Relativistic Calculations of the Charge-Transfer Cross Sections for Low-Energy Heavy Ion Collisions

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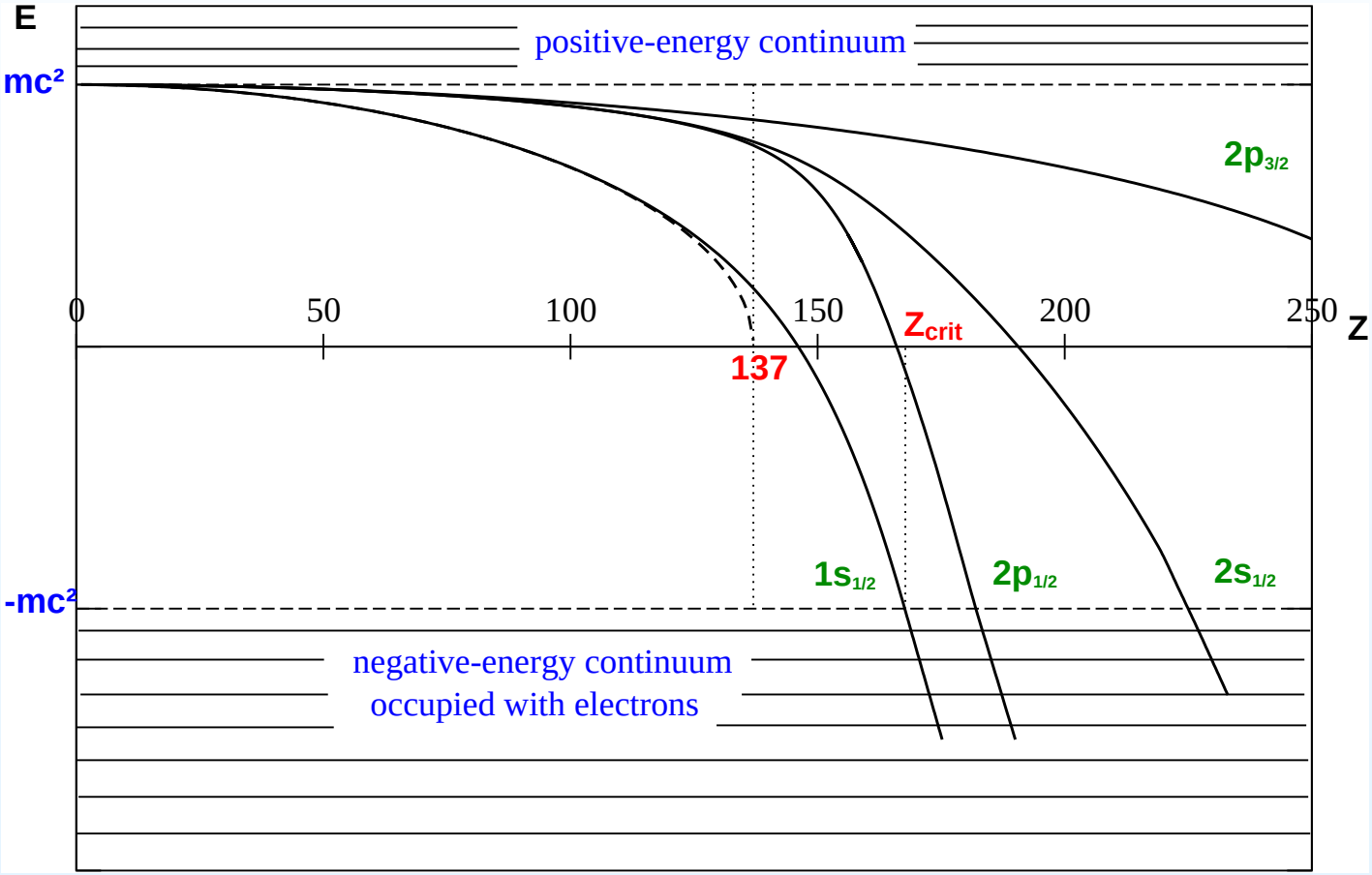
Motivation

