

Relativistic calculation of inner-shell atomic processes in low-energy ion-atom collisions

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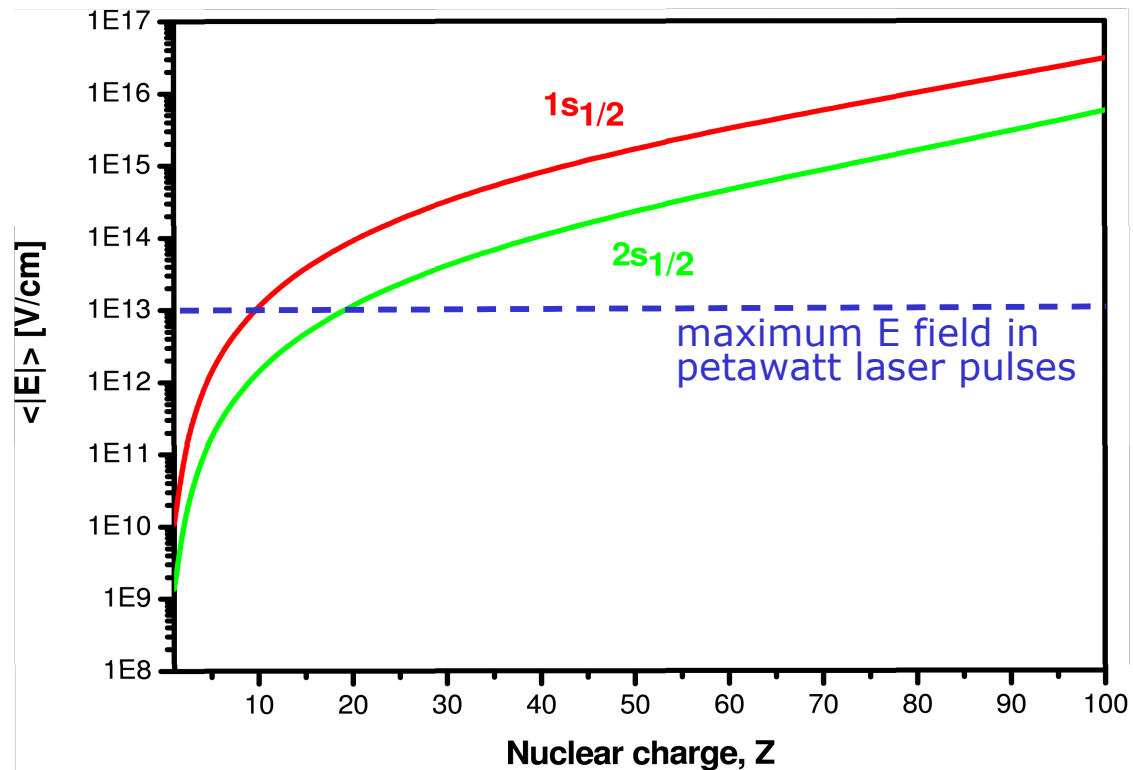
Outline

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



Introduction

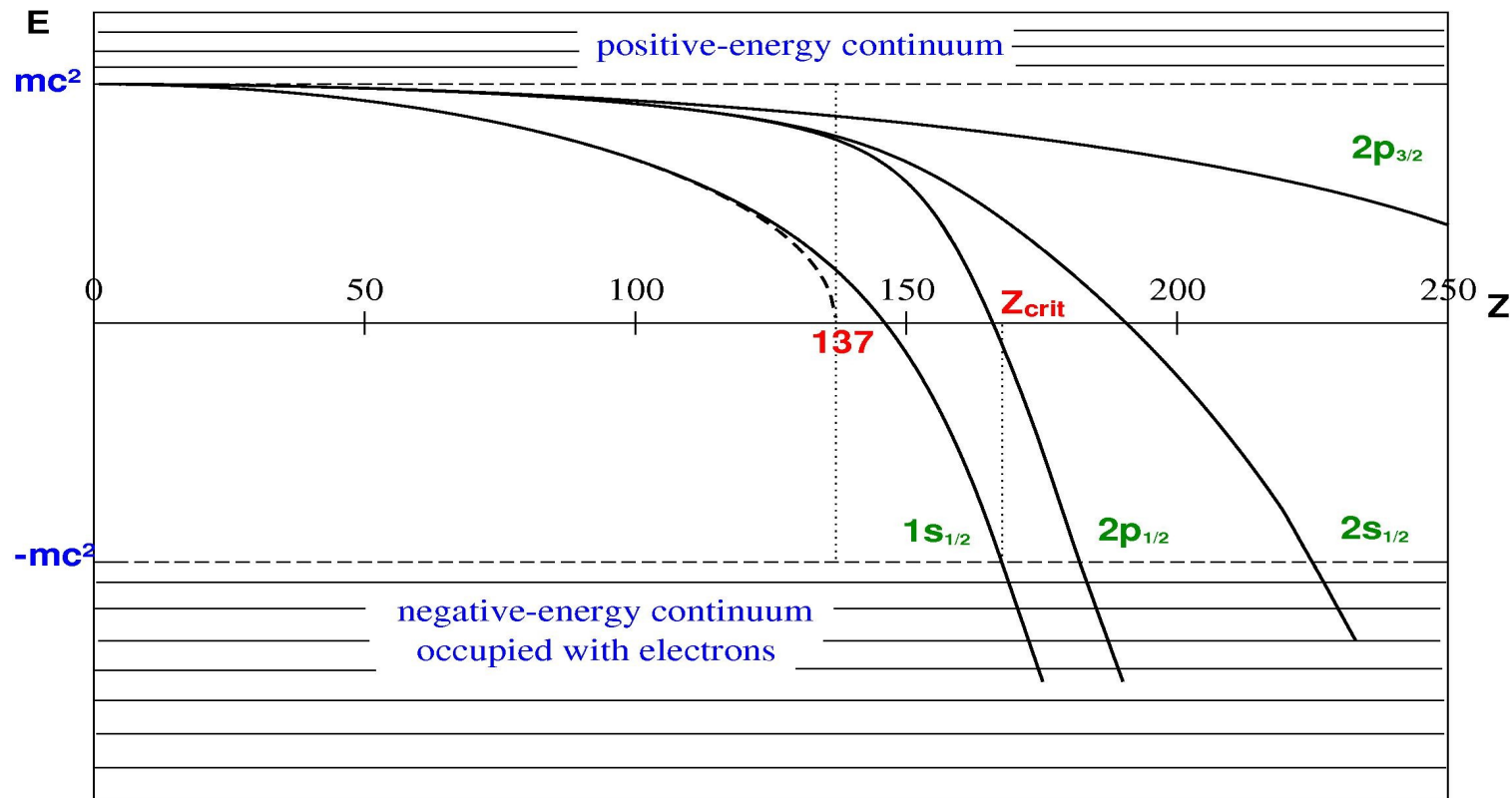
Heavy few-electron ions provides possibility to test of QED at extremely strong electromagnetic fields



