Relativistic Evaluation of the Charge-Transfer Probabilities and Cross Sections for Low-nergy Collisions of H-like Ions with Bare Nuclei

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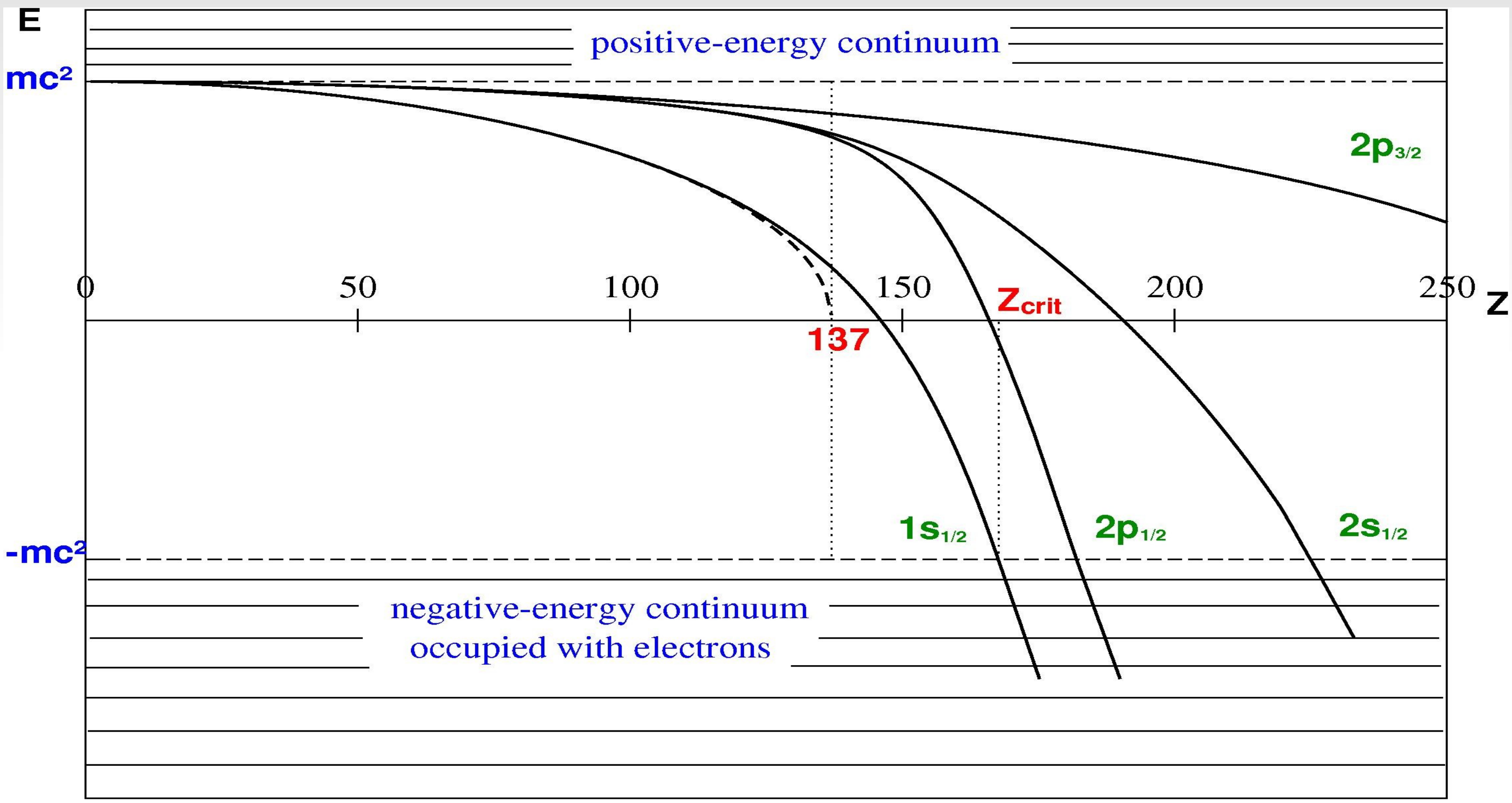
Outline:

- Introduction and motivation
- Theoretical description
- Numerical results
- Summary

