Ab initio Studies of Rubidium Ionisation Processes

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1. Overview of the Applied Theory
2. Results and Further Plans
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Photoionisation processes are studied via *ab initio* calculations.

One active electron approach has been applied.

The Hamilton operator has the form of

$$H = H_{Rb} + V_I \tag{1}$$

Hamilton operator of the Rb atom [1]:

$$H_{Rb} = -\frac{1}{2}\nabla^2 - \frac{1}{r}(1 - be^{-dr}) \tag{2}$$

with $b = 4.5$ and $d = 1.09993$.

The interaction operator [2]:

$$V_I = -\frac{1}{2}\Omega_{kj}(t)\exp\left[i\varepsilon_{kj}(t)t\right] \tag{3}$$

with the Rabi frequency being:

$$\Omega_{kj}(t) = d_{kj}A(t) \tag{4}$$

with d_{kj} being the dipole matrix element between the $|k\rangle$ and $|j\rangle$ states, $A(t)$ amplitude of the electromagnetic field. The EM field may have the following type:

- Planewave pulse with $\sin^2$ temporal envelope
- Gaussian beam [3]
- Maxwell–Gaussian beam [4]

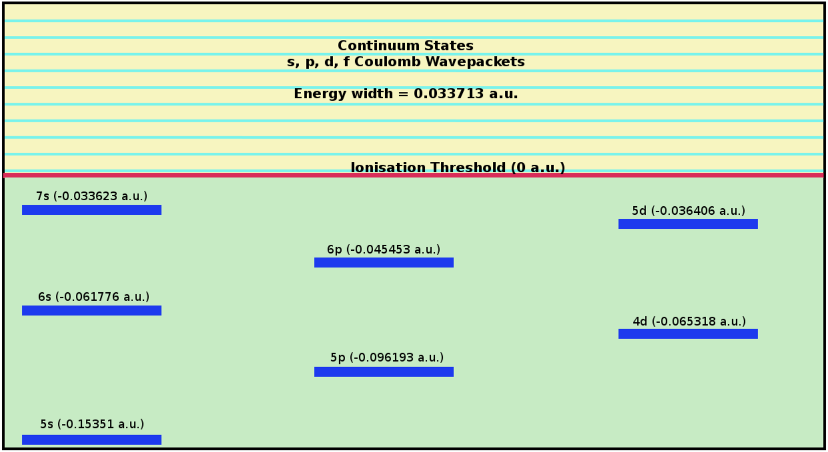

FIGURE : Graphical overview of the spectrum of the Rubidium atom and ion.

The bound and the continuum states of the valence electron are described with Slater-type orbitals and Coulomb wavepackets [5], respectively:

$$\chi_{n,l,m,\kappa}(\vec{r}) = C(n,\kappa) r^{n-1} e^{-\kappa r} Y_{l,m}(\theta,\varphi) \tag{5}$$

$$\varphi_{k,l,m,\tilde{Z}}(\vec{r}) = N(k,\Delta k) \int_{k-\Delta k/2}^{k+\Delta k/2} F_{l,\tilde{Z}}(k',r) dk' \, Y_{l,m}(\theta,\varphi) \tag{6}$$

$$F_{l,\tilde{Z}}(k,r) = \sqrt{\frac{2k}{\pi}} \exp\left(\frac{\pi \tilde{Z}}{2k}\right) \frac{(2kr)^l}{(2l+1)!} \exp(-ikr) \left|\Gamma(l+1-i\tilde{Z}/k)\right| \times {}_1F_1(1+l+i\tilde{Z}/k, 2l+2, 2ikr) \tag{7}$$

The variation principle yields the spectrum of the bound states. Since the Slater-functions are not orthogonal to each other, one has to solve a generalized eigenvalue problem:

$$\mathbf{Hc} = E\mathbf{Sc} \tag{8}$$

with

$$H_{ij} = \left\langle \psi_i \middle| \hat{H} \middle| \psi_j \right\rangle \tag{9}$$

and

$$S_{ij} = \langle \psi_i | \psi_j \rangle \tag{10}$$

The variational parameters are the κ screening factors.

The energy and width of the Coulomb wavepackets depends on the integration limits. Since the Slater–packet overlap is nonzero—it has an order of magnitude of 10^{-2}—the presence of the packets slightly shifts the energy of the bound states.