Introduction

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

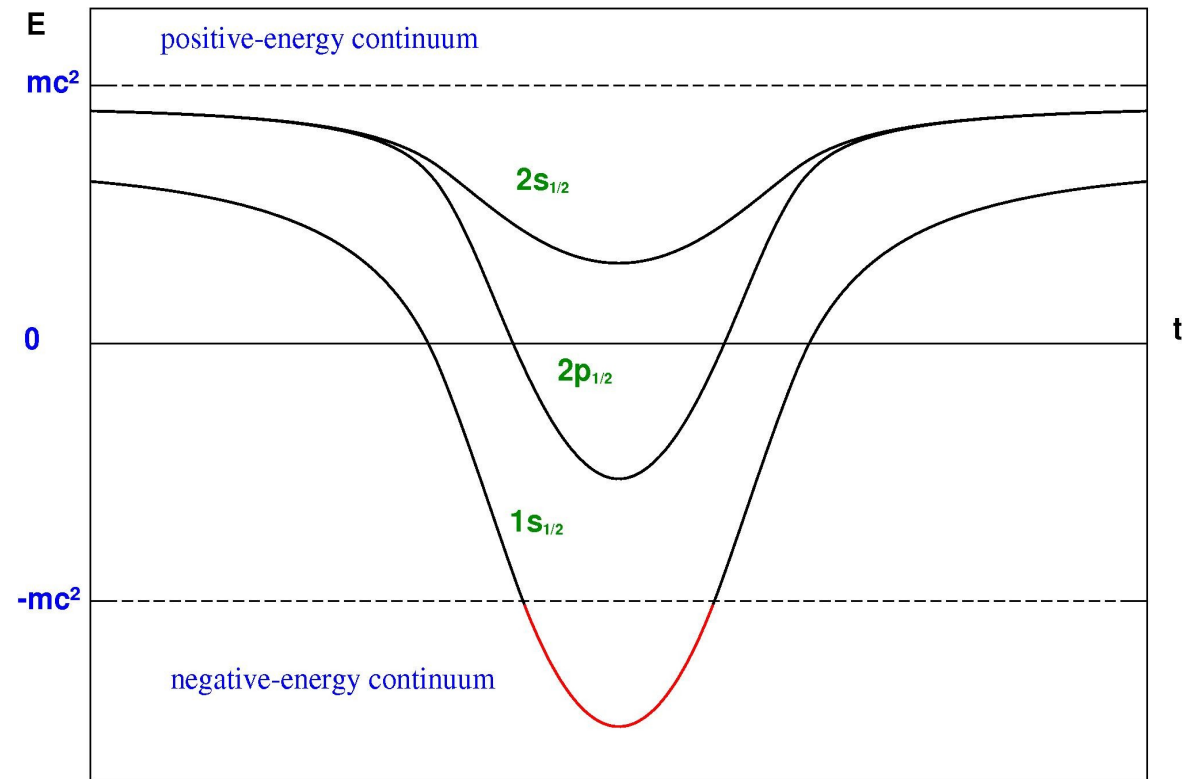
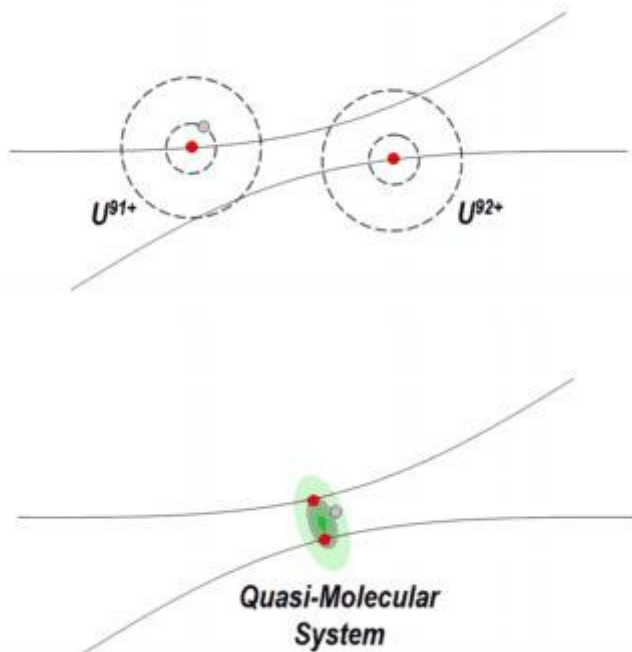
Existence of point charge with value more than $\alpha Z > 1$ is forbidden
[Gätner et al., 1981].



