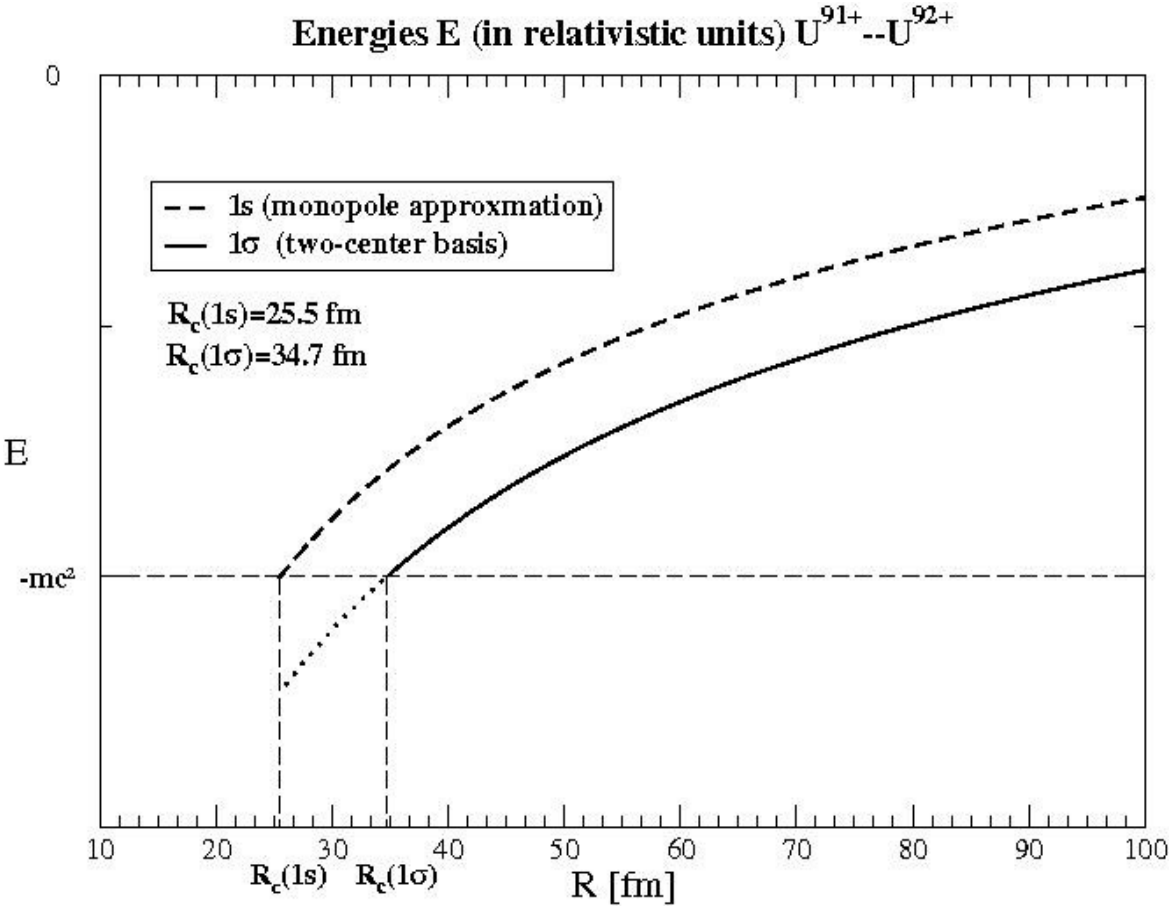
The $1\sigma+$ state energy of the U_2^{183+} quasimolecule as a function of the internuclear distance R.

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

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

$R_{nucl} = 5.9$ fm





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., Phys. Lett. **69B**, 2 (1977)];* [b] *[A. Artemyev et al., J. Phys. B 43, 235207 (2010)]*
[c] *[J. Rafelski, B. Müller, Phys. Lett. **65B**, 205 (1976)];* [d] *[V. Lisin et al., Phys. Lett. **91B**, 20 (1980)]*
[f] *[B. Müller and W. Greiner, Z. Naturforsch. **31a**, 1 (1975)]*

Charge-transfer and Ionization Probabilities

The probabilities of the charge transfer $W_{nk}^{(ct)}$ and direct excitations $W_{nk}^{(d)}$ from the 1s state of nuclear A to the state nκ are given by

$$W_{nk}^{(d)} = \lim_{t\to\infty} \sum_{\mu} |\langle \Psi(\vec{r},t)|\varphi_{nk\mu}(\vec{r}_A,t)\rangle|^2$$
$$W_{nk}^{(ct)} = \lim_{t\to\infty} \sum_{\mu} |\langle \Psi(\vec{r},t)|\varphi_{nk\mu}(\vec{r}_B,t)\rangle|^2$$