Introduction

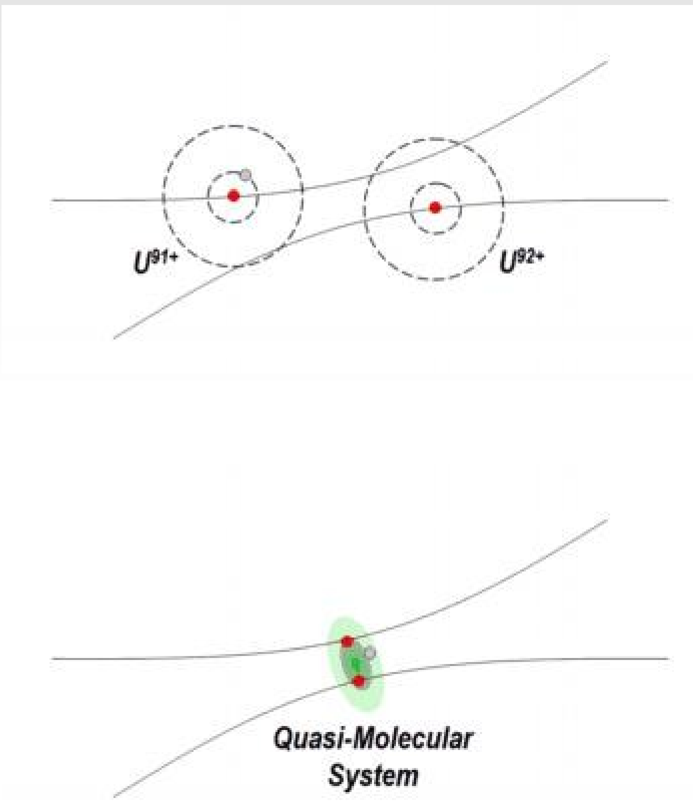
The *1s* level dives into the negative-energy continuum at Z_{crit} ~173.

