Continuum processes in GRASP

... with a strong emphasis on autoionization and the Auger effect

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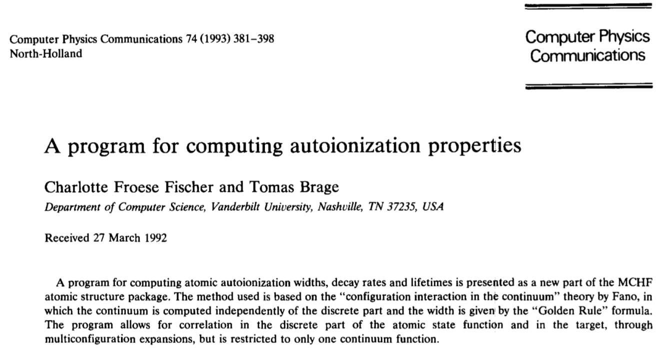
June 14, 2025

CompAS meeting 12 – 14 June 2025, Lund

A long journey ...



Computer Physics Communications 74 (1993) 381–398
North-Holland

Computer Physics Communications

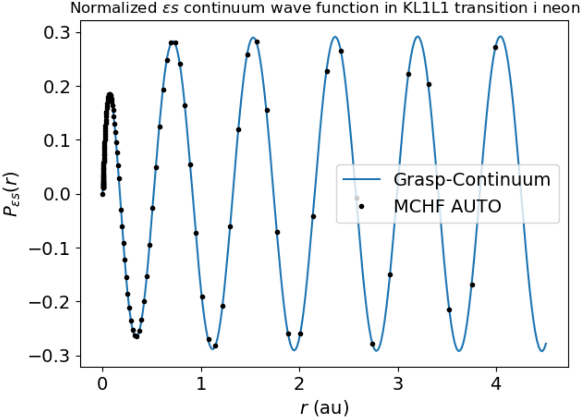
A program for computing autoionization properties

Charlotte Froese Fischer and Tomas Brage
Department of Computer Science, Vanderbilt University, Nashville, TN 37235, USA

Received 27 March 1992

A program for computing atomic autoionization widths, decay rates and lifetimes is presented as a new part of the MCHF atomic structure package. The method used is based on the "configuration interaction in the continuum" theory by Fano, in which the continuum is computed independently of the discrete part and the width is given by the "Golden Rule" formula. The program allows for correlation in the discrete part of the atomic state function and in the target, through multiconfiguration expansions, but is restricted to only one continuum function.

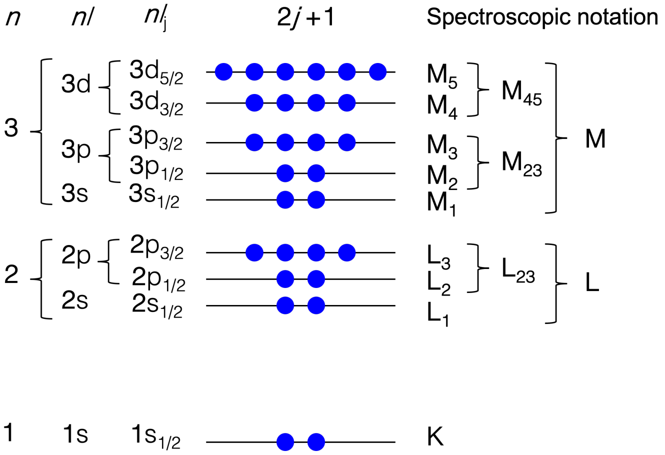
A long journey ...



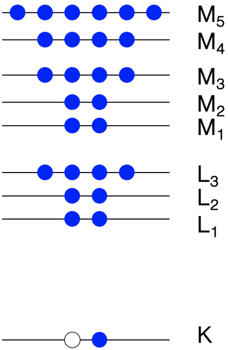
A long journey ...

- Email discussions about a possible continuum solver in GRASP since (at least) 2013 in my mailbox.
- In April 2016, during a visit to ANU/Australia, tests were made suggesting that it was indeed possible to compute Auger decay rates using non-orthogonal basis sets with GRASP.
- But the continuum solver was still missing ...
- In the meanwhile, calculations utilizing GRASP together with RATIP continued.
- And then recently GRASPC :). Thank you Paweł and collaborators!
- And then, very recently, the first prototype of an Auger module for GRASP (RAUGER)
- And then today, the very first results ...