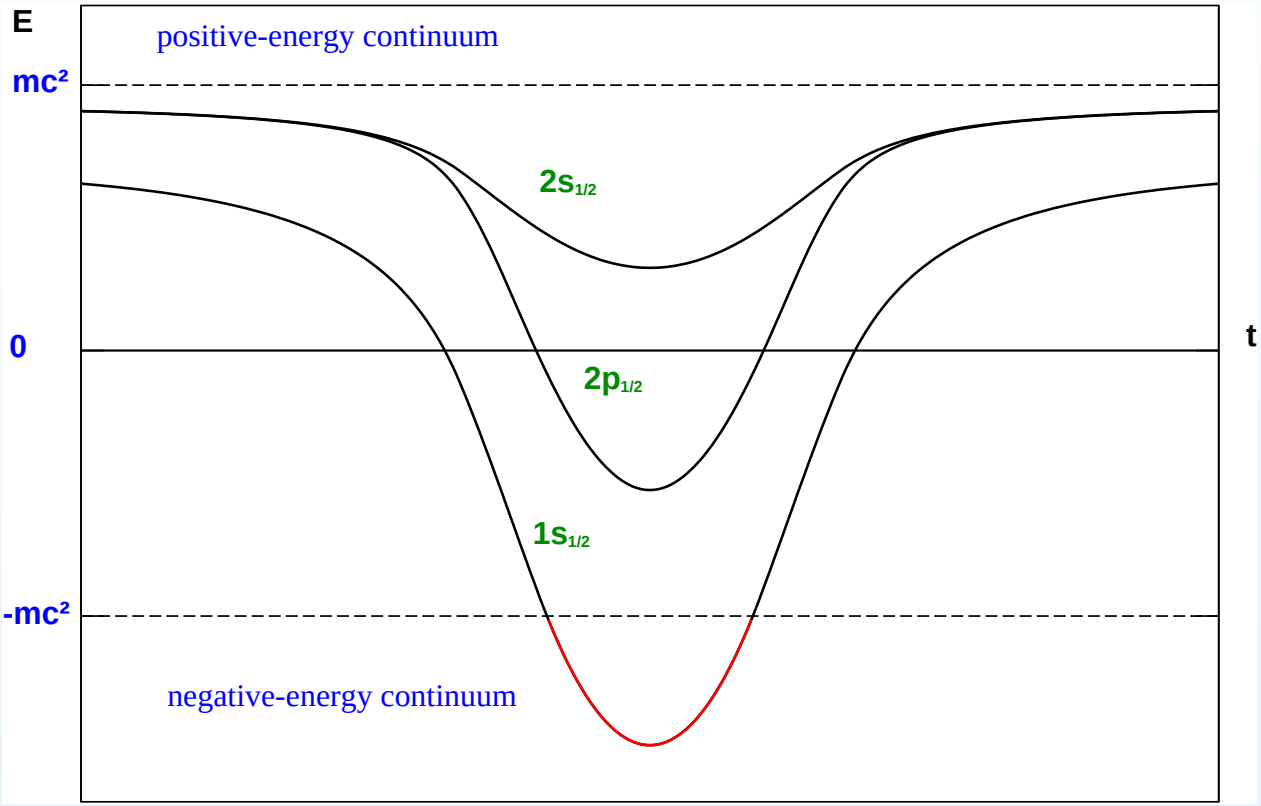
The $1s$ level dives into the negative-energy continuum at $Z_{\text{crit}} \approx 173$.



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

Motivation

The “diving” of the bound-state levels into the negative-energy continuum in heavy-ion collisions with $Z_1 + Z_2 > 173$.



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

Spontaneous e^+e^- pair creation time is about 10^{-19} sec. *[B. Müller et al., Phys. Rev. Lett., 28, 1235 (1972)]*

Two-center Dirac equation

Features of the investigated process:

Low-energy ions: ~ 6 MeV/u for U^{91+}-U^{92+}, $V_{\rm nucl} \sim 0.1c$

(~ 1 keV in the case of H-H^+)

Relativistic electron: $v_{\rm e} \sim (\alpha Z)c$

Nuclei ($\vec{R}_A, \vec{R}_B$) move according to the Rutherford trajectory.

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

$$i\frac{\partial \Psi(\vec{r},t)}{\partial t} = \hat{h}_{\rm D}\,\Psi(\vec{r},t), \qquad \hat{h}_{\rm D}\psi_n(\vec{r}) = \varepsilon_n\,\psi_n(\vec{r})\,, \tag{1}$$

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

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

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

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

$$H_{ij} = \langle \varphi_i \mid \hat{h}_{\mathrm{D}} \mid \varphi_j \rangle \, , \qquad T_{ij} = i \langle \varphi_i \mid \frac{\partial}{\partial t} \mid \varphi_j \rangle \, , \qquad S_{ij} = \langle \varphi_i \mid \varphi_j \rangle \, .$$

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.

Central field Dirac orbitals

$$\varphi_{n\kappa m}(\vec{r},\sigma) = \begin{pmatrix} \dfrac{P_{n\kappa}(r)}{r}\,\chi_{\kappa m}(\Omega,\sigma) \\ \\ i\,\dfrac{Q_{n\kappa}(r)}{r}\,\chi_{-\kappa m}(\Omega,\sigma) \end{pmatrix}$$

where $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small components, respectively.

The large and small radial components are obtained by solving numerically the Dirac equation in the central field potential $V(r)$ ($\hbar = e = m = 1$)

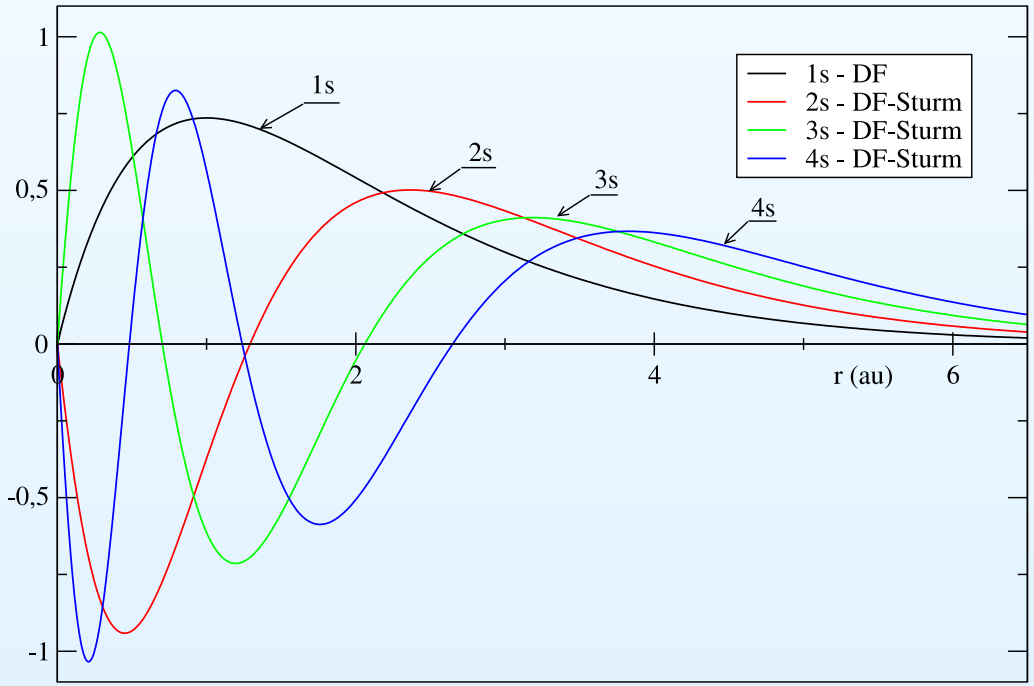
$$\begin{cases} c\left(-\dfrac{d}{dr} + \dfrac{\kappa}{r}\right) Q_{n\kappa}(r) + \left(V(r) + c^2\right)\, P_{n\kappa}(r) &= \varepsilon_{n\kappa}\, P_{n\kappa}(r) \\ c\left(\dfrac{d}{dr} + \dfrac{\kappa}{r}\right) P_{n\kappa}(r) + \left(V(r) - c^2\right)\, Q_{n\kappa}(r) &= \varepsilon_{n\kappa}\,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