The $1s$ level dives into the negative-energy continuum at $Z_{crit} \sim 173$
[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: $\sim 6 \text{ MeV/u}$ for U
- Relativistic electron: $v_e \sim (\alpha Z) c$
- $m_e \ll M_{nucl} \rightarrow$ Nuclei ($\mathbf{R}_A, \mathbf{R}_B$) move according to the Rutherford trajectory

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

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

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

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

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.):

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

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

$$\left\{ \begin{array}{l} i \sum_j S_{ij} \frac{dC_j(t)}{dt} = \sum_j (H_{ij} - T_{ij}) C_j(t) \\ \lim_{t \rightarrow -\infty} \mathbf{C}(t) = \mathbf{C}^0 \end{array} \right.$$

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

Finite Basis Expansion

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

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

$$\phi_{nkm}(\vec{r}, \sigma) = \begin{pmatrix} \frac{P_{nk}(r)}{r} \chi_{km}(\Omega, \sigma) \\ i \frac{Q_{nk}(r)}{r} \chi_{-km}(\Omega, \sigma) \end{pmatrix}; \quad \begin{aligned} k &= (-1)^{l+j+1/2} (j+1/2) \\ j &= |k| - 1/2, \quad l = j + \frac{1}{2} \frac{k}{|k|} \end{aligned}$$

The large P_{nk} and small Q_{nk} radial components are obtained by solving numerically the Dirac equation in the center field potential $V(r)$

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

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

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

where (for the point nucleus case)

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

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

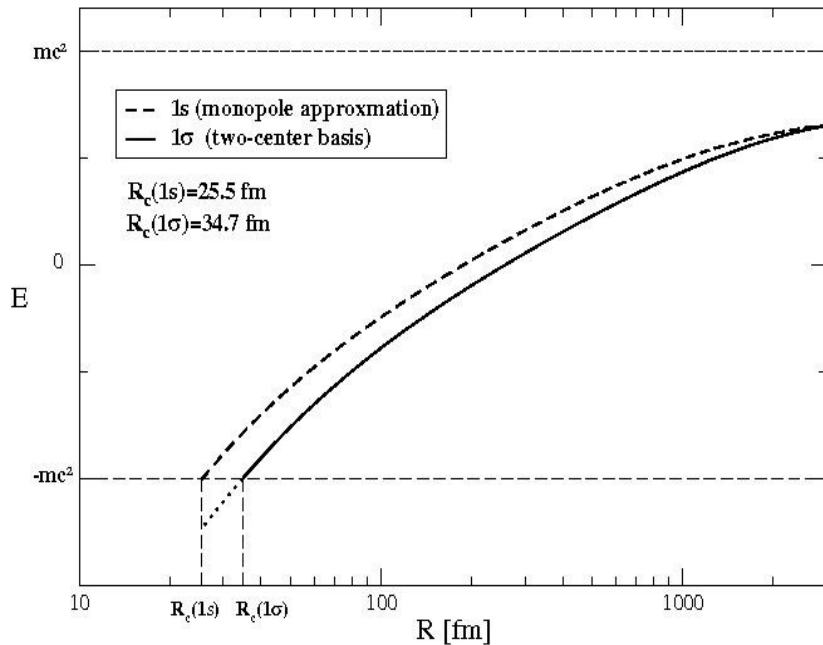
The $1\sigma_+$ state energy of the U_2^{183+} quasimolecule as a function of the internuclear distance R .

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

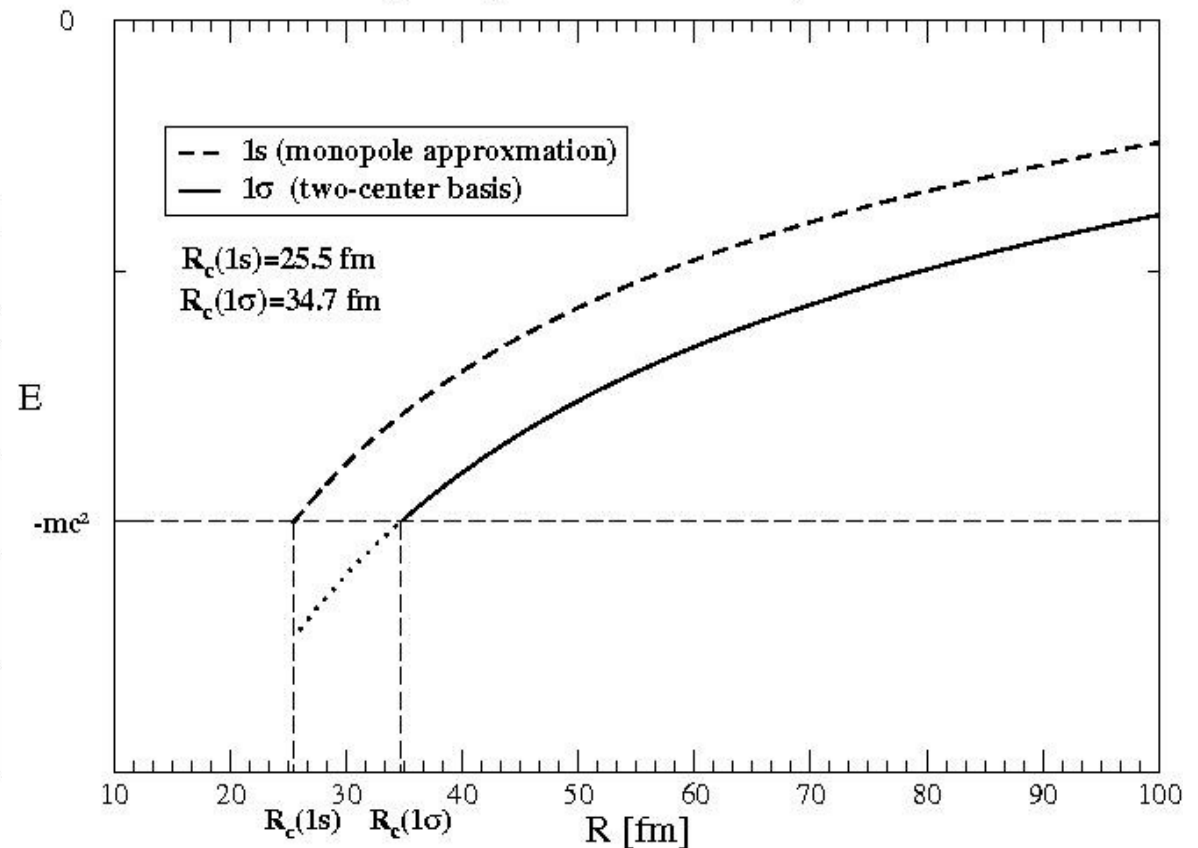
$$R_{\text{crit}}(1\sigma_+) = 34.7 \text{ fm}$$