The Auger effect

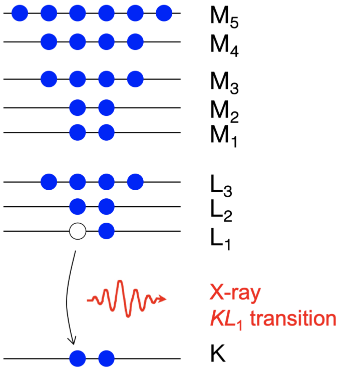


The Auger effect

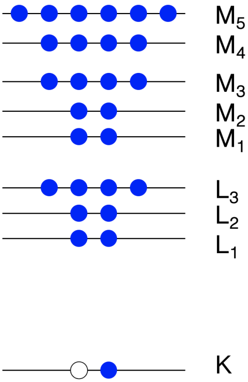


An initial vacancy is created

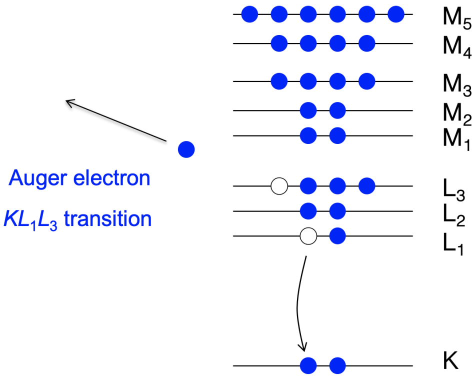
The Auger effect



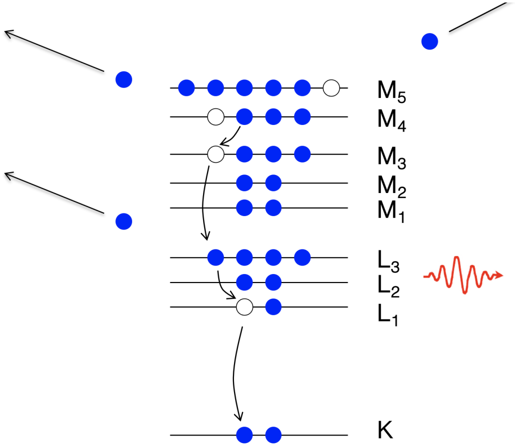
The Auger effect



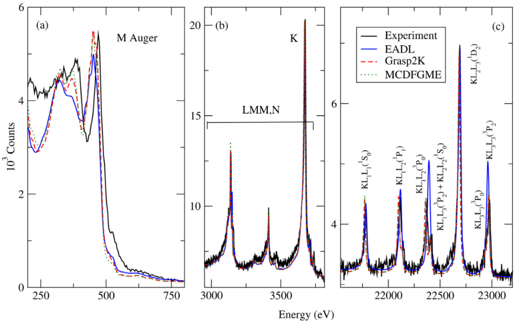
The Auger effect



The Auger effect



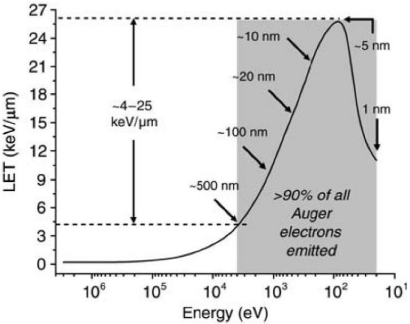
Radiation therapy of tumours with the Auger-electron emitter ^{125}I

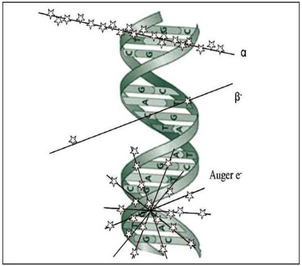


- ^{125}I is an Auger-electron emitter which decay via Electron Capture (EC) with a half-life of 60 days
- In each decay, on average around 20 Auger electrons are ejected

J.M. Sampaio et al. Journal of Quantitative Spectroscopy & Radiative Transfer 277 (2022) 107964