Central field Dirac-Sturm orbitals

$$\begin{cases} c\left(-\frac{d}{dr}+\frac{\kappa}{r}\right)\overline{Q}_{n\kappa}(r)+\left(V(r)+c^2-\varepsilon_{n_0\kappa}\right)\overline{P}_{n\kappa}(r) & =\lambda_{n\kappa}\,W_\kappa(r)\,\overline{P}_{n\kappa}(r) \\ c\left(\frac{d}{dr}+\frac{\kappa}{r}\right)\overline{P}_{n\kappa}(r)+\left(V(r)-c^2-\varepsilon_{n_0\kappa}\right)\overline{Q}_{n\kappa}(r) & =\lambda_{n\kappa}\,W_\kappa(r)\,\overline{Q}_{n\kappa}(r) \end{cases}$$

Here $\varepsilon_{n_0\kappa}$ is the fixed energy, $\lambda_{n\kappa}$ is an eigenvalue of the Dirac-Sturm operator, $W(r)$ is a weight function: $W(r) = -\frac{1-\exp(-(\alpha\,r)^2)}{(\alpha\,r)^2}$.

Sturmian orbitals. Hydrogen



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

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

where (for the point nucleas case)

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

Basis set advantages

- 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 **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.

Two-center problem. Energy levels of quasi-molecule

Finite basis expansion

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

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

Basis 1: Positive: $1s$-$3s$, $2p$, $3p$, $3d$, $\overline{4s}$-$\overline{6s}$, $\overline{4p}$-$\overline{6p}$, $\overline{4d}$-$\overline{6d}$, $\overline{4f}$, $\overline{5f}$: 220 functions

Negative: $-\overline{1s}$-$(-\overline{6s})$, $-\overline{2p}$-$(-\overline{6p})$ $\ldots$: 220 functions

Basis 2: Positive: $1s$, $\overline{2s}$-$\overline{8s}$, $\overline{2p}$-$\overline{8p}$, $\overline{3d}$-$\overline{8d}$, $\overline{4f}$-$\overline{6f}$, $\overline{4f}$, $\overline{6f}$: 392 functions

Negative: $-\overline{1s}$-$(-\overline{6s})$, $-\overline{2p}$-$(-\overline{6p})$ $\ldots$: 392 functions

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

The "chemical" inter-nuclear distance R_{AB}=2.0/Z (a.u.).

Calculations are performed for the Point Nucleus case.

	H_2^+ $(Z=1)$		Th_2^{+179} $(Z=90)$	
	$\varepsilon_{1\sigma_+}$	Relative Error	$\varepsilon_{1\sigma_+}$	Relative Error
Basis 1	-1.1026248	$1.5 \cdot 10^{-5}$	-9504.573	$1.9 \cdot 10^{-5}$
Basis 2	-1.1026405	$1.0 \cdot 10^{-6}$	-9504.732	$2.5 \cdot 10^{-6}$
“Exact"	-1.1026416^a		-9504.756^b	

^{a} *[L. Yang, D. Heinemann, D. Kolb, Chem. Phys. Lett., 178, 213 (1991)]*

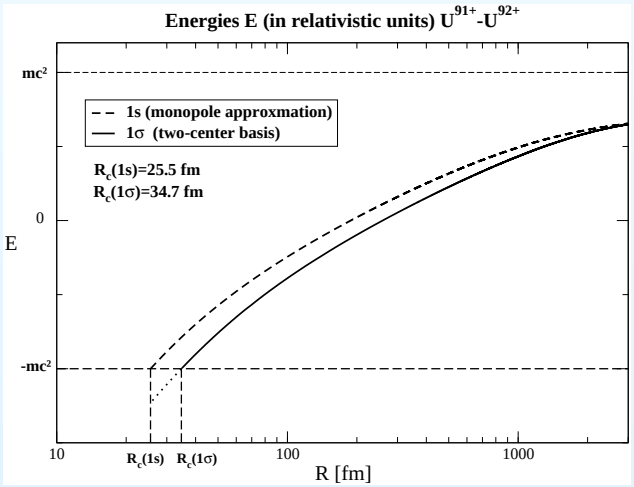
^{b} *[O. Kullie, D. Kolb, Eur. Phys. J. D, 17, 167 (2001)]*

