Hollow-atom probing of surfaces
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Atomic Units

Atomic units are based on typical dimensions of the Hydrogen atom. The *length* is the classical radius of the hydrogen electron orbital in the 1s ground state. The *velocity* is the classical hydrogen ground state electron velocity and *time* is given by the ratio of length and velocity. *Charge* is the charge of the electron, *mass* is the mass of the electron and *energy* is the sum of the kinetic and potential energy of the hydrogen 1s electron (≈ 2 × 13.604 eV).

<table>
<thead>
<tr>
<th></th>
<th>Formula</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>length</td>
<td>Bohr radius $a_0$</td>
<td>$5.2918 \cdot 10^{-11}$ m</td>
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<tr>
<td>velocity</td>
<td>$ac$</td>
<td>$2.1877 \cdot 10^6$ m/s</td>
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<tr>
<td>time</td>
<td>$a_0/ac$</td>
<td>$2.4188 \cdot 10^{-17}$ s</td>
</tr>
<tr>
<td>charge</td>
<td>$e$</td>
<td>$1.6022 \cdot 10^{-19}$ C</td>
</tr>
<tr>
<td>mass</td>
<td>$m_e$</td>
<td>$9.1095 \cdot 10^{-31}$ kg</td>
</tr>
<tr>
<td>energy</td>
<td>$E_0 = m(ac)^2$</td>
<td>$4.3593 \cdot 10^{-18}$ J</td>
</tr>
<tr>
<td>angular momentum</td>
<td>$\hbar$</td>
<td>$1.0546 \cdot 10^{-34}$ J s</td>
</tr>
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</table>
This appendix presents a short evaluation of the time spread of the beam pulses produced by the Sirifo chopper–sweeper system. In principle the working of the chopper is such that, at the moment the plate voltage switches from positive to negative potential, only those ions which reside halfway the plates will pass through without effectively being deflected. Ions outside the center at the moment of the switching will experience a net acceleration towards one of the plates. For the negative flank, ions “running ahead” experience an acceleration towards the grounded plate which is not completely compensated by an opposite acceleration after the chopper switch. For ions “running behind”, the situation is just reversed. The width $\tau_c$ of the beam pulse results from the chopper voltage $V_c$ and rise time $\tau_r$; the ion velocity $v_0$; the source acceleration voltage $V_{acc}$, and the given geometry. Hoekstra\textsuperscript{173} calculated $\tau_c$ assuming ions whose traversing time through the plates is longer than the rise time $\tau_r$:

$$\tau_c \simeq \frac{0.035 V_{acc}}{v_0 V_c}$$

(B.1)

with $\tau_c$ in ns, $V_{acc}$ in V, and $v_0$ in atomic units.

B.1 Bunching effects

The ion pulses passing the chopper plates are subject to bunching effects. Ion pulses, transmitted on the negative flank of the chopper voltage, are
Figure B.1: (a) plots of the pulse width $\tau_c$ and bunching correction $\Delta \tau_c$ versus $V_e/V_{eer}$ for $v_0 = 0.1$, (10 keV Ar) and $v_0 = 0.5$ (25 keV He). Figures (b) and (c) show the geometrically induced widths $\Delta t_i - \Delta t_e$ calculated for the two tubes at $\theta_0 = 10^\circ$ and $\theta_0 = 30^\circ$ assuming a typical 10 keV Ar beam incident on an Al target. The velocity after reflection $v_r$ is calculated for reflected Ar and recoil O and H particles.
subject to a twofold deceleration. Firstly, upon entering the plates, $V_c$ is positive decelerating the incoming ions. After passage, $V_c$ has become negative, now decelerating the ions leaving the plates$^1$. For ions on the beam axis, halfway in between the plates, the energy loss equals $qV_c(d/2 + d/2)/d = qV_c$. Ions off axis suffer a different energy loss, depending on their position $y$ in between the plates. With respect to the beam centered at $y = d/2$, this induces a total energy spread of $\Delta E = 4qV_c y/d$ around the central energy of ions traveling on axis. This energy spread shortens ("bunches") the ion pulse, irrespective of the chosen chopper flank. The slowest ions will always be swept through diaphragm $D_3$ first, followed by faster ones leading to temporal focusing, until the fast ions overtake the slow ones. The maximum radius $y_{max}$ of a transmitted beam pulse is roughly given by half the radius of diaphragm $D_3 = 1$ mm (see Hoekstra$^{29}$). This gives an energy spread $\Delta E$:

$$\Delta E = \frac{2}{3}qV_c; \quad \text{(B.2)}$$

and:

$$\frac{\Delta E}{E} = \frac{2}{3} \frac{\Delta v}{v} = \frac{2V_c}{3V_{ecr}} \quad \text{(B.3)}$$

which, at the target located 293 mm behind $D_3$, gives a decrease in time spread $\Delta \tau_e \simeq 45V_e/(v_0V_{ecr})$ ns. Therefore, at the target the time spread is given by:

$$\tau_t = \tau_e - \Delta \tau_e$$

$$= \frac{0.035 V_{ecr}}{v_0} - \frac{45}{V_e} \frac{V_e}{V_{ecr}}. \quad \text{(B.4)}$$

The optimum setting of $V_c/V_{ecr}$ is found for $\tau_t = 0$, which is at $V_c/V_{ecr} \simeq 0.028$ (for all $v_0$). For $V_c/V_{ecr}$ values larger than this, the pulse width increases again. Figure B.1 (a) shows plots of the pulse width $\tau_e$ and bunching correction $\Delta \tau_e$ versus $V_c/V_{ecr}$ for two typical ion velocities $v_0 = 0.1$, (10 keV Ar) and $v_0 = 0.5$ (25 keV He).

### B.2 Lens system

Deceleration of the beam pulses by the 180 mm four-element lens system mounted 55 mm behind diaphragm $D_3$ affects the bunching contribution $\Delta \tau_e$. The energy of a decelerated beam pulse is lowered stepwise each time a new lens element is entered. Therefore, the travel time to the target

$^1$Ions passing on the positive chopper flank will be accelerated instead of decelerated.
becomes dependent on each individual lens setting, and consequently also the bunching spread. For decelerated beams the optimum $V_c/V_{acc}$ setting is best determined experimentally, by minimizing the time spread of the particles scattered off the target into one of the time of flight tubes.

### B.3 Geometry effect

Opposed to the bunching effect, leading to a decrease in width of the chopped pulse, the target itself induces a broadening of the pulse during reflection. This *geometry effect* stems from different trajectory lengths of particles scattered into a time of flight tube mounted at an angle $\theta_0$ from different parts of the pulse. The reflected ions are subject to (elastic and inelastic) energy losses and have velocity $v_r < v_0$ after the collision. Consider a beam with a diameter of 2 mm incident at an angle $\psi$. This gives a time difference (ns) in incident path length of $\Delta t_i = 0.92/(v_0 \tan \psi)$ and in the reflected path of $\Delta t_r = 0.92 \cos(\theta_0 - \psi)/(v_r \sin \psi)$. The time spread $\tau_d$ at the detector is given by:

$$
\tau_d = \tau_i + \Delta t_i - \Delta t_r
= \tau_i + 0.92 \left\{ \frac{1}{v_0 \tan \psi} - \frac{\cos(\theta_0 - \psi)}{v_r \sin \psi} \right\}
$$

(F.5)

Figures B.1 (b) and (c) show the geometrically induced widths $\Delta t_i - \Delta t_r$ calculated for the two tubes at $\theta_0 = 10^\circ$ and $\theta_0 = 30^\circ$ assuming a typical 10 keV Ar beam incident on an Al target. The velocity after reflection $v_r$ is calculated for reflected Ar and recoil O and H particles. Inelastic losses are omitted. The figures show that the best time resolution is obtained for incident angles as large as possible. Deflection over $\theta_0 = 30^\circ$ gives less broadening for all $\psi$ as compared to deflection over 10°.
Solution of Coster-Kronig rate equations

Here we briefly give the solutions of the rate equations from section 6.3. The general structure of the rate equation for the population of a given state $i$ is

$$ \dot{n}_i = \frac{dn_i}{dt} = -\Gamma_{ii} n_i(t) + \sum_k A_{ki} \Gamma_{ki} n_k(t) $$ \hspace{1cm} (C.1)

where the coefficients $A_{ki}$ may be zero and the loss rate is defined as the sum over all rates to the final states $j$ accessible from the given state $i$, i.e.

$$ \Gamma_{ii} = \sum_{j \neq i} \Gamma_{ij} $$ \hspace{1cm} (C.2)