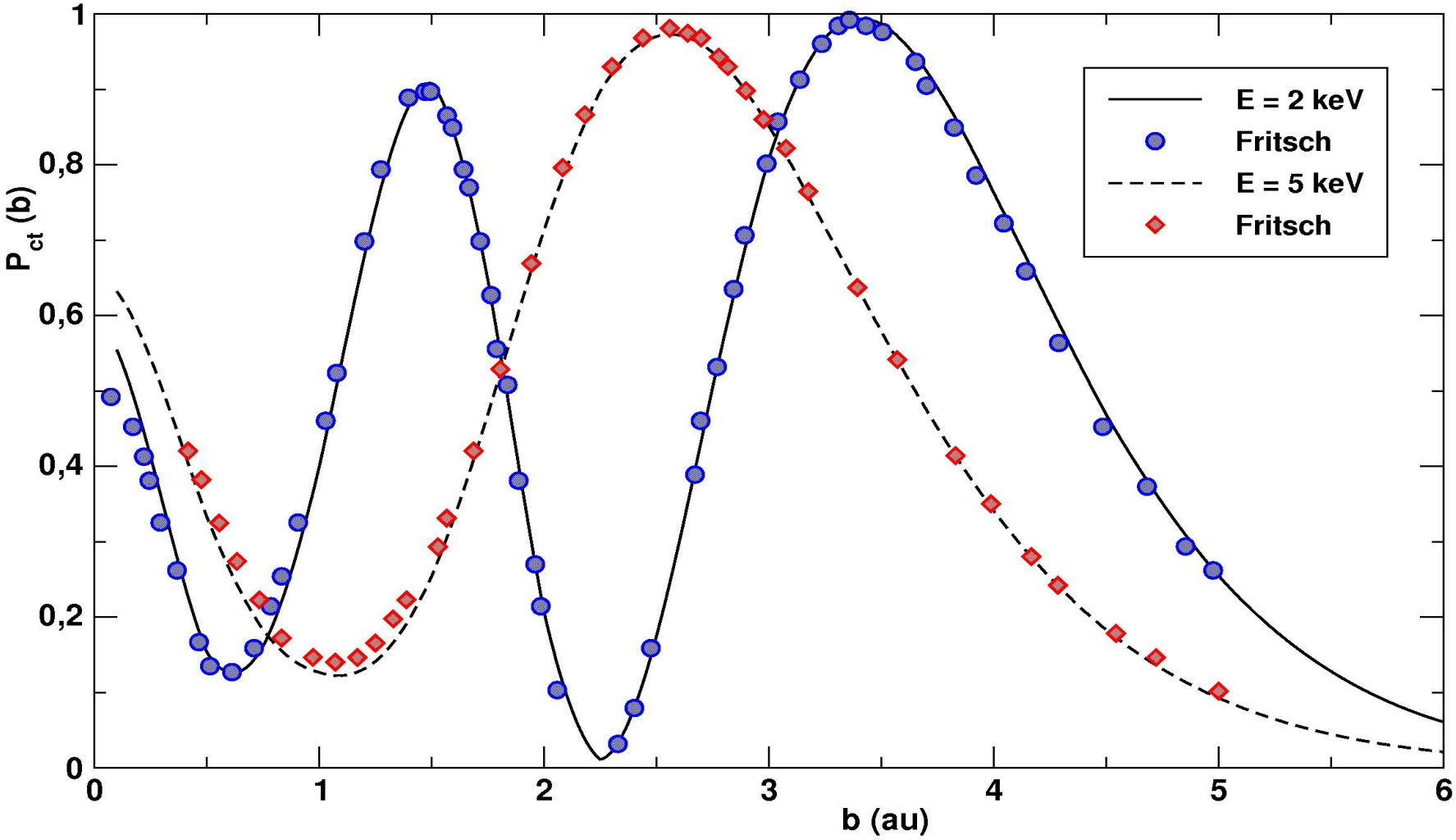
The total direct excitation P_d, charge-transfer P_{ct} and ionization P_{ion} probabilities are defined by

$$P_d = \sum_{nk\neq 1s} W_{nk}^{(d)}, \quad P_{ct} = \sum_{nk} W_{nk}^{(ct)}, \quad P_{ion} = 1 - P_d - P_{ct} - W_{1s}^{(d)}.$$

The cross sections for the charge-transfer and ionization processes are then calculated by integrating the probabilities over the impact parameter b

$$\sigma_{ct} = 2\pi \int_0^\infty db\, b\, P_{ct}(b), \quad \sigma_{ion} = 2\pi \int_0^\infty db\, b\, P_{ion}(b).$$