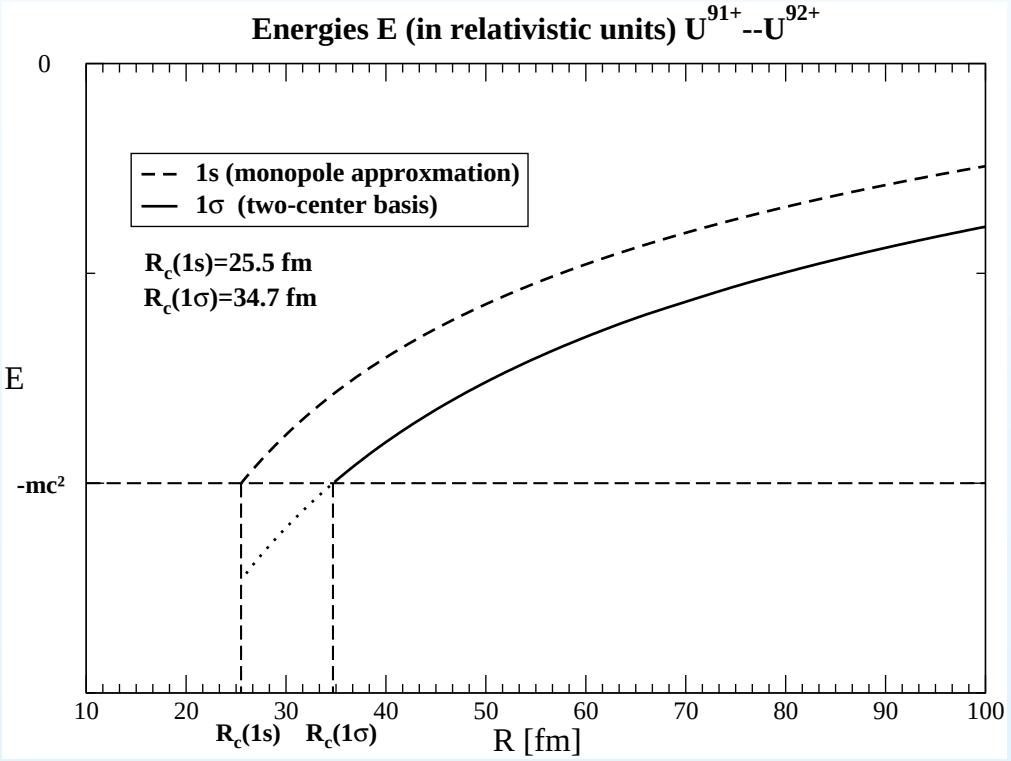
Energies of the $1\sigma_+$ ground states of quasi-molecules

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

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

$R_{\rm crit}(1\sigma_+) = 34.7$ 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)]*

Charge-transfer and Ionization Probabilities

The probabilities of the charge transfer $W_{n\kappa}^{(\mathrm{ct})}$ and direct excitations $W_{n\kappa}^{(\mathrm{d})}$ to the state $n\kappa$ are given by

$$\begin{aligned} W_{n\kappa}^{(\mathrm{d})} &= \lim_{t\to\infty} \sum_{\mu} \left| \langle \Psi(\vec{r},t) \mid \psi_{n\kappa\mu}(\vec{r}_A,t) \rangle \right|^2 , \\ W_{n\kappa}^{(\mathrm{ct})} &= \lim_{t\to\infty} \sum_{\mu} \left| \langle \Psi(\vec{r},t) \mid \psi_{n\kappa\mu}(\vec{r}_B,t) \rangle \right|^2 . \end{aligned}$$