$$R_{\text{nucl}} = 5.9 \text{ fm}$$

Energies E (in relativistic units) $U^{91+} - U^{92+}$



Energies E (in relativistic units) $U^{91+} - U^{92+}$



Critical Distances

Critical Distances R_c (fm)

Z	Point nucleus		Extended nucleus	
	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

^aV. Lisin et al., PRL 1977

^cJ. Rafelski and B. Müller, PL 1976

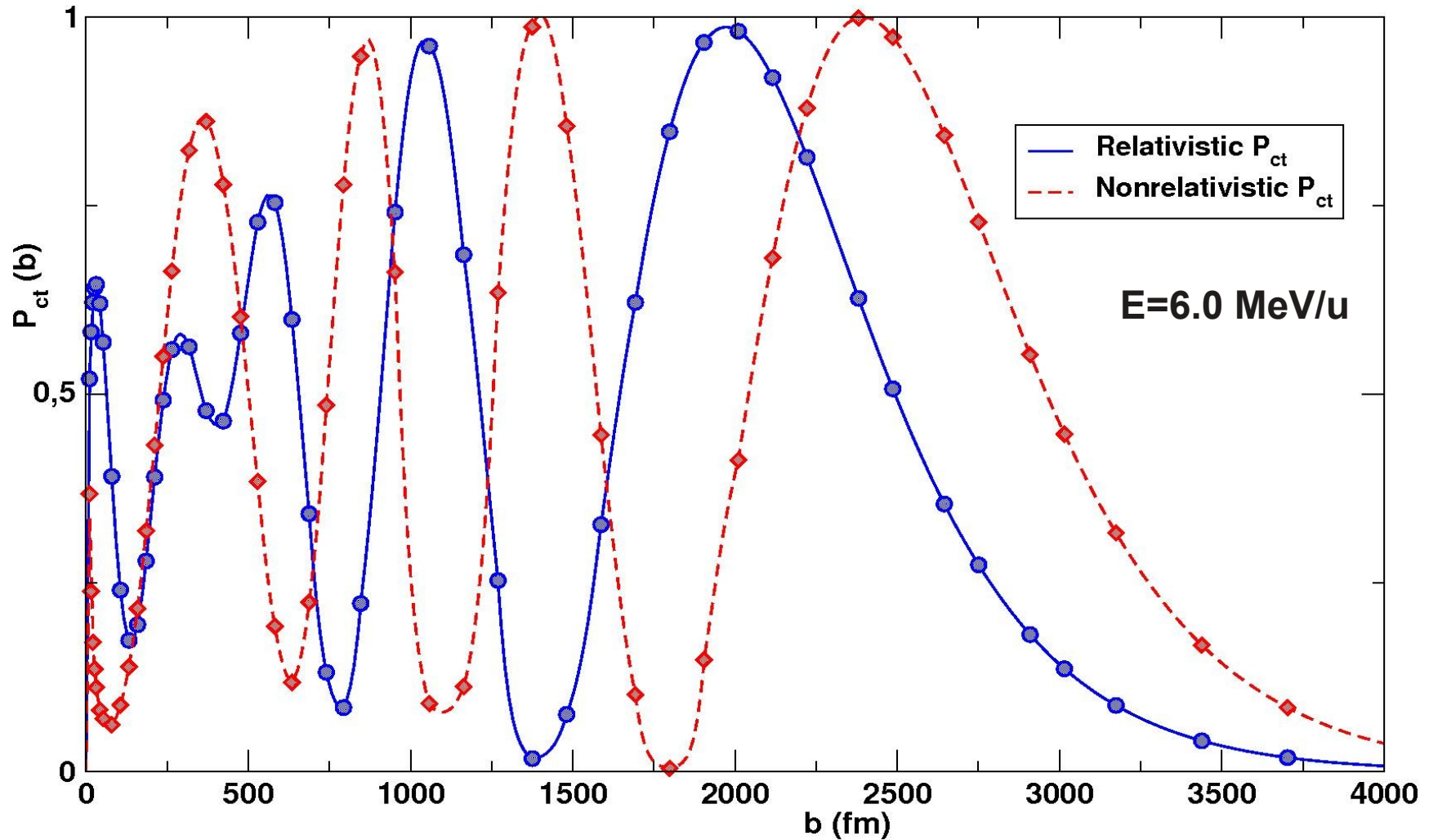
^fB. Müller and W. Greiner, ZN 1975

^bA. Artemyev et al., JPB 2010

^dV. Lisin et al., PL 1980

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

Many-electron case

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

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

$$\left\{ \begin{array}{l} i \frac{d\psi_i(t)}{dt} = h_i^{\text{eff}} \psi_i(t) \\ \lim_{t \rightarrow -\infty} (\psi_i(t) - \psi_i^0(t)) = 0 \end{array} \right.$$

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

Dirac-Kohn-Sham equation

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

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