H(1s)-H$^+$

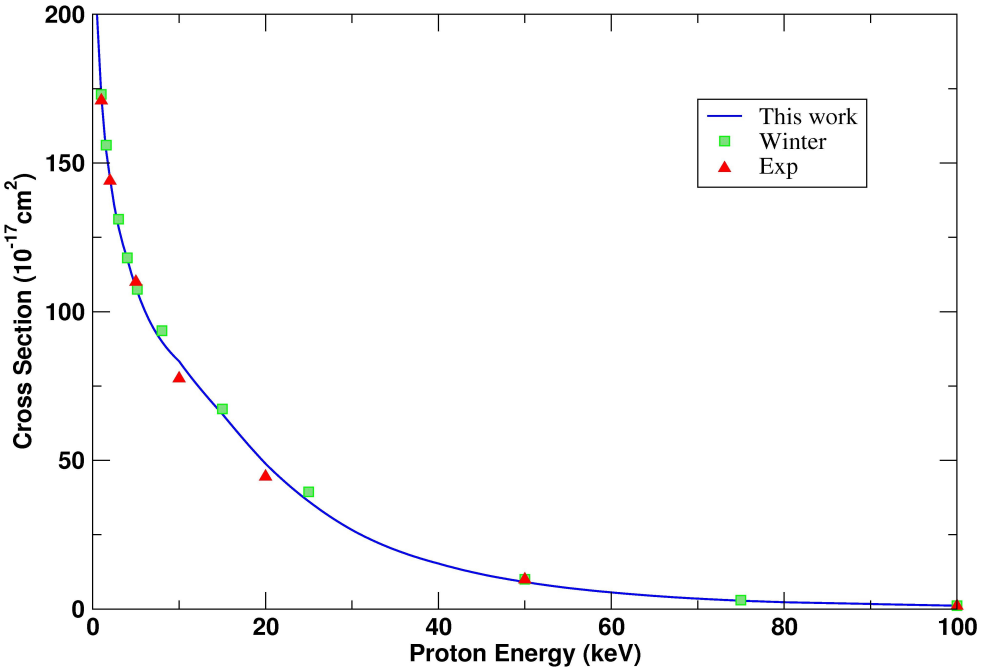


Charge-transfer probability as a function of the impact parameter *b*.
Comparison with the results of work *[Fritsch et al., PR, 202, 1 (1991)]*.

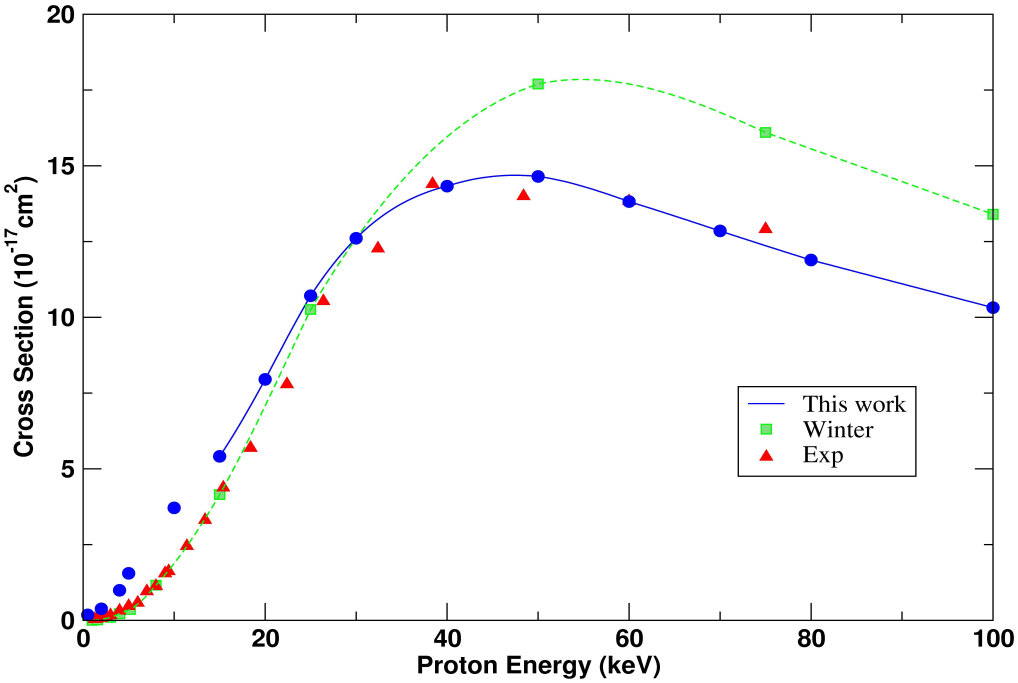
H(1s)-H$^+$

Charge-transfer and Ionization cross sections as functions of the collision energy

Charge-transfer



Ionization



Other calculations *[G. Winter, PRA **80**, 032701 (2009)]*

Experimental data *[R. Janev et al., At. and Pl. Mat. Int. Data for Fusion, Nucl. Fusion Suppl **4** (1993); M. Shah et al., JPB **31**, L757 (1998); **20**, 2481 (1987)]*

Scaling Transformation

Z Scaling transformation takes place in the case of nonrelativistic straight-line collision of symmetric systems. For the $A^{(Z-1)+}(1s)$-A^{Z+} and $H(1s)$-H^{+} collisions could be established links between the charge transfer parameters.

$$
\begin{aligned}
\vec{r}\,' &= Z\vec{r} \\
\vec{R}'_A &= Z\vec{R}_A \\
\vec{R}'_B &= Z\vec{R}_B \\
t' &= Z^2 t \\
E' &= E/Z^2 \\
\vec{V}'_A &= \vec{V}_A/Z \\
\vec{V}'_B &= \vec{V}_B/Z \\
\sigma' &= \sigma Z^2
\end{aligned}
$$

Here V_a is the velocity of the ion a = A, B,
E is the collision energy.
Values with and without a prime symbol (') correspond to the $H(1s)$-H^{+} and $A^{(Z-1)+}(1s)$-A^{Z+} collisions, respectively.