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

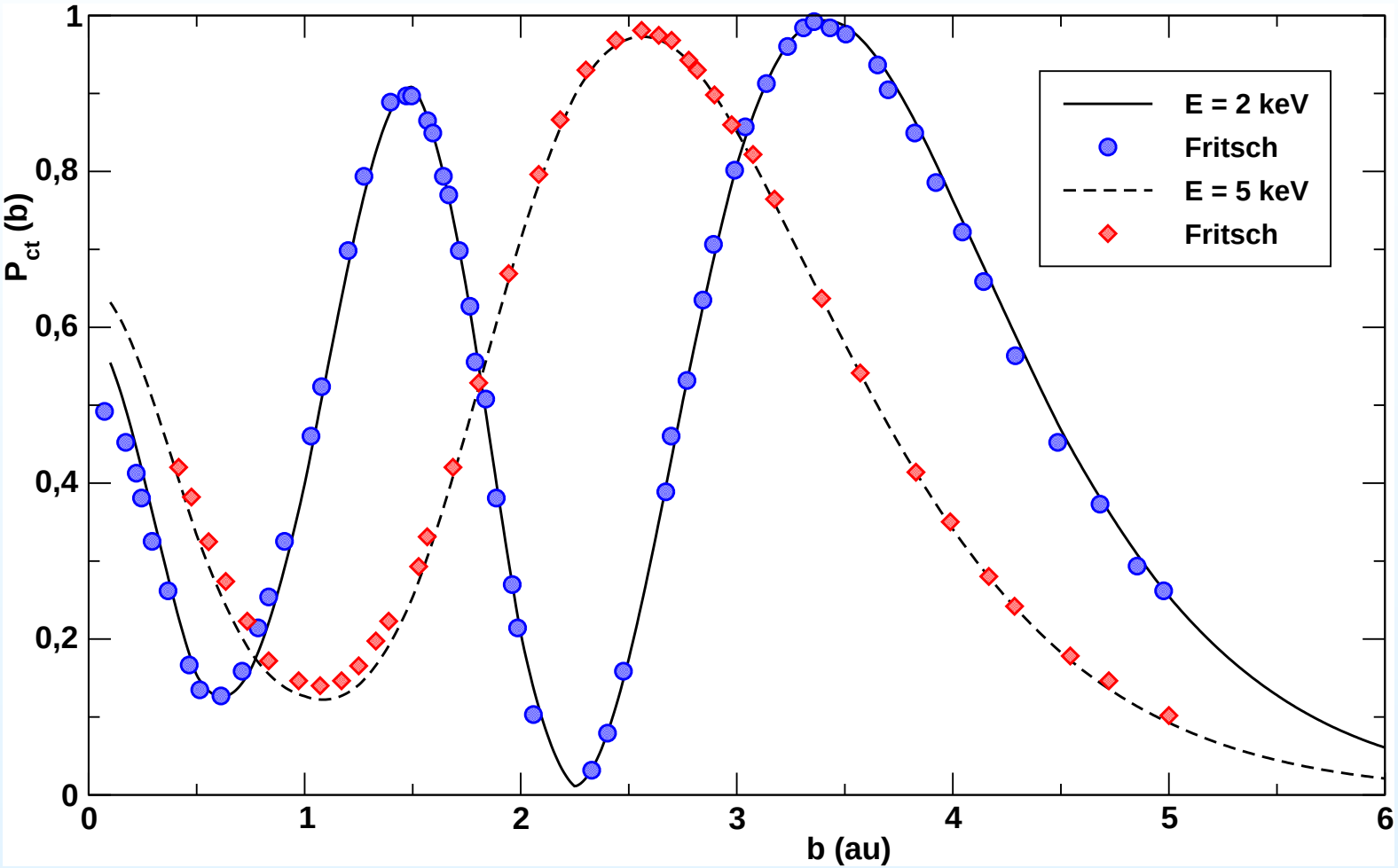
$$P_{\mathrm{d}} = \sum_{n\kappa \neq 1s} W_{n\kappa}^{(\mathrm{d})} , \quad P_{\mathrm{ct}} = \sum_{n\kappa} W_{n\kappa}^{(\mathrm{ct})} , \quad P_{\mathrm{ion}} = 1 - P_{\mathrm{d}} - P_{\mathrm{ct}} - W_{1s}^{(\mathrm{d})} .$$

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

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

$H(1s)–H^+$ collision

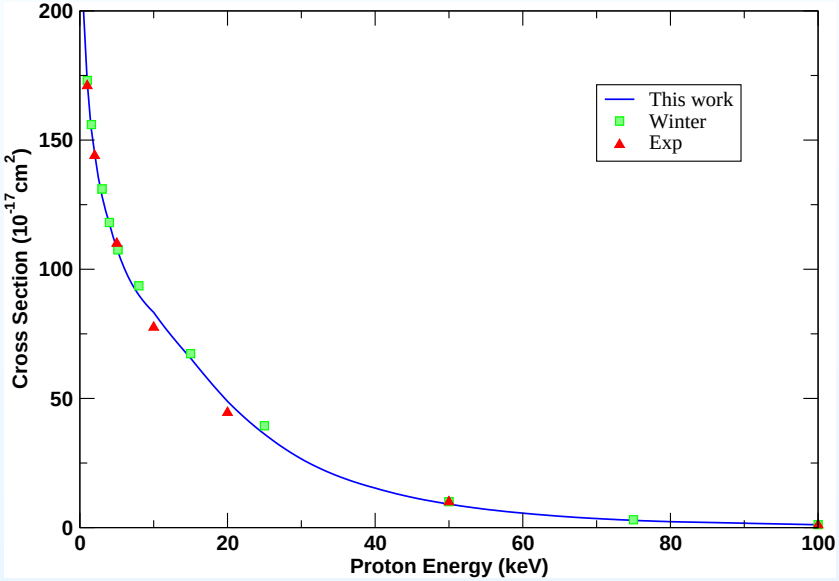
Charge-transfer probability as a function of the impact parameter b

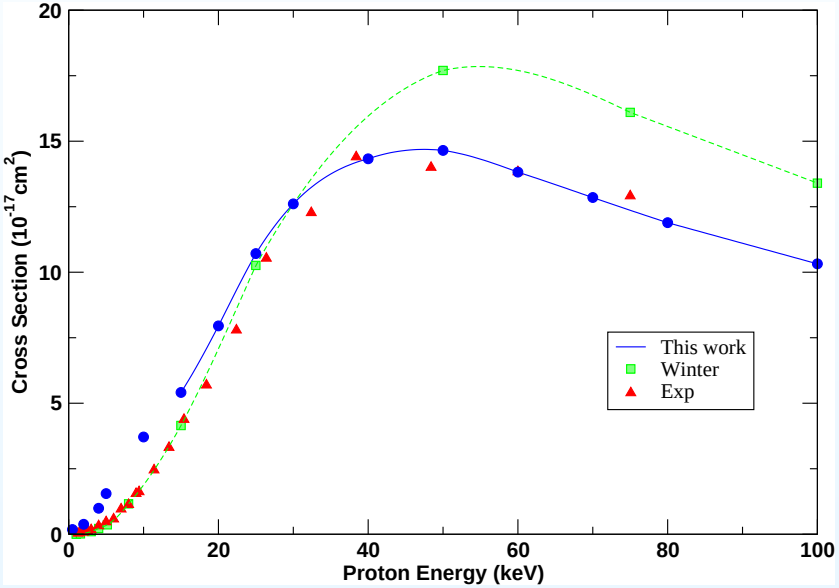


Comparison with the results of work *[W. Fritsch et al., Phys. Rep., 202, 1 (1991)]*