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

$$V_H[\rho] = V_{\text{nucl}}^A(\vec{r}_A) + V_{\text{nucl}}^B(\vec{r}_B) + V_C[\rho]$$

$$V_{\text{nucl}}(\vec{r}) = \int d^3 \vec{r}' \frac{\rho_{\text{nucl}}(\vec{r}')}{|\vec{r} - \vec{r}'|} \quad V_C[\rho] = \int d^3 \vec{r}' \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|}$$

$V_{xc}[\rho]$ is the exchange-correlation potential
in the Perdew-Zunger parametrization

Perdew and Zunger, PRB 23, 5048 (1981)

Inclusive probability

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

$$P_{f_1, \dots, f_N} = \det(\gamma_{nn'}) \quad n, n' = 1, \dots, N$$

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

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

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

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

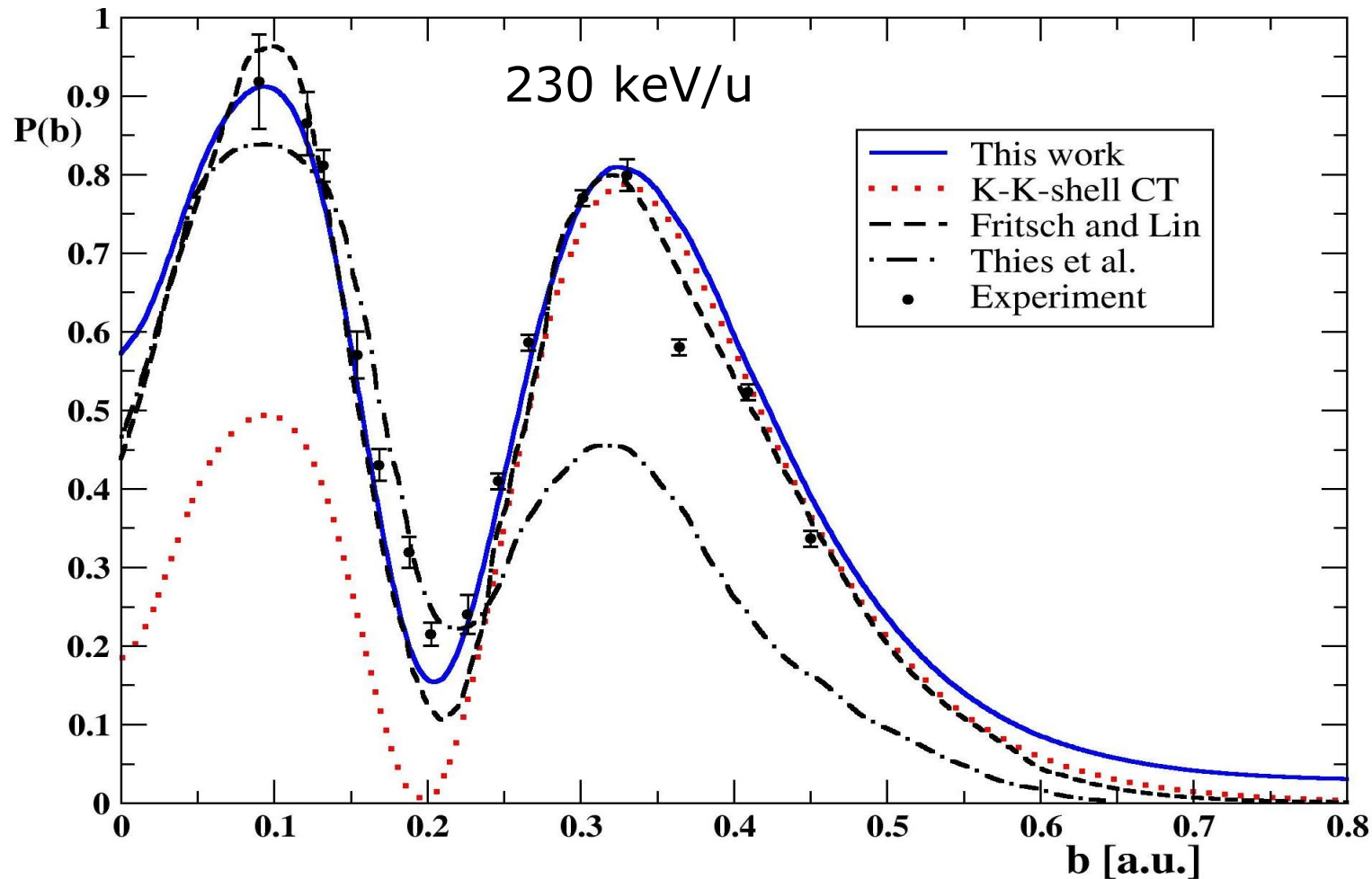
Numerical calculation

Test system: $\text{Ne}(1s^2 2s^2 2p^6) - \text{F}^{8+}(1s)$
 $\text{Ne}(1s^2 2s^2 2p^6) - \text{F}^{6+}(1s^2 2s)$