We apply the following Ansatz for the time-dependent Schrödinger equation:

$$\Psi(\vec{r},t) = \sum_{j=1}^{N} a_j(t)\Phi_j(\vec{r})e^{-iE_j t} \tag{11}$$

We get the following system of equations for the $a_j(t)$ coefficients:

$$\frac{\mathrm{d}a_k(t)}{\mathrm{d}t} = -i\sum_{j=1}^{N} V_{kj}(t)e^{-i(E_j-E_k)t}a_j(t) \quad (k = 1\dots N) \tag{12}$$

with

$$V_{kj}(t) = \langle\Phi_k|\hat{V}(t)|\Phi_j\rangle \tag{13}$$

being the couplings matrix, $\Phi_k(\vec{r})$ is either a Slater-type orbital or a Coulomb wavepacket.

Initial conditions:

$$a_k\left(t \to -\infty\right) = \begin{cases} 1 & k = 1 \\ 0 & k \neq 1 \end{cases} \tag{14}$$

Final state probabilities:

$$P_k(t \to \infty) = \left|a_k(t \to \infty)\right|^2 \tag{15}$$

Electron density after the ionisation has happened:

$$\varrho(\vec{r}) = \left\langle \Psi(\vec{r}', t \to \infty) \middle| \delta(\vec{r}) \middle| \Psi(\vec{r}', t \to \infty) \right\rangle \tag{16}$$

The ionisation caused by a 400 GeV proton beam originates in photoionisation via the Weizsäcker–Williams method.

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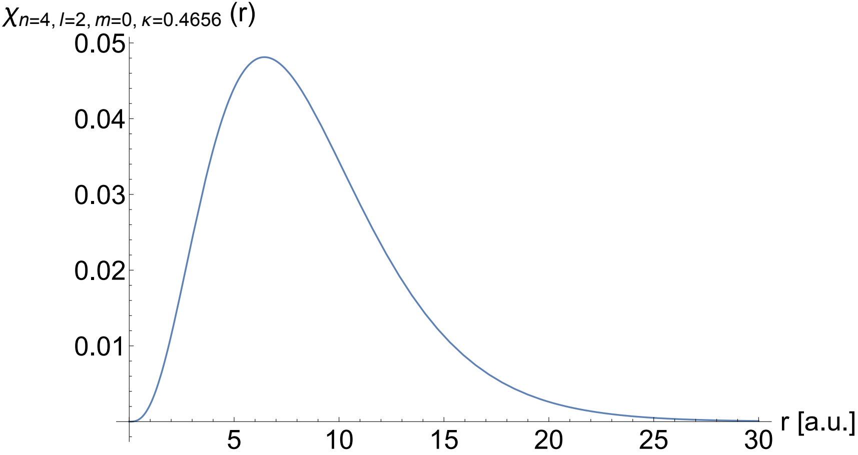

FIGURE : Slater-type orbital corresponding to the 4*d* state.

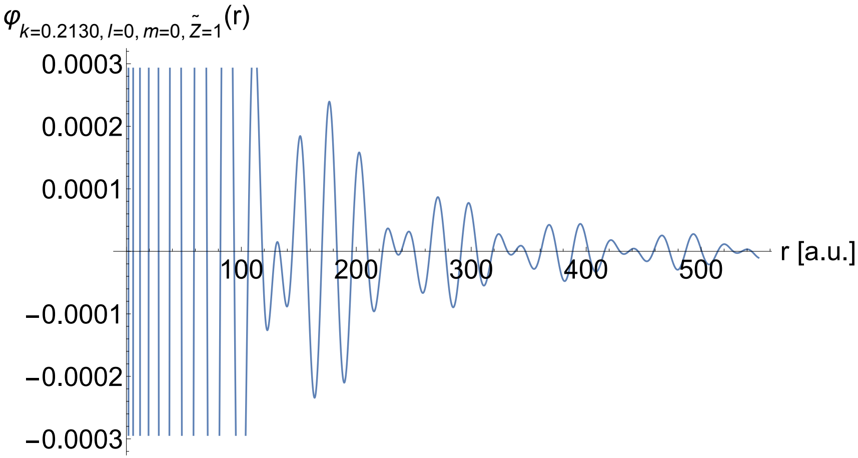

FIGURE : *s* wavefunction of the electron after absorbing a photon.