$Ne^{9+}(1s)$-Ne^{10+}

Charge-transfer cross section σ_{ct} (10^{-17} см^2) for the $Ne^{9+}(1s)$-Ne^{10+} collision

	$H(1s)$-H^+	$Ne^{9+}(1s)$-Ne^{10+}		
E/Z^2 (keV/u)	σ_{ct}	$\sigma_{ct} \cdot Z^2$ Rel.	$\sigma_{ct} \cdot Z^2$ Nonrel.	$\sigma_{ct} \cdot Z^2$ Born Appr.
1.0	172.4	171.6	172.2	188.4
2.0	144.9	144.3	144.8	150.7
4.0	117.5	117.1	117.5	114.8
5.0	107.8	107.3	107.8	107.3
10.0	81.3	80.8	81.3	76.2
15	63.5	63.0	63.5	57.6
20	48.9	48.5	48.9	48.2
30	26.6	26.4	26.6	30.1
50.0	9.1	9.0	9.1	13.7
70.0	3.5	3.5	3.5	5.4
100.0	1.1	1.1	1.1	2.0

$Xe^{53+}(1s)$-Xe^{54+}

Charge-transfer cross section σ_{ct} (10^{-17} см^2) for the $Xe^{53+}(1s)$-Xe^{54+} collision

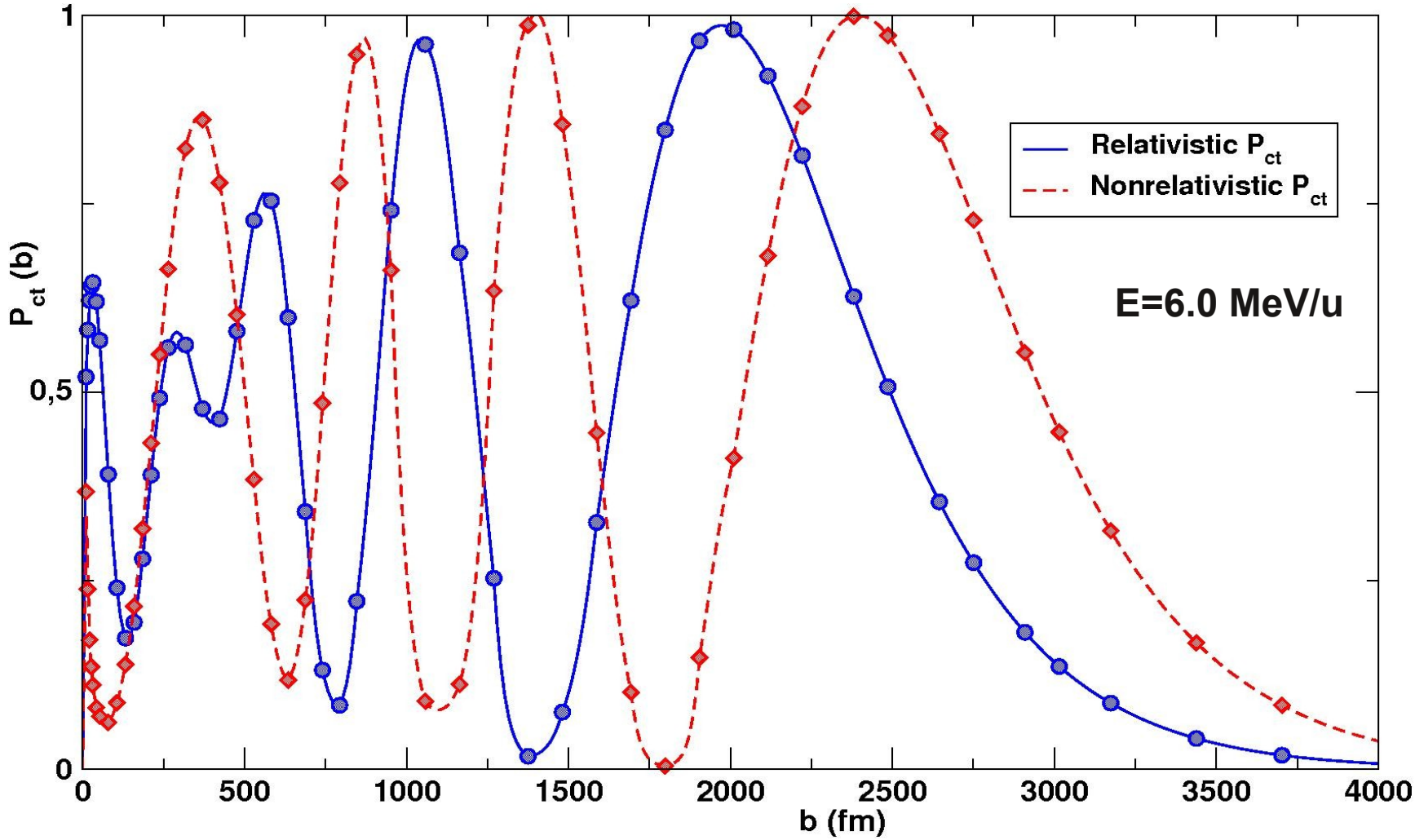
	$H(1s)$-H^+	$Xe^{53+}(1s)$-Xe^{54+}		
E/Z^2 (keV/u)	σ_{ct}	E (MeV/u)	$\sigma_{ct} \cdot Z^2$ Rel.	$\sigma_{ct} \cdot Z^2$ Nonrel.
1.23457	165.0	3.6	148.3	163.3
2.02332	144.9	5.9	129.4	143.0
3.42936	124.8	10.0	109.1	123.8
34.2936	20.7	100.0	13.3	20.6

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

Charge-transfer cross section σ_{ct} (10^{-17} см^2) for the $U^{91+}(1s)$-U^{92+} collision