Auger effect - Applications





Amin I Kassis, Radiation Protection Dosimetry (2010) pp. 1-7

Autoionization in Grasp

Autoionization is essentially a transition from a discrete state to a state in the continuum, and can be described by Fermi's Golden rule

$$\Gamma = 2\pi \left| V_{E_0} \right|^2 ,$$

where Γ is the (full) width (at half maximum) of the autoionizing state and V_{E_0} is the interaction element. The decay rate is then given by

$$A = \frac{\Gamma}{\hbar} .$$

Autoionization in GRASP

If the interaction between the discrete state and the continuum state is not too strong, the interaction element, based on the theory by Fano, can be written

$$V_{E_0} = \langle \Psi_b(N; E_0\gamma J) | H - E_0 | \Psi_k(N-1; \widetilde{\gamma}\widetilde{J}) \cdot \phi(\epsilon\kappa)\gamma' J' \rangle \,,$$

where $\phi(\epsilon\kappa)$ is a continuum orbital with appropriate symmetry computed using GRASPC.

Autoionization in GRASP

$$V_{E_0} = \langle \Psi_b(N; E_0\gamma J) | H - E_0 | \Psi_k(N-1; \widetilde{\gamma}\widetilde{J}) \cdot \phi(\epsilon\kappa)\gamma' J' \rangle \,.$$

- The bound states $\Psi_b(N; E_0\gamma J)$ and $\Psi_k(N-1; \widetilde{\gamma}\widetilde{J})$ are expansions of configuration state functions (CSF:s) and can be constructed from a common basis set or from different basis sets.
- If a common (orthogonal) basis set is used, only two-electron interactions contribute in $H - E_0$.
- If different (non-orthogonal) basis sets are used, the interaction element is computed using bi-orthogonal transformation and target states must be closed under de-excitation (but this is a good thing!)

Autoionization in GRASP

Example: $|\Psi_b(N; E_0\gamma J)\rangle$ represents a K-vacancy ($1s^{-1}$) in argon and is constructed using three CSF:s.

```
  1s ( 2)  2s ( 2)  2p-( 2)  2p ( 4)  3s ( 1)  3p-( 2)  3p ( 4)
                                         1/2
                                                              1/2+
  1s ( 2)  2s ( 1)  2p-( 2)  2p ( 4)  3s ( 2)  3p-( 2)  3p ( 4)
               1/2
                                                              1/2+
  1s ( 1)  2s ( 2)  2p-( 2)  2p ( 4)  3s ( 2)  3p-( 2)  3p ( 4)
      1/2
                                                              1/2+
```

The CSF list above is closed under de-excitation (CUD), which is a requirement for bi-orthogonal transformation.

Autoionization in GRASP

Example: $|\Psi_k(N-1;\widetilde{\gamma}\widetilde{J}) \cdot \phi(\epsilon\kappa)\gamma' J'\rangle$ represents a $L_1 L_1$ $(2s^{-2})$ state, coupled to a continuum orbital $(4s)$.

```
 1s ( 2)  2s ( 2)  2p-( 2)  2p ( 4)  3p-( 2)  3p ( 4)  4s ( 1)
                                                          1/2
                                                           1/2+
 1s ( 2)  2s ( 1)  2p-( 2)  2p ( 4)  3s ( 1)  3p-( 2)  3p ( 4)  4s ( 1)
              1/2                         1/2                       1/2
                                              0                      1/2+
 1s ( 2)  2p-( 2)  2p ( 4)  3s ( 2)  3p-( 2)  3p ( 4)  4s ( 1)
                                                          1/2
                                                           1/2+
```

Again, the CSF list is closed under de-excitation (CUD).

Preliminary results - *KLL*-transitions i argon

Transition	EADL	MCDFGME	GRASPC/RAUGER
KL_1L_1	5.897E+13	7.491E+13	6.488E+13
KL_2L_2	1.162E+13	4.316E+11	4.470E+11
KL_3L_3	1.640E+14	4.544E+13	3.664E+13

Table: Decay rates in s^{-1} for *KLL*-transitions in argon using non-orthogonal basis sets.

Outlook

- More tests ...
- Facilitated grid-handling
- Automatized generation of CSF-lists (CUD) representing continuum states
- Inclusion of Breit and first order QED interactions
- Inclusion of other continuum processes (work in progress with photo-ionization - Per)
- More tests ...

Thank you for your attention!