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

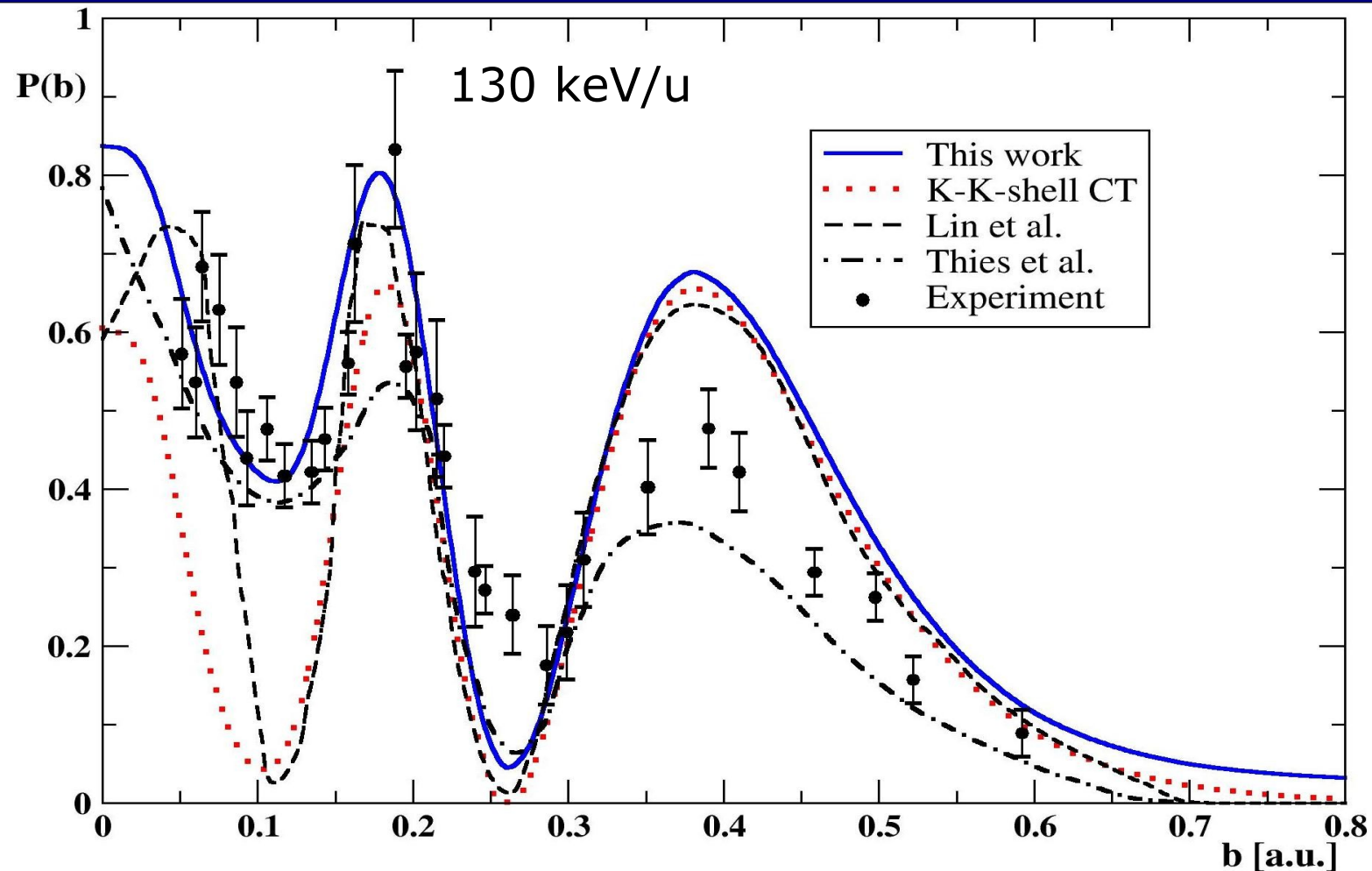
Theoretical calculations: W. Fritsch and C.D. Lin, PRA 1985
A. Toepfer et al., PLA 1987
B. Thies et al., PLA 1989