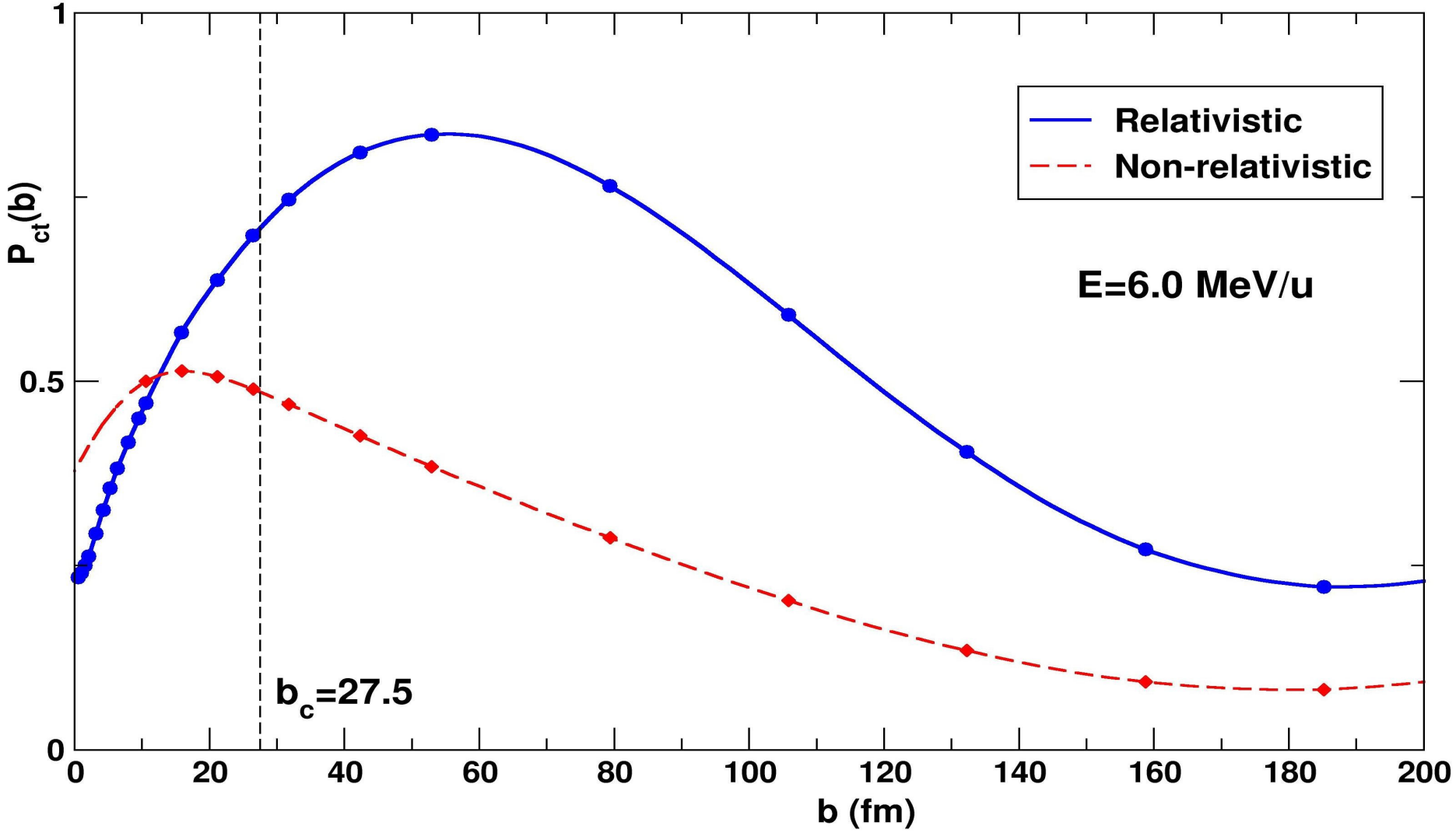
$U^{91+}(1s)$-U^{92+}				$H(1s)$-H^+	
Energy E (MeV/u)	$\sigma_{ct} \cdot Z^2$ Rel.	$\sigma_{ct} \cdot Z^2$ Nonrel.	$\sigma_{ct} \cdot Z^2$ Nonrel. staight-line	Energy E (keV/u)	σ_{ct}
6.0	135.3	184.2	185.0	0.709	186.4
6.5	132.7	181.3	182.0	0.768	183.1
7.0	130.3	178.2	179.1	0.827	180.1
10.0	117.1	165.8	166.7	1.181	167.6