$H(1s)–H^+$ 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 A$^{(Z-1)+}$(1s)– A^{Z+} and H(1s)–H^{+} collisions

$$
\begin{cases}
\vec{r}' &= Z\,\vec{r} \\
\vec{R}'_A &= Z\,\vec{R}_A \\
\vec{R}'_B &= Z\,\vec{R}_B \\
t' &= Z^2\,t \\
E' &= E/Z^2 \\
\vec{V}'_A &= \vec{V}_A/Z \\
\vec{V}'_B &= \vec{V}_B/Z \\
\sigma'_{\rm ct} &= \sigma_{\rm ct}\,Z^2
\end{cases}
\qquad
\begin{cases}
\vec{r} &= \vec{r}'/Z \\
\vec{R}_A &= \vec{R}'_A/Z \\
\vec{R}_B &= \vec{R}'_B/Z \\
t &= t'/Z^2 \\
E &= E'\,Z^2 \\
\vec{V}_A &= \vec{V}'_A\,Z \\
\vec{V}_B &= \vec{V}'_B\,Z \\
\sigma_{\rm ct} &= \sigma'_{\rm ct}/Z^2
\end{cases}
$$

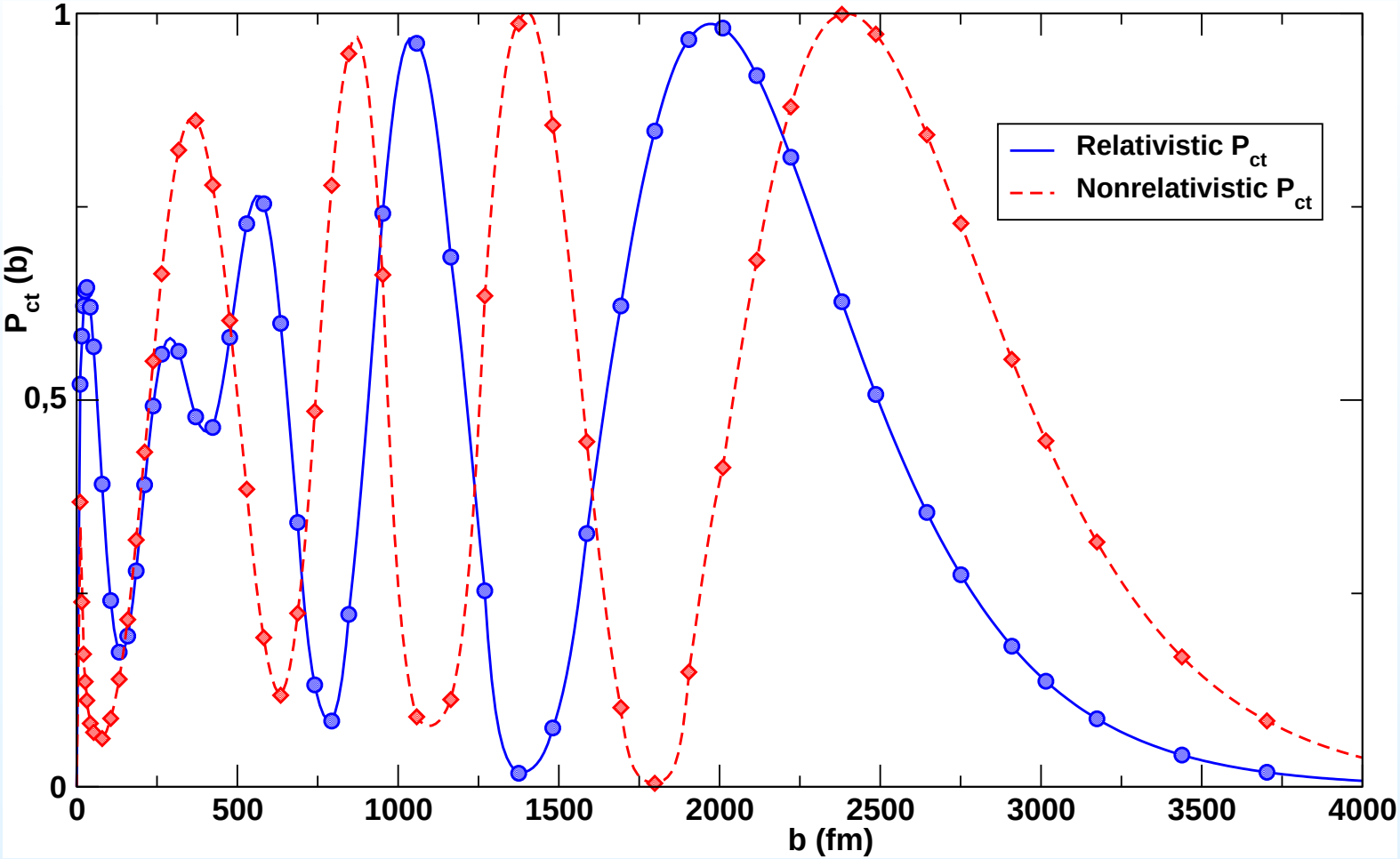
$U^{91+}(1s)$–U^{92+}

Charge-transfer cross section $\sigma_{\rm ct}$ (10^{-17} cm^2) for the $U^{91+}(1s)$–U^{92+} and $H(1s)$–H^+ collisions

$U^{91+}(1s)$–U^{92+}				$H(1s)$–H^+	
Energy E (MeV/u)	$\sigma_{\rm ct} \cdot Z^2$ Rel.	$\sigma_{\rm ct} \cdot Z^2$ Nonrel.	$\sigma_{\rm ct} \cdot Z^2$ Nonrel. straight-line	Energy E (keV/u)	$\sigma_{\rm ct}$
6.0	135.3	184.4	185.7	0.709	186.1
6.5	132.7	182.0	183.2	0.768	183.4
7.0	130.3	179.5	180.6	0.827	181.2
10.0	118.0	165.0	166.1	1.181	166.4

$U^{91+}(1s)$–U^{92+}

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



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**

For more details:

I.I. Tupitsyn, Y.S. Kozhedub, V.M. Shabaev, G.B. Deyneka, S. Hagmann,

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e-print arXiv:1004.5131; PRA in press.