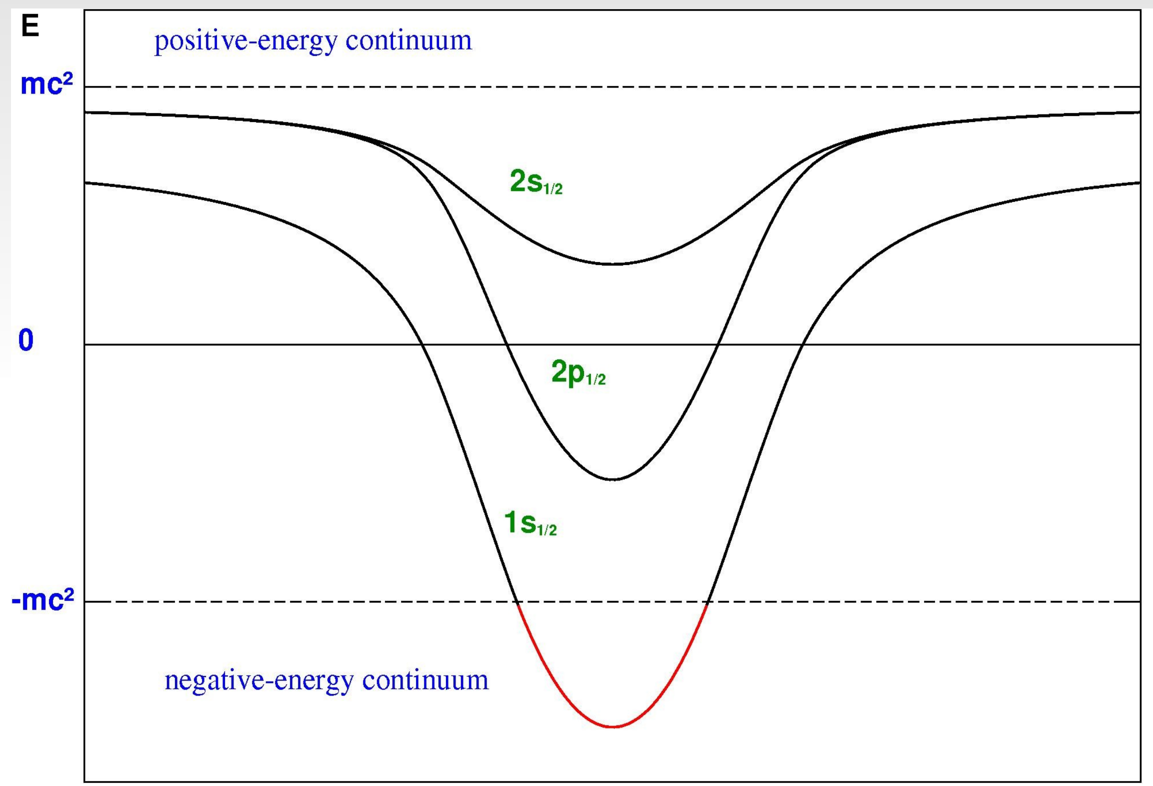


[S.S. Gershtein, Ya.B. Zeldovich, 1969; W. Pieper, W. Greiner, 1969]

Motivation: super-heavy quasi-molecules

A way to create super-critical field is to collide 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: $v_e \sim (\alpha Z)c$
- $m_e \ll M_{nucl} \rightarrow$ 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.)

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

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

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

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

Finite Basis Expansion

$$\Psi(\vec{r}) = \sum_i c_i \varphi_i(\vec{r}),$$

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

Stationary case: $$\sum_j S_{ij} c_j = \sum_j H_{ij} c_j$$

Time-dependent case: $$i \sum_j S_{ij} \frac{dC_j(t)}{dt} = \sum_j (H_{ij} - T_{ij}) C_j(t),$$

where

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

Basis set

- Our basis is constructed as a sum of the Dirac and Dirac-Sturm orbitals, localized on each ion.
- The Dirac and Dirac-Sturm orbitals are obtained by solving numerically the finite-difference one-center Dirac and Dirac-Sturm equations.

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

$\varphi_{\alpha,\mu}$ is the Dirac or the Dirac-Sturm orbital localized on the center α.

Basis set advantages

- Spectrum of the Dirac-Sturm operator is red discrete and complete (including functions of the negative Dirac spectrum).
- Relativistic DSO satisfy the dual kinetic balance condition *[V. Shabaev et al., PRL **93**, 130405 (2004)].*
- 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.