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



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

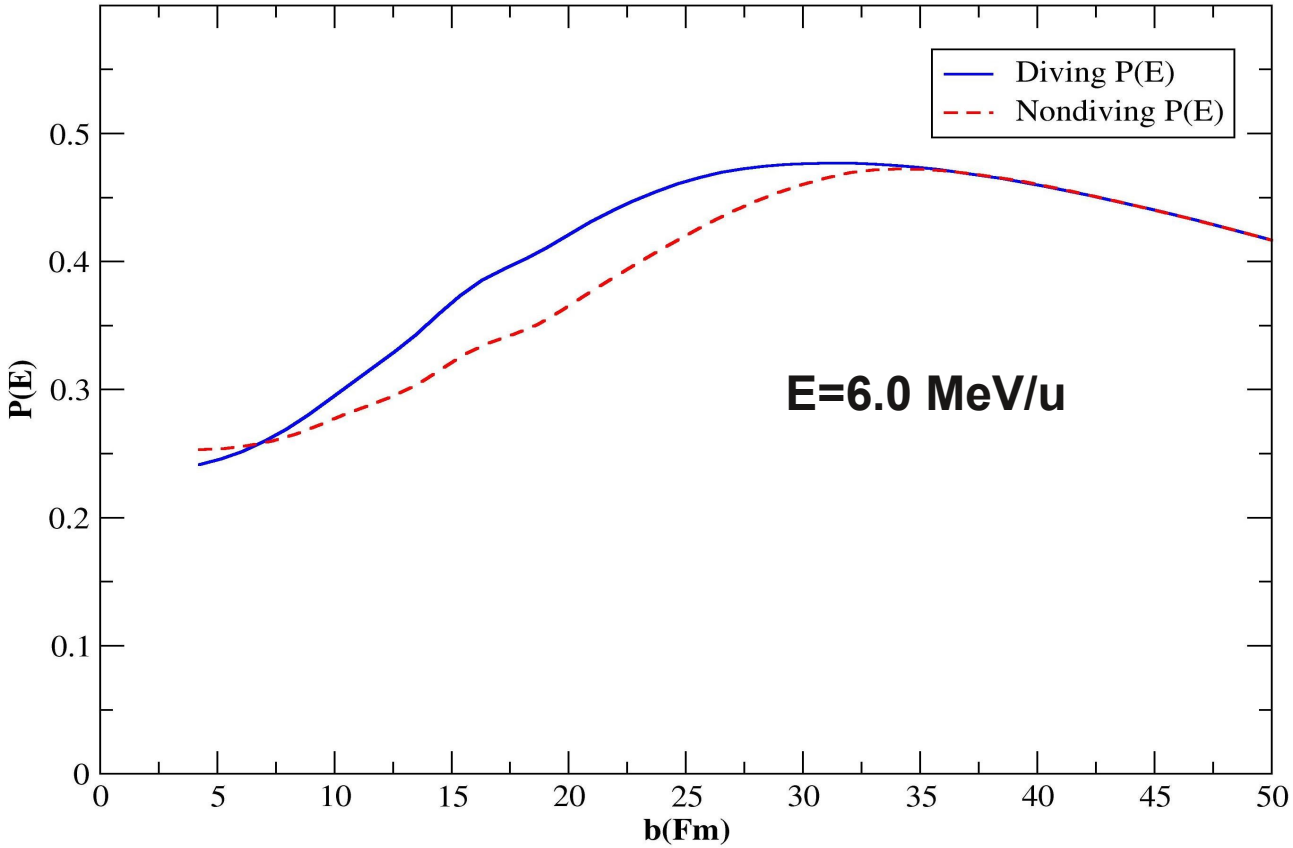
$U^{91+}(1s)$-U^{92+}



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

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

$$\Delta H = \left|\psi_{1\sigma_+}\right\rangle\left(-mc^2 - E_{1\sigma_+}\right)\left\langle\psi_{1\sigma_+}\right|$$



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

Summary and Outlook

Summary

- A new method employing the Dirac-Sturm basis functions for evaluation of various electron-excitation processes in low-energy heavy-ion collisions has been developed
- Systematic calculations of the charge transfer for low-energy collisions of H-like ions with bare nuclei have been carried out
- The "diving" of the ground state of the quasi-molecular U^{91+}–U^{92+} system into the negative-energy Dirac continuum is studied

Outlook

- Extending our method to collisions involving many-electron ions and neutral atoms
- Studing in more details the diving effect