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



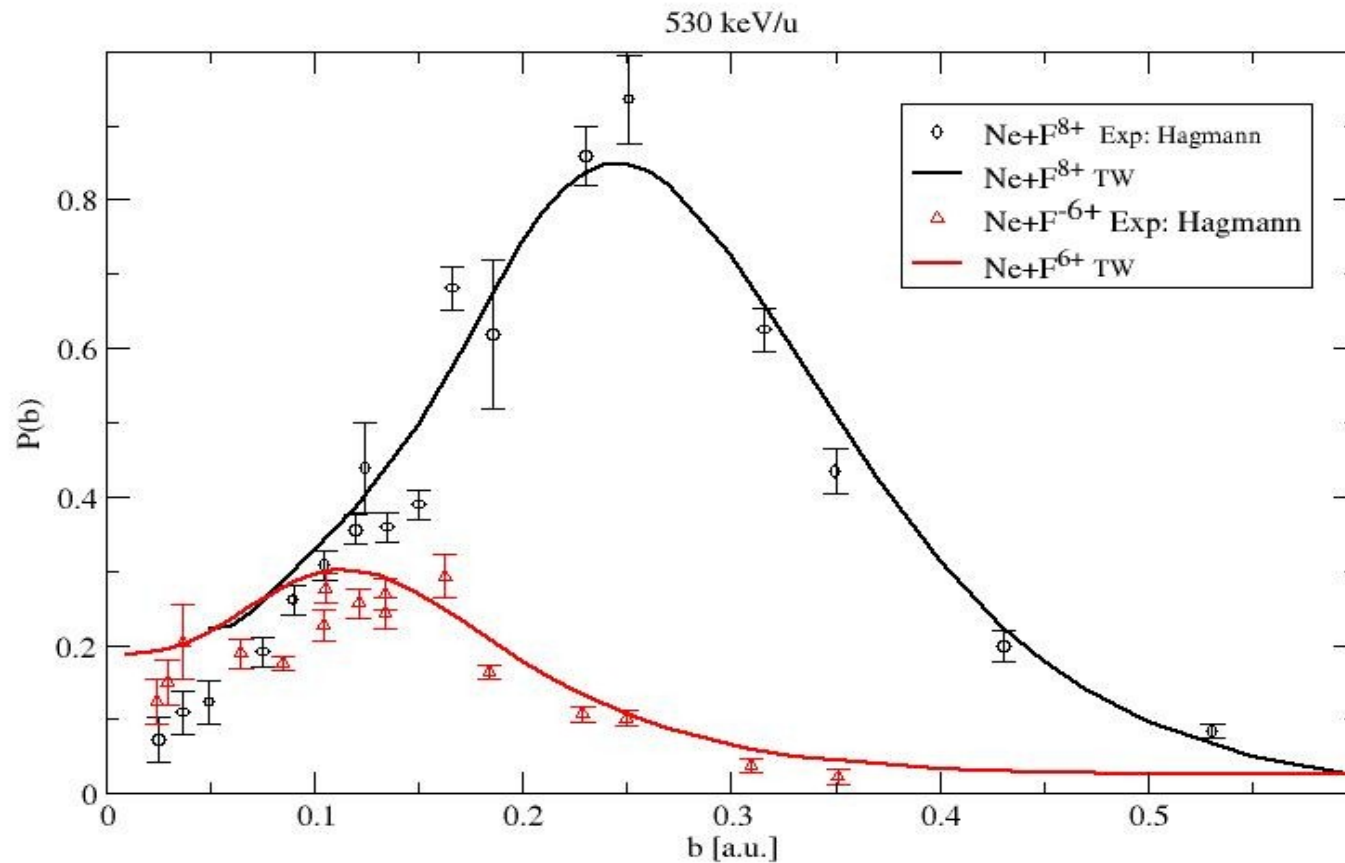
The probability of Ne K-shell-vacancy production as a function of the impact parameter b

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



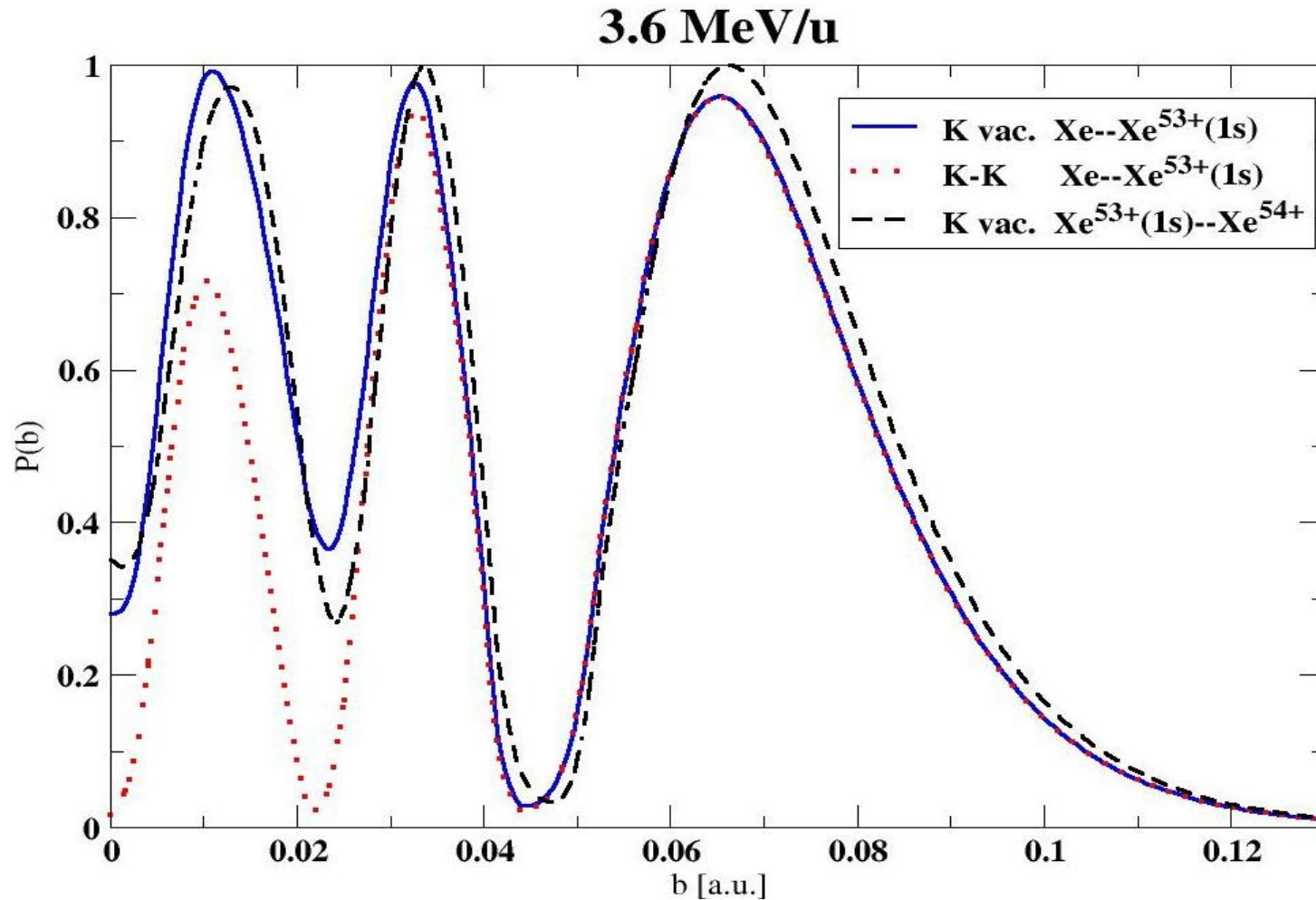
The probability of Ne K-shell-vacancy production as a function of the impact parameter b