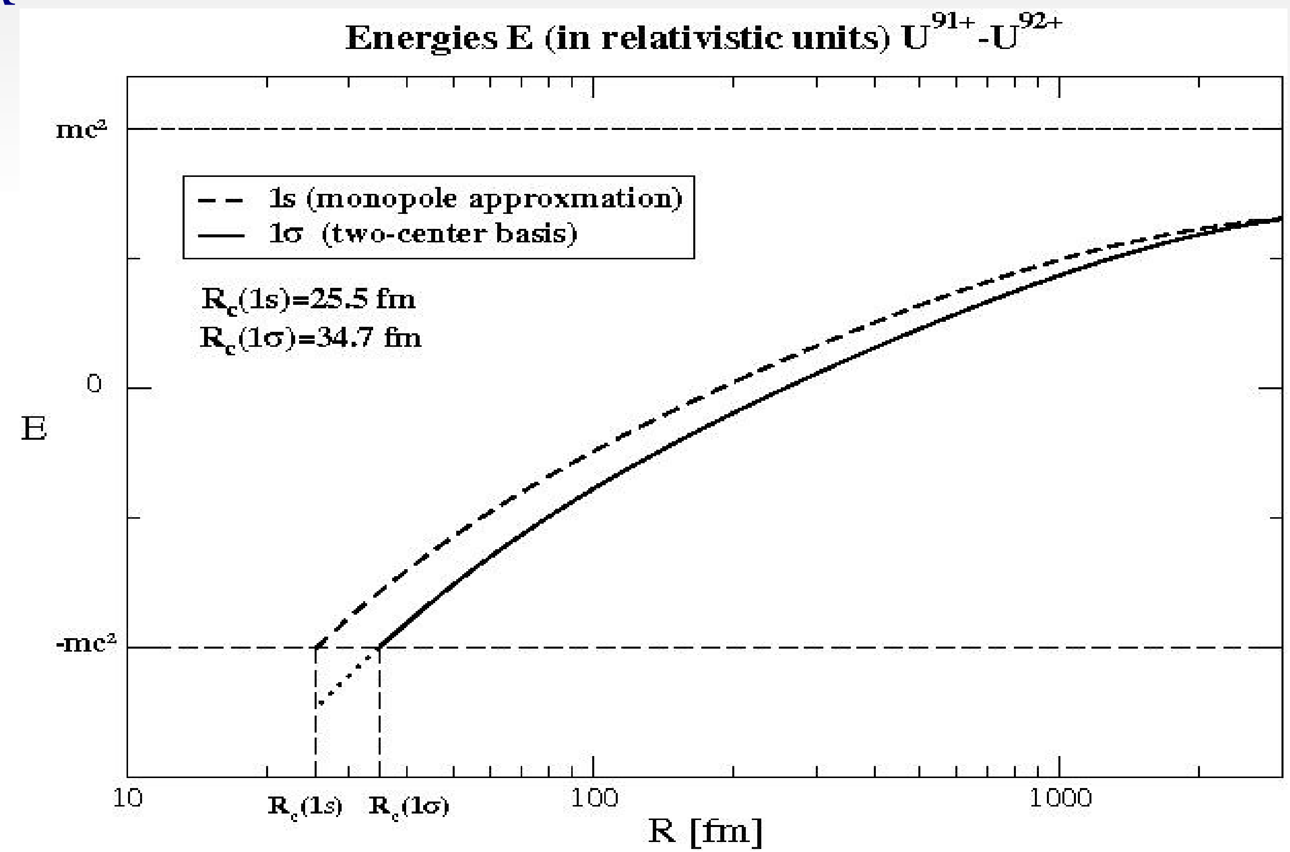
The Basis set

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

Energies of the $1\sigma_+$ ground states of quasi-molecules

The $1\sigma_+$ state energy of the U_2^{183+} quasi-molecule as a function of the internuclear distance *R*

$R(1\sigma_+)$=34.7 fm



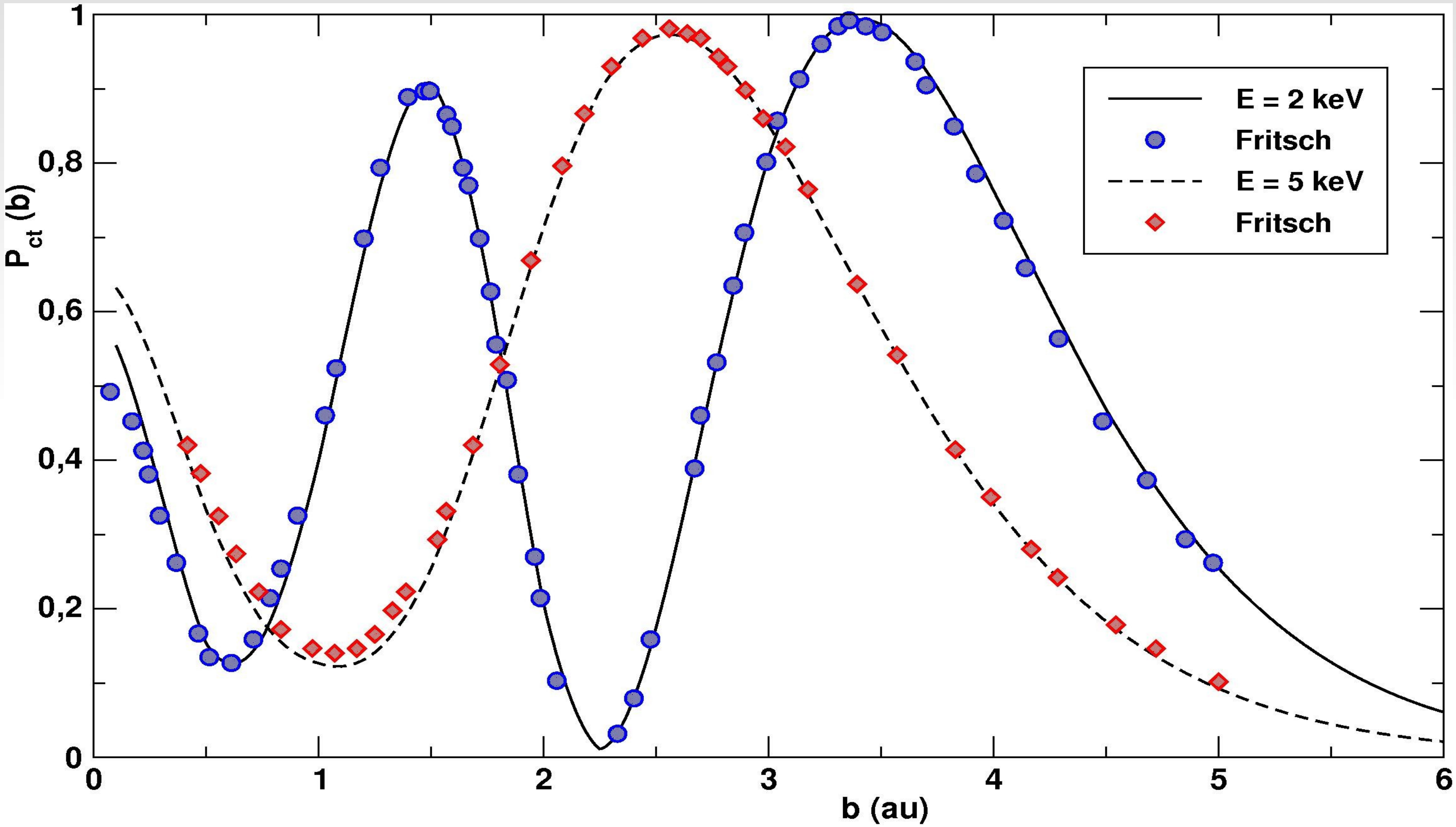
Critical Distances R_c (fm)