Since none of the states $k$ decaying to state $i$ is among the states $j$ the set of rate equations, equations 6.1 - 6.6 can readily be solved consecutively starting with the upper states of the Coster-Kronig cascade where the coefficients $A_{ki}$ are zero, i.e.

$$ n_F(t) = n_F(0) \cdot \exp(-\Gamma_{FF} t) , $$
$$ n_E(t) = n_E(0) \cdot \exp(-\Gamma_{EE} t) , $$
$$ n_D(t) = n_D(0) \cdot \exp(-\Gamma_{DD} t) . $$

Inserting these solutions equations 6.4 and 6.5 rewrite to
\[
\dot{n}_C = -\Gamma_{CC} \cdot n_C \\
+ \Gamma_{EC} n_E(0) \cdot \exp(-\Gamma_{EE} t) \\
+ \Gamma_{FC} n_F(0) \cdot \exp(-\Gamma_{FF} t).
\]

\[
\dot{n}_B = -\Gamma_{BB} \cdot n_B \\
+ \Gamma_{DB} n_D(0) \cdot \exp(-\Gamma_{DD} t).
\]

Their solutions are:

\[
n_C(t) = n_C(0) \cdot \exp(-\Gamma_{CC} t) \\
- \frac{\Gamma_{EC}}{\Gamma_{CC} - \Gamma_{EE}} \cdot \left\{ \exp(-\Gamma_{EE} t) - \exp(-\Gamma_{CC} t) \right\} \\
- \frac{\Gamma_{FC}}{\Gamma_{CC} - \Gamma_{FF}} \cdot \left\{ \exp(-\Gamma_{FF} t) - \exp(-\Gamma_{CC} t) \right\},
\]

\[
n_B(t) = n_B(0) \cdot \exp(-\Gamma_{BB} t) \\
- \frac{\Gamma_{DB}}{\Gamma_{BB} - \Gamma_{DD}} \cdot \left\{ \exp(-\Gamma_{DD} t) - \exp(-\Gamma_{BB} t) \right\}.
\]

Insertion of these solutions into equation 6.6 finally leads to

\[
n_A(t) = n_A(0) \cdot \exp(-\Gamma_{AA} t) \\
- \left( n_C(0) \cdot \frac{\Gamma_{CA}}{\Gamma_{CC} - \Gamma_{AA}} \\
+ n_E(0) \cdot \frac{\Gamma_{EC}}{\Gamma_{EE} - \Gamma_{AA}} \\
+ n_F(0) \cdot \frac{\Gamma_{FC}}{\Gamma_{FF} - \Gamma_{AA}} \right) \\
\cdot \left\{ \exp(-\Gamma_{CC} t) - \exp(-\Gamma_{AA} t) \right\} \\
+ n_E(0) \cdot \frac{\Gamma_{EC}}{\Gamma_{EE} - \Gamma_{CC}} \cdot \frac{\Gamma_{CA}}{\Gamma_{EE} - \Gamma_{AA}} \\
\cdot \left\{ \exp(-\Gamma_{EE} t) - \exp(-\Gamma_{AA} t) \right\} \\
+ n_F(0) \cdot \frac{\Gamma_{FC}}{\Gamma_{FF} - \Gamma_{CC}} \cdot \frac{\Gamma_{CA}}{\Gamma_{FF} - \Gamma_{AA}} \\
\cdot \left\{ \exp(-\Gamma_{FF} t) - \exp(-\Gamma_{AA} t) \right\}.
\]
According to equation C.2 the loss rates in particular are defined as:

\[
\begin{align*}
\Gamma_{FF} &= \Gamma_F + \Gamma_{FC} , \\
\Gamma_{EE} &= \Gamma_E + \Gamma_{EC} , \\
\Gamma_{DD} &= \Gamma_D + \Gamma_{DB} , \\
\Gamma_{CC} &= \Gamma_C + \Gamma_{CA} , \\
\Gamma_{BB} &= \Gamma_B , \\
\Gamma_{AA} &= \Gamma_A .
\end{align*}
\]

Throughout this work we have chosen

\[
\Gamma_{FC} = \Gamma_{EC} = \Gamma_{DB} = \Gamma_{BA}
\]

for the Coster-Kronig rates. The KLL-Auger rates are taken from table 5.2.