I.I. Tupitsyn, Y.S. Kozhedub, V.M. Shabaev, G.B. Deyneka, S. Hagmann,

C. Kozhuharov, G. Plunien, Th. Stöhlker,
Phys.Rev.A, v.82, p.042701 (2010).

Dirac Equation in the Finite Basis Set.

- Central field Dirac Bispinors

$$\Psi_{n\kappa\mu}(\vec{r},\tau) = \begin{pmatrix} \dfrac{P_{n\kappa}(r)}{r}\,\chi_{\kappa\mu}(\Omega,\sigma) \\ i\,\dfrac{Q_{n\kappa}(r)}{r}\,\chi_{-\kappa\mu}(\Omega,\sigma) \end{pmatrix} \qquad \kappa = (-1)^{l+j+1/2}(j+1/2)$$

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

where $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are large and small components, respectively.

- Dirac Equation in the central field ($\hbar$=e=m=1)

$$\begin{cases} c\left(-\dfrac{d}{dr}+\dfrac{\kappa}{r}\right) Q_{n\kappa}(r) + \hat{V}(r)\,P_{n\kappa}(r) &= \varepsilon_{n\kappa}\,P_{n\kappa}(r) \\ c\left(\dfrac{d}{dr}+\dfrac{\kappa}{r}\right) P_{n\kappa}(r) + \left(\hat{V}(r)-2c^2\right) Q_{n\kappa}(r) &= \varepsilon_{n\kappa}\,Q_{n\kappa}(r) \end{cases}$$

For the point nucleus $V(r) = -Z/r$

Finite Basis set expansion

$$\begin{cases} P_{n\kappa}(r) &= \sum_{i=1}^{M} C_{in}^{P}(\kappa)\,\varphi_i(r) \\ Q_{n\kappa}(r) &= \sum_{i=1}^{M} C_{in}^{Q}(\kappa)\,\varphi_i(r)\,. \end{cases} \qquad , \qquad \langle \varphi_i \mid \varphi_j \rangle = \delta_{ij}$$

Matrix Eigenvalue Problem

$$H^D(\kappa) \begin{pmatrix} \vec{C}_n^P(\kappa) \\ \vec{C}_n^Q(\kappa) \end{pmatrix} = \begin{pmatrix} V & cA^+(\kappa) \\ cA(\kappa) & V - 2c^2 \end{pmatrix} \begin{pmatrix} \vec{C}_n^P(\kappa) \\ \vec{C}_n^Q(\kappa) \end{pmatrix} = \varepsilon_{n\kappa} \begin{pmatrix} \vec{C}_n^P(\kappa) \\ \vec{C}_n^Q(\kappa) \end{pmatrix},$$

where $M \times M$ matrices $A(\kappa)$ and V are given by

$$A_{ij}(\kappa) = \langle i \mid \hat{A}(\kappa) \mid j \rangle\,, \qquad V_{ij} = \langle i \mid \hat{V} \mid j \rangle\,.$$

Nonrelativistic limit. $c \to \infty$.

$$
\begin{aligned}
Q_{n\kappa}(r) &\to \frac{1}{2c}\,\hat{A}(\kappa)\,P_{n\kappa}(r) = \frac{1}{2c}\left(\frac{d}{dr} + \frac{\kappa}{r}\right) P_{n\kappa}(r) \\
\vec{C}^{Q}(\kappa) &\to \frac{1}{2c}\,A(\kappa)\,\vec{C}^{P}(\kappa)\,,
\end{aligned}
$$

Then

$$
\begin{aligned}
\left(\frac{1}{2}\,\hat{A}^{+}(\kappa)\,\hat{A}(\kappa) + \hat{V}\right) P_{n\kappa}(r) &= \varepsilon_{n\kappa}\,P_{n\kappa}(r) \\
\left(\frac{1}{2}\,A^{+}(\kappa)\,A(\kappa) + V(r)\right) \vec{C}^{P}_{n}(\kappa) &= \varepsilon_{n\kappa}\,\vec{C}^{P}_{n}(\kappa)
\end{aligned}
$$

$$
\hat{H}_{\rm nr} = \frac{1}{2}\hat{A}^{+}(\kappa)\,\hat{A}(\kappa) + \hat{V} = -\,\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + \hat{V}(r)
$$

For matrices

$$
\left(A^{+}(\kappa)\,A(\kappa)\right)_{ij} \neq \left\langle i \mid \hat{A}^{+}(\kappa)\,\hat{A}(\kappa) \mid j \right\rangle = \left(-\,\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}\right)_{ij}
$$