	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.I. Lisin et al., Phys. Lett.* ***69B****, 2 (1977)]*
[b] *[A. Artemyev et al., to be published]*
[c] *[J. Rafelski, B. Müller, Phys. Lett.* ***65B****, 205 (1976)]*
[d] *[V.I. Lisin et al., Phys. Lett.* ***91B****, 20 (1980)]*
[f] *[B. Müller and W. Greiner, Z. Naturforsch.* ***3la****, 1 (1975)]*

H(1*s*)-H$^+$ collision

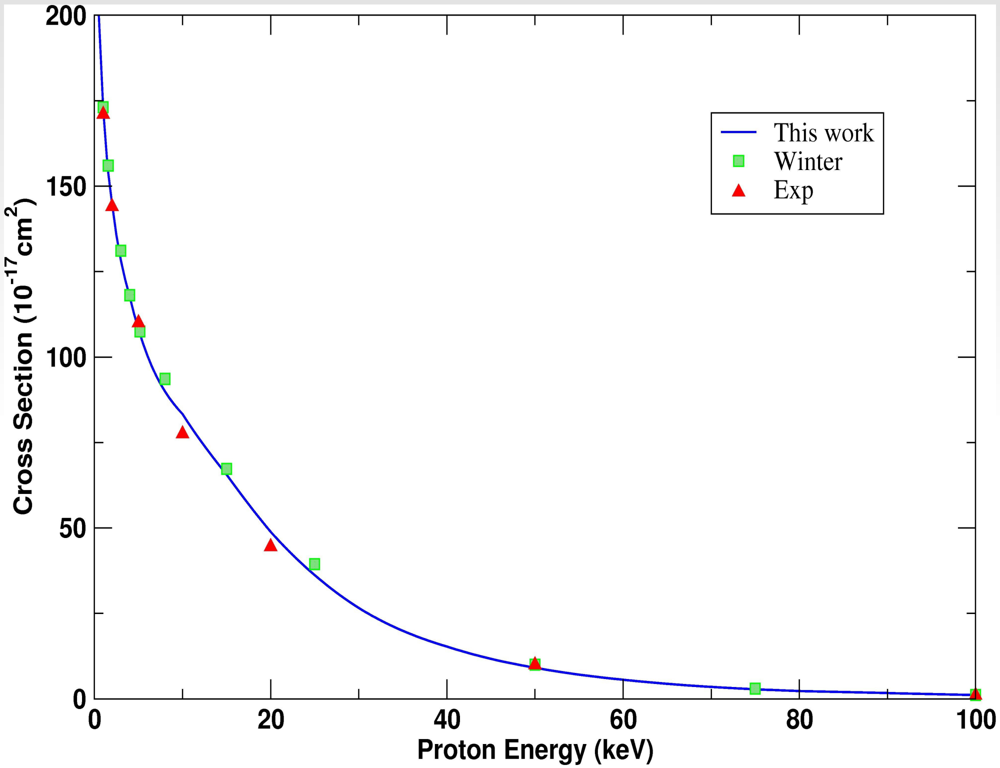
Charge-transfer probability as a function of the impact parameter *b*