Ne(1s²2s²2p⁶)-F⁶⁺(1s²2s)



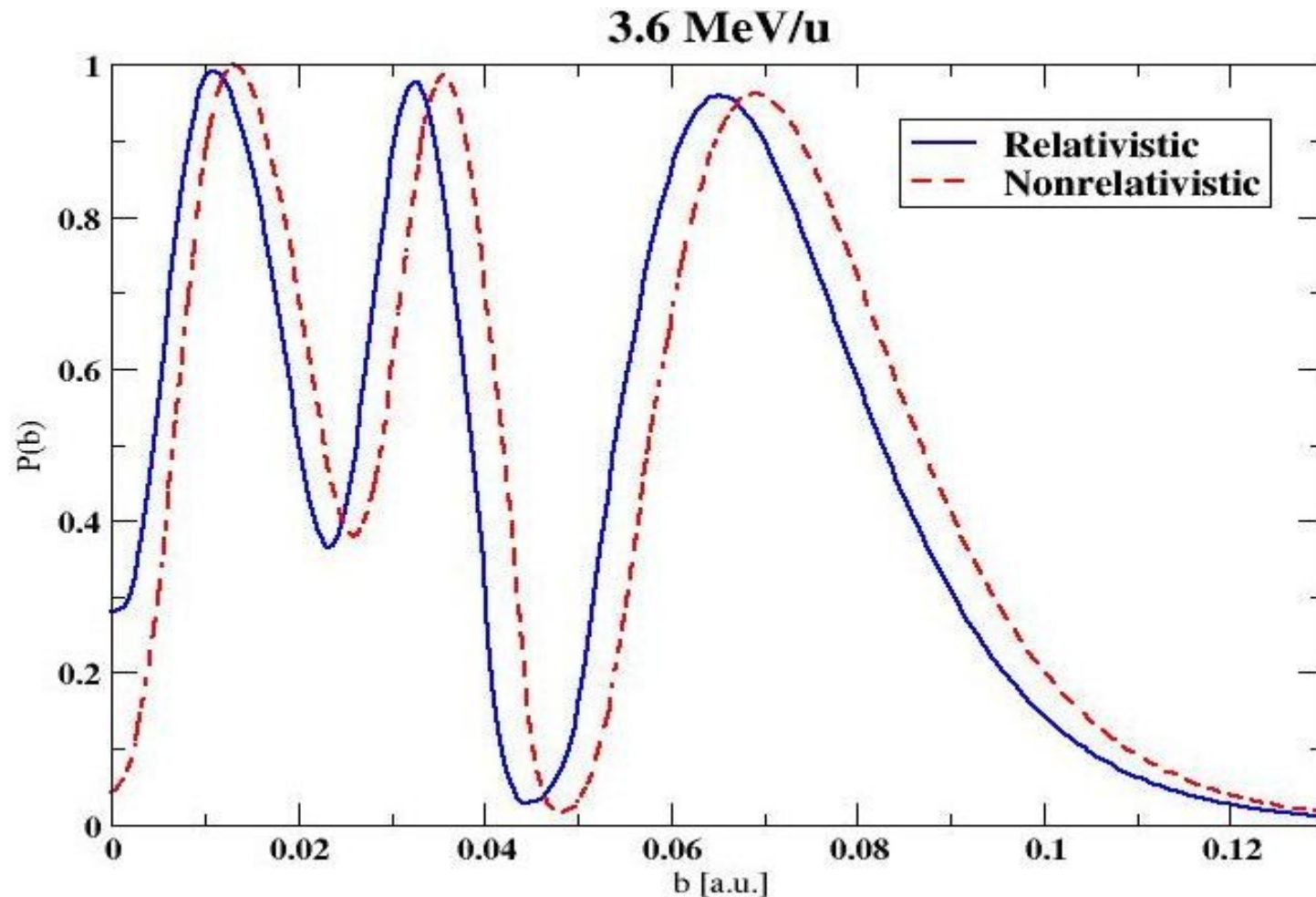
The probability of Ne K-shell-vacancy production as a function of the impact parameter b

Xe-Xe⁵³⁺(1s)



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

Xe-Xe⁵³⁺(1s)



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

Summary

- A new method employing the Dirac-Sturm (Dirac-Fock-Sturm) basis functions for evaluation of various electron-excitation processes 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 effects are investigated
-

Collaboration



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Many thanks to



Thank you very much for your attention!