Thank You for Your Attention

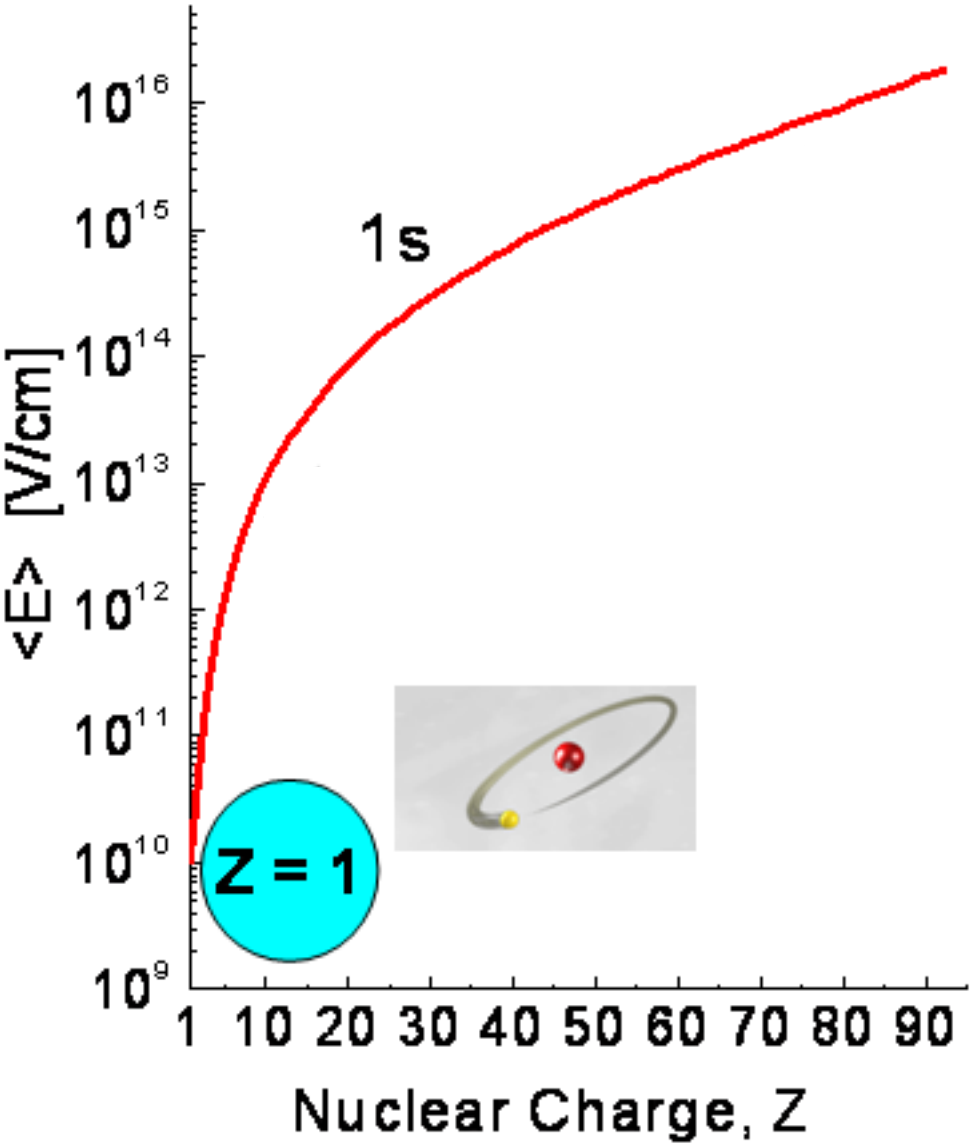
Thank You for Your Attention

I.I. Tupitsyn *et al.*, Phys Rev A **82**, 042701 (2010).

St. Petersburg State University

Winter, 2011

Introduction

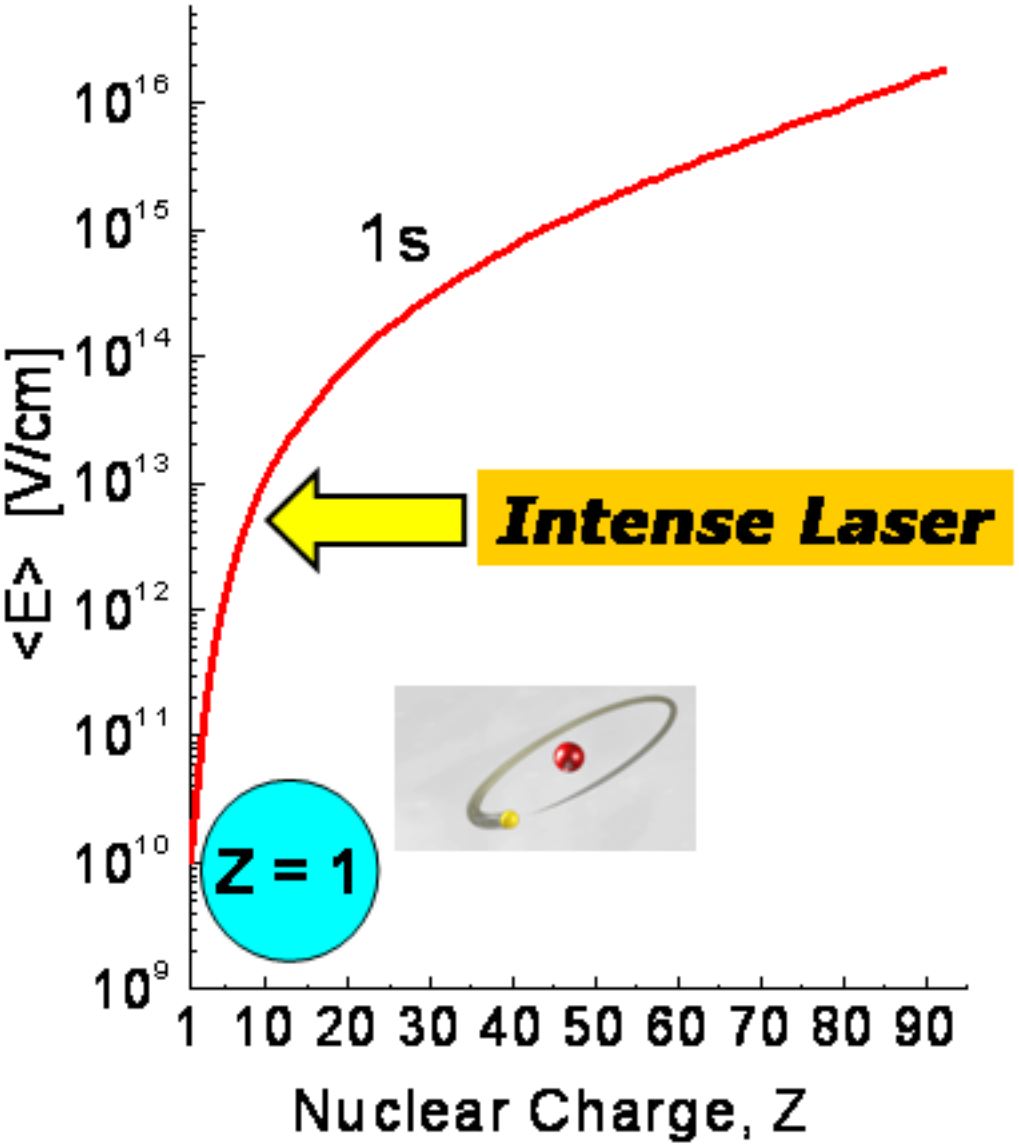


Hydrogen

E_K = -13.6 eV

$\langle E \rangle = 1 \cdot 10^{10}$ V/cm

Introduction



Hydrogen

E_K = -13.6 eV

$\langle E \rangle = 1 \cdot 10^{10}$ V/cm

Basis set properties

- Spectrum of the Dirac-Sturm operator is discrete and complete (including functions of the negative Dirac spectrum)
- Relativistic DSO satisfy the dual kinetic balance condition *[V. Shabaev et al, PRL 2*
- ОДШ позволяют легко строить функции отрицательного спектра
- 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