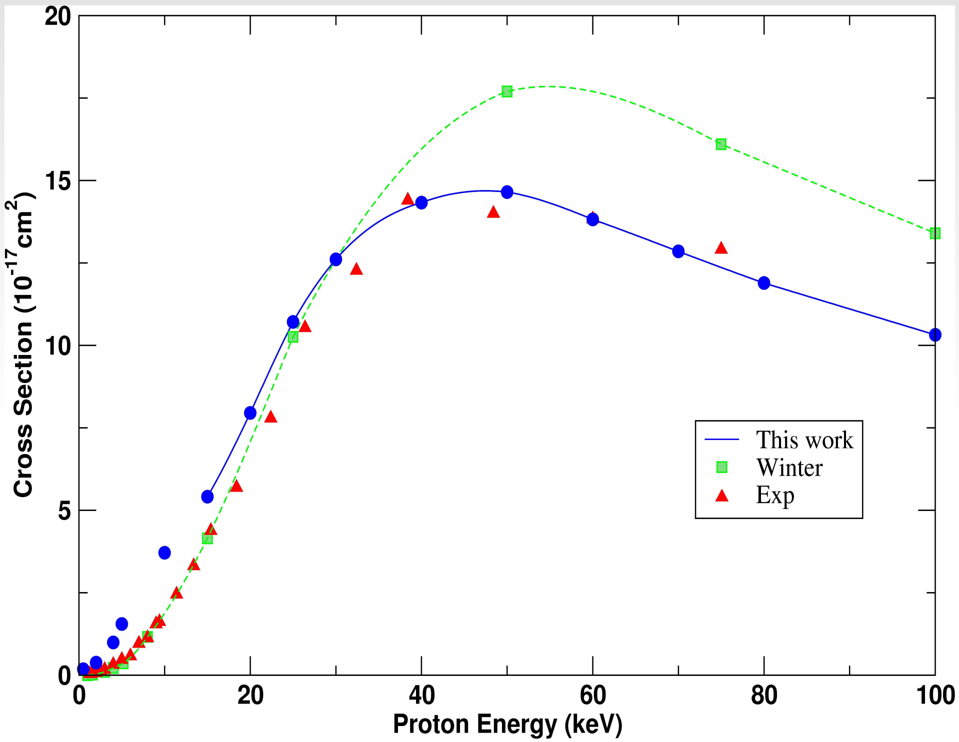


Comparison with the results of work *[W. Fritsch et al., Phys. Rep., 202, 1 (1991)]*

H(1*s*)-H^+ collision

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





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)]*

Z Scaling Transformation

In the nonrelativistic case, using the scale transformation it is possible to establish a link between the charge-transfer parameters in the $H(1s)\text{-}H^+$ and $A^{(Z-1)+}(1s)\text{-}A^{Z+}$ collisions

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

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

Charge-transfer cross section σ_{ct} (10^{-17} cm^2) for the $Ne^{10+}(1s)$-Ne^{9+} and $H(1s)$-H^{+} collisions

	$Ne^{10+}(1s)$-Ne^{9+}			$H(1s)$-H^{+}
Energy E/Z^2(keV/u)	$\sigma_{ct} \cdot Z^2$ Rel.	$\sigma_{ct} \cdot Z^2$ Nonrel.	$\sigma_{ct} \cdot Z^2$ Born approx.[a]	$\sigma_{ct} \cdot Z^2$
1.0	171.6	172.2	188.4	172.4
4.0	117.1	117.5	114.8	117.5
10.0	80.8	81.3	76.2	81.3
20.0	48.5	48.9	48.2	48.9