The Coulomb packets have been constructed according to

$$E_\gamma(800nm) = 0.0570\,\mathrm{a.u.} \tag{17}$$
$$E_{7s} = -0.0315\,\mathrm{a.u.} \tag{18}$$
$$\Delta E = E_\gamma/4 \tag{19}$$
$$E_{max} = E_{7s} + 3E_\gamma \tag{20}$$

The total energy range given above can be split into ten ΔE width parts. For every part there exists a package with s, p, d and f azimuthal quantum number, respectively (40 total).

The spectrum of the bound states:

κ [1]	E_{exp} [a.u.]	E_{opt}	E_{calc} [a.u.]
1.35789	-0.153507	-0.144606	-0.148578
0.747335	-0.0617762	-0.0590814	-0.0649904
0.162072	-0.0336229	-0.0317344	-0.0370498
0.285925	-0.0211596	-0.0196661	-0.0236445
0.563253	-0.0145428	-0.0132598	-0.0161758
0.0995939	-0.0106093	-0.0093473	-0.011617
0.177069	-0.00808107	-0.00685427	-0.00856655
0.192805	-0.00636018	-0.00463121	-0.00653549

TABLE : The spectrum of the bound states: E_{ns}. $n = 5 \ldots 13$

The spectrum of the bound states:

κ [1]	E_{exp} [a.u.]	E_{opt}	E_{calc} [a.u.]
0.934074	-0.0961927	-0.0961927	-0.102753
0.0606182	-0.0454528	-0.0454529	-0.0500378
0.593825	-0.0266809	-0.0266805	-0.0293907
0.360146	-0.0175686	-0.0175692	-0.0191912
0.257965	-0.0124475	-0.0124474	-0.0134602
0.10425	-0.00928107	-0.00928073	-0.00994177
0.117591	-0.00718653	-0.00718617	-0.00763469
0.0654625	-0.00572873	-0.00572882	-0.00604301
0.111322	-0.0046738	-0.004674	-0.00489973
0.0972476	-0.0038856	-0.00388597	-0.00405129
0.0594662	-0.00328125	-0.0032817	-0.00340454
0.091899	-0.00280771	-0.00280802	-0.00290064
0.0660554	-0.00242976	-0.00242971	-0.00250062
0.0886535	-0.00212316	-0.00212282	-0.00217684
0.0606625	-0.0018712	-0.00187064	-0.00190818

The spectrum of the bound states:

κ [1]	E_{exp} [a.u.]	E_{opt}	E_{calc} [a.u.]
0.465587	-0.0653178	-0.0543145	-0.0544901
0.260371	-0.0364064	-0.0306089	-0.0307153
0.142432	-0.0227985	-0.0196441	-0.019709
0.231017	-0.0155403	-0.0136696	-0.0137109
0.12431	-0.0112513	-0.0100561	-0.0100841
0.144521	-0.00851559	-0.00770051	-0.0077216
0.107533	-0.00666683	-0.00606339	-0.00608392

TABLE : The spectrum of the bound states: E_{nd}. $n = 4 \dots 10$

The spectrum of the bound states:

κ [1]	E_{exp} [a.u.]	E_{opt}	E_{calc} [a.u.]
0.247252	-0.0314329	-0.0312247	-0.031225
0.164201	-0.0201073	-0.019978	-0.0199783
0.115393	-0.0139554	-0.0138729	-0.0138734
0.108716	-0.0102476	-0.0101934	-0.0101937
0.187485	-0.00784234	-0.007803	-0.00780359

TABLE : The spectrum of the bound states: E_{nf}. $n = 4 \dots 8$

Ionisation cross-sections as a function of laser intensity: approx. $0.1\,\mathrm{Mb}$–$10-15\,\mathrm{Mb}$, e.g. [6] Estimation of the collision-ionisation cross-section (proton beam):

$$\lg\left(\frac{\sigma}{Z_p}\right) = 3.86 - 0.87\lg\left(\frac{v_p^2}{Z_p}\right) \tag{21}$$

$\sigma \approx 35\,\mathrm{Mb}$

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Thank you for your attention!