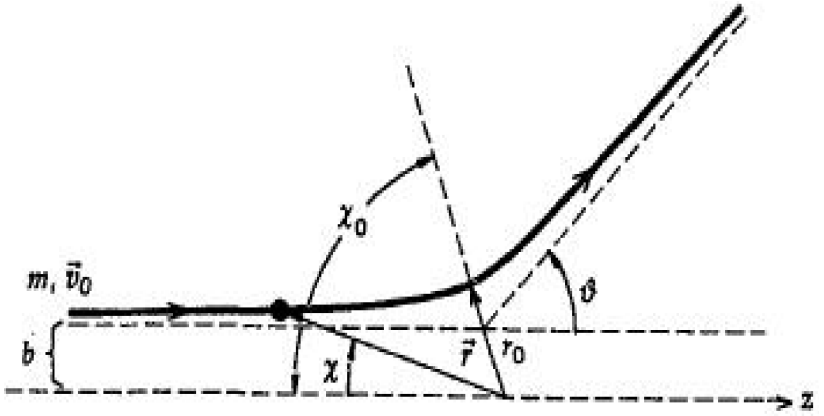
Basis of DO and DSO, localized on each ion:

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

Rutherford Scattering

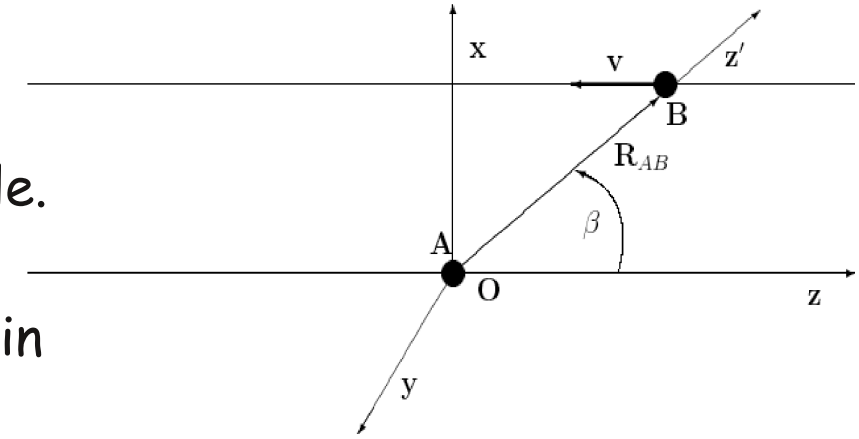
The trajectories $\mathbf{R}_A$ (t) and $\mathbf{R}_B$ (t) of the motion of the target (A) and the projectile (B) can be obtained as explicit solution of the classical motion equation in the interval $t \in (-\infty, \infty)$

$$\begin{cases} R_{AB} = a(\varepsilon \cosh\xi + 1) \\ t = \dfrac{a}{V_\infty}(\varepsilon \sinh\xi + \xi) \end{cases}, \quad \text{where } \xi \in (-\infty, \infty).$$



$$R_{AB} = |\vec{R}_A - \vec{R}_B|, \quad a = \frac{Z_T Z_P e^2}{M_r V_\infty^2}, \quad \varepsilon = \left(1 + \frac{b^2}{a^2}\right)^{1/2},$$

b is the impact parameter, M_r is the reduced mass, V_∞ is the initial velocity of the projectile.



Assuming that Z_T or Z_P equal to zero, we obtain a straight line trajectory for the projectile.

Time-depending Dirac equation

$$\begin{cases} iS\dfrac{d\boldsymbol{C}(t)}{dt}=(H-T)\boldsymbol{C}(t) \\ C_j(t)\big|_{t\to-\infty}=\delta_{j,1s} \end{cases}$$

orthogonalization

$$\begin{cases} i\dfrac{d\boldsymbol{C}^{\boldsymbol{L}}(t)}{dt}=M\,\boldsymbol{C}^{\boldsymbol{L}}(t) \\ C_j^L(t)\big|_{t\to-\infty}=\delta_{j,1s} \end{cases}$$

M is Hermitian.

$$\boldsymbol{C}^{\boldsymbol{L}}(t+\Delta t)=\exp(-i\,\overline{M}\,\Delta t)\,\boldsymbol{C}^{\boldsymbol{L}}(t)+O(\Delta^3 t)$$

$$\overline{M}=M(t+\Delta t/2)$$

Preserving the norm at each time step: $\langle\Psi(\boldsymbol{r},t)|\Psi(\boldsymbol{r},t)\rangle=\sum_j|C_j^L(t)|^2=1$

$$\begin{aligned} \overline{M} &= V\,\Lambda\,V^{+} \\ \exp(-i\,\overline{M}\,\Delta t) &= V\exp(-i\,\Lambda\,\Delta t)\,V^{+} \end{aligned}$$