[a] *V. Shevelko, 2010*

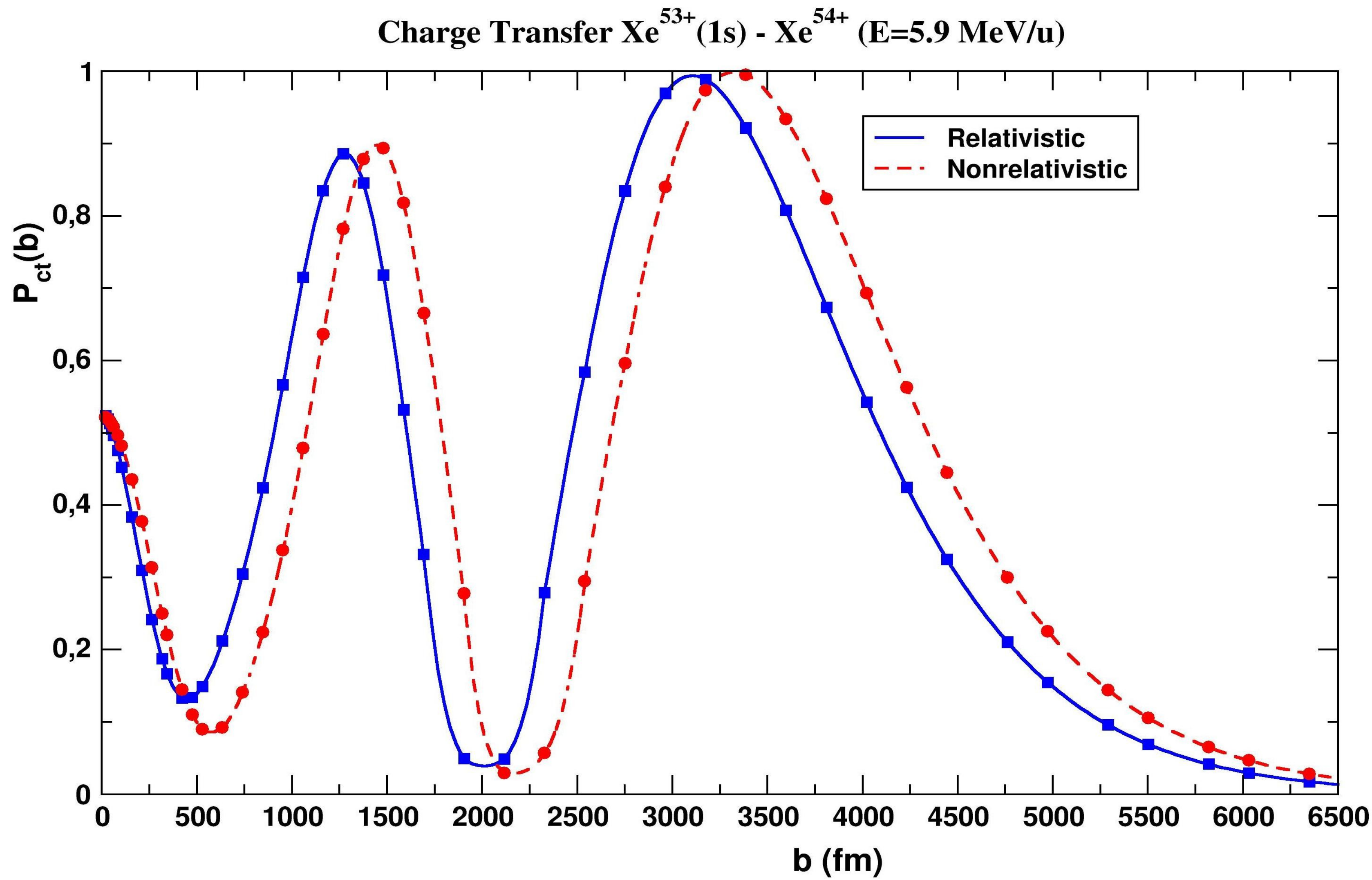
$Xe^{53+}(1s)$-Xe^{54+} collision

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

	$Xe^{54+}(1s)$-Xe^{53+}			$H(1s)$-H^+
E/Z^2 (keV/u)	E (MeV/u)	$\sigma_{ct} \cdot Z^2$ Rel.	$\sigma_{ct} \cdot Z^2$ Nonrel.	$\sigma_{ct} \cdot Z^2$
1.234 57	3.6	148.3	163.3	165.0
2.023 32	5.9	129.4	143.0	144.9
3.429 36	10.0	109.1	123.8	124.8
34.293 6	100.0	13.3	20.6	20.7

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

Charge-transfer probability as a function of the impact parameter *b*, *E=5.9 MeV/u*



Summary

Conclusion:

- 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
- Relativistic calculations of the charge transfer for low-energy collisions of H-like ions with bare nuclei have been carried out

Outlook:

- Calculations of the charge-transfer probabilities at supercritical regime, $Z_1+Z_2 > 173$
- Investigation of a possibility of indirect observation of the diving effect

Thank You for Your Attention