Operator $\hat{B}(\kappa)$ and matrix $B(\kappa)$

$$\hat{B}(\kappa) = \hat{A}(\kappa) - Z/\kappa = \left(\frac{d}{dr} + \frac{\kappa}{r}\right) - Z/\kappa\,, \qquad B(\kappa) = A(\kappa) - Z/\kappa\,.$$

$$\hat{B}^+(\kappa) = -\hat{B}(-\kappa)\,, \qquad B^+(\kappa) = -B(-\kappa)\,.$$

Then for $V(r) = -Z/r$

$$\begin{aligned}
\hat{B}^+(\kappa)\,\hat{B}(\kappa) &= \hat{A}^+(\kappa)\,\hat{A}(\kappa) + 2\,\hat{V} + \frac{Z^2}{\kappa^2}\,. \\
B^+(\kappa)\,B(\kappa) &= A^+(\kappa)\,A(\kappa) + 2\,V + \frac{Z^2}{\kappa^2}\,.
\end{aligned}$$

and

$$\begin{aligned}
\hat{B}^+(-\kappa)\,\hat{B}(-\kappa) &= \hat{B}(\kappa)\,\hat{B}^+(\kappa) \\
B^+(-\kappa)\,B(-\kappa) &= B(\kappa)\,B^+(\kappa)
\end{aligned}$$

Another form of the H-like Schrödinger equation

$$\hat{H}_{\rm nr}(\kappa) = -\frac{1}{2}\,\hat{A}(\kappa)\,\hat{A}^{+}(\kappa) + \hat{V}(r) = \frac{1}{2}\,\hat{B}^{+}(\kappa)\,\hat{B}(\kappa) \;-\; \frac{Z^2}{2\kappa^2}\,.$$

Define the operator $\hat{H}_\lambda(\kappa)$ and eigenvalues $\lambda_n(\kappa)$

$$\hat{H}_\lambda(\kappa) \;=\; \hat{H}_{\rm nr}(\kappa) + \frac{Z^2}{2\kappa^2} \;=\; \frac{1}{2}\,\Big[\hat{B}^{+}(\kappa)\,\hat{B}(\kappa)\Big]\,, \quad \lambda_n(\kappa) \;=\; \varepsilon_{n\kappa} \;+\; \frac{Z^2}{2\kappa^2}\,.$$

Then

$$\hat{H}_\lambda(\kappa)\,P_{n\kappa}(r) \;=\; \frac{1}{2}\,\Big[\hat{B}^{+}(\kappa)\,\hat{B}(\kappa)\Big]\;P_{n\kappa}(r) \;=\; \lambda_n(\kappa)\,P_{n\kappa}(r)\,,$$

and

$$\hat{H}_\lambda(-\kappa) \;=\; \frac{1}{2}\,\hat{B}^{+}(-\kappa)\,\hat{B}(-\kappa) = \frac{1}{2}\,\hat{B}(\kappa)\,\hat{B}^{+}(\kappa)$$

Spurious States in the Nonrelativistic Limit.

The nonzero eigenvalues of the operators $\hat{B}\hat{B}^+$ and $\hat{B}^+\hat{B}$ coincide.

$$\hat{B}^+\,\hat{B}\,\varphi = \lambda\,\varphi \quad \Longrightarrow \quad \hat{B}\,\hat{B}^+\left(\hat{B}\,\varphi\right) = \lambda\left(\hat{B}\,\varphi\right).$$

If $B\,\varphi = 0$, then $\lambda = 0$.

Conclusion.

The eigenvalues of the operators $\hat{H}_{\rm nr}(\kappa)$ and $\hat{H}_{\rm nr}(-\kappa)$ coincide, except $\varepsilon_{n\kappa} = -Z^2/2\kappa^2$.
The states

$$\begin{aligned} \kappa &< 0: \quad 2s_{1/2}, \quad 3p_{3/2}, \quad 4d_{5/2}, \quad 5f_{7/2}, \quad \ldots \\ \kappa &> 0: \quad 2p_{1/2}, \quad 3d_{3/2}, \quad 4f_{5/2}, \quad 5g_{7/2}, \quad \ldots \end{aligned}$$

have the same energies.

Finite basis equations in the nonrelativistic limit.

In the nonrelativistic limit for the finite basis set we have

$$\overline{H}_\lambda(\kappa)\,\vec{C}^P_{n\kappa} \;=\; \lambda_{n\kappa}\,\vec{C}^P_{n\kappa}\,,$$

where

$$\overline{H}_\lambda(\kappa) = \frac{1}{2}\,B^+(\kappa)\,B(\kappa)\,, \qquad \lambda_{n\kappa} = \varepsilon_{n\kappa} - \frac{Z^2}{2\kappa^2}\,.$$

Thorem.

All eigenvalues (including zero eigenvalues) of the $M \times M$ matrices BB^+ and B^+B coincide.

Conclusion.

All eigenvalues of the matrices $\overline{H}_{\rm nr}(\kappa)$ and $\overline{H}_{\rm nr}(-\kappa)$ coincide.
The states

$$\begin{aligned}
\kappa < 0: &\quad 1s_{1/2}, \quad 2s_{1/2}, \quad 2p_{3/2}, \quad 3p_{3/2}, \quad 3d_{5/2}, \quad 4d_{5/2}, \quad \ldots \\
\kappa > 0: &\quad \overline{1p}_{1/2}, \quad 2p_{1/2}, \quad \overline{2d}_{3/2}, \quad 3d_{3/2}, \quad \overline{3f}_{5/2}, \quad 4f_{5/2}, \quad \ldots
\end{aligned}$$

have the same energies.

Spurious States in the the nonrelativistic limit

The Spurious states are:

$$\kappa > 0: \quad \overline{1p}_{1/2}, \quad \overline{2d}_{3/2}, \quad \overline{3f}_{5/2}, \quad \overline{4g}_{7/2}, \quad \ldots$$