Assessment of RBED electron-impact ionization cross sections for Monte Carlo electron transport

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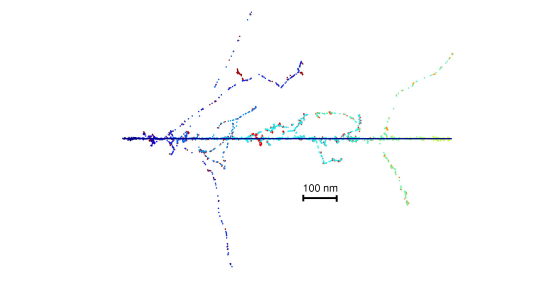
Motivation

- Improving cross sections for MC simulation of electron transport
- Accurate track structures in microdosimetry and other applications in medical physics



- Need differential and total (integrated) cross sections (DCSs and TCSs)
- Present work: ionization of atomic inner shells by electron impact

Ionization of atoms by electron impact

- Empirical, semi-empirical, and *ab initio* (first principles) calculations
- Current gold standard is DWBA (Bote and Salvat, 2008):
    - Projectile wavefunctions distorted by target, not plane waves
    - Valid from low E ($\sim$ 50 eV) to relativistic regime
    - Thoroughly validated against experiment (Llovet *et al*, 2014)
    - TCS data tabulated in NIST (all atoms; K, L, M shells)
    - DCS data not tabulated
    - Much more computationally expensive than PWBA
- Focus here on semi-empirical RBED model (Kim and Rudd, 2000)
- Yields both DCS and ICS and is very simple

Purpose: compare RBED with DWBA and assess limitations of the model

Relativistic binary-encounter-dipole (RBED) model

Model which combines Møller cross section with Bethe equation

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}w}\right)_{\mathrm{RBED}} = \frac{4\pi a_0^2 \alpha^4 N}{(\beta_t^2 + \beta_u^2 + \beta_b^2)\, 2b'} \left\{ \frac{(N_i/N) - 2}{t+1} \left(\frac{1}{w+1} + \frac{1}{t-w} \right) \frac{1+2t'}{(1+t'/2)^2} \right.$$
$$+ \left(2 - \frac{N_i}{N}\right) \left[\frac{1}{(w+1)^2} + \frac{1}{(t-w)^2} + \frac{b'^2}{(1+t'/2)^2} \right]$$
$$\left. + \frac{1}{N(w+1)} \frac{\mathrm{d}f}{\mathrm{d}w} \left[\ln \frac{\beta_t^2}{1-\beta_t^2} - \beta_t^2 - \ln(2b') \right] \right\}$$

Required input:

- Kinetic energy of the projectile (T)
- Binding (B) & average kinetic (U) energies of the N target electrons
- Optical oscillator strength (OOS), $\mathrm{d}f(w)/\mathrm{d}w$

W is the kinetic energy of outgoing electron, $w = W/B$

N_i is the effective number of electrons in the shell, $N_i = \int_0^\infty \frac{\mathrm{d}f}{\mathrm{d}w}\,\mathrm{d}w$

Optical Oscillator Strength models

1. RBEB model:
   - If nothing is known about OOS, use the empirical function

$$\left(\frac{\mathrm{d}f}{\mathrm{d}w}\right)_{\mathrm{RBEB}} = \frac{N}{(w+1)^2}$$

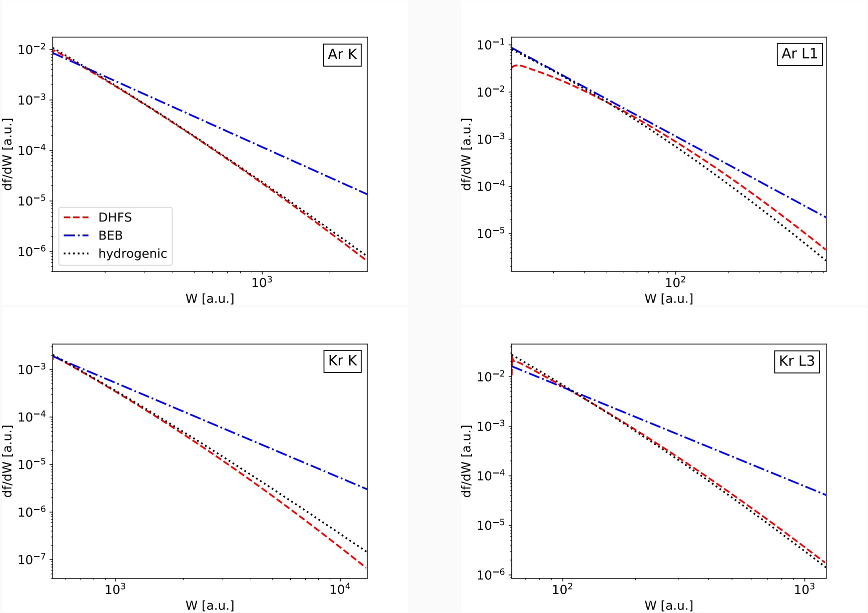
   - This choice yields analytical DCS and TCS, hence the popularity of RBEB
2. Hydrogenic OOS:
   - Fully analytical, non relativistic
   - Obtained by setting $Q = 0$ in GOS expressions
   - Can be applied to any Z by using Z_{eff} according to Slater's rules
3. Numerical (*ab initio*) OOS:

$$\begin{aligned}\frac{\mathrm{d}f}{\mathrm{d}W} \quad = \quad & \frac{2m_{\mathrm{e}}}{3\hbar^2}(B+W)\,N_W \sum_{\kappa'} \left\langle \ell \tfrac{1}{2} j \middle\| \mathbf{C}^{(1)} \middle\| \ell' \tfrac{1}{2} j' \right\rangle^2 \\ & \times \left\{ \int_0^\infty \left[P_{W\kappa'}(r)\, P_{n\kappa}(r) + Q_{W\kappa'}(r)\, Q_{n\kappa}(r) \right] r\,\mathrm{d}r \right\}^2\end{aligned}$$

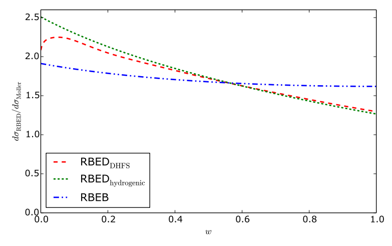
Overview of results

- Self-consistent DHFS potential used to calculate numerical OOS
- Calculations done for Z spanning periodic table, and K, L, M (sub)shells
- Inner shell electrons: $B \gtrsim 200$ eV
- Results shown here: OOSs, DCSs and TCSs
- Emphasis: comparison of RBED (using the three OOS models) with DWBA

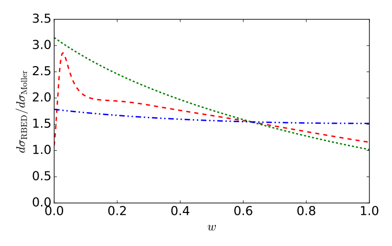
Results: OOSs



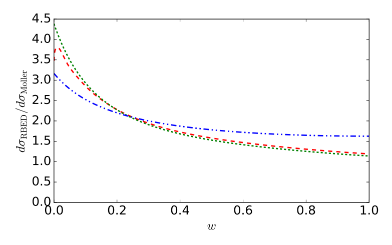
Results: DCSs



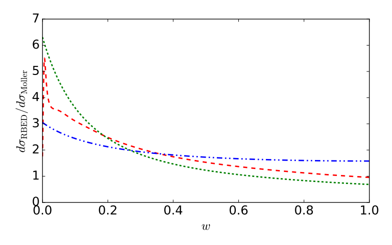
(a) Neon 1s, T = 3B



(b) Argon $2p_{3/2}$, T = 3B



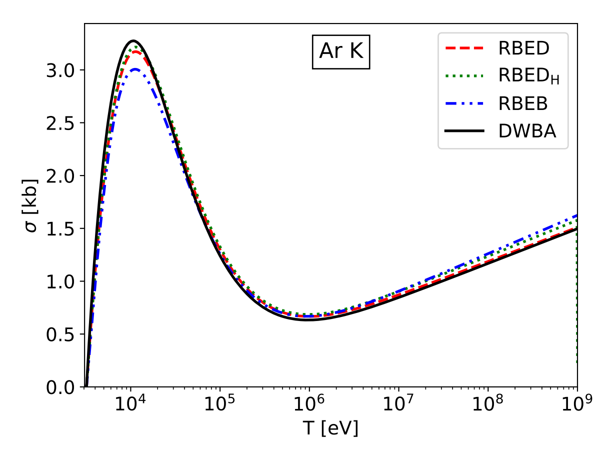
(c) Neon 1s, T = 10B



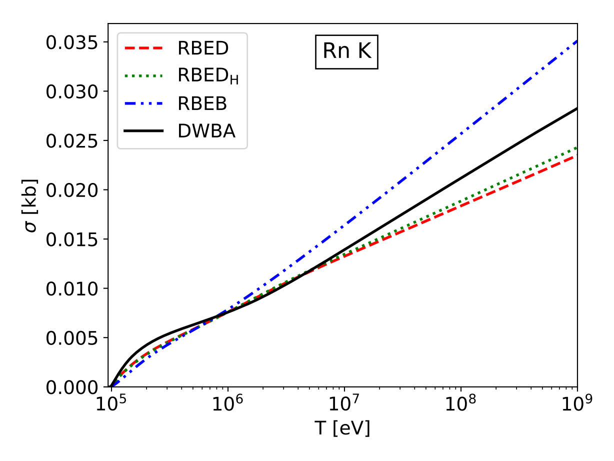
(d) Argon $2p_{3/2}$, T = 10B

Results: TCSs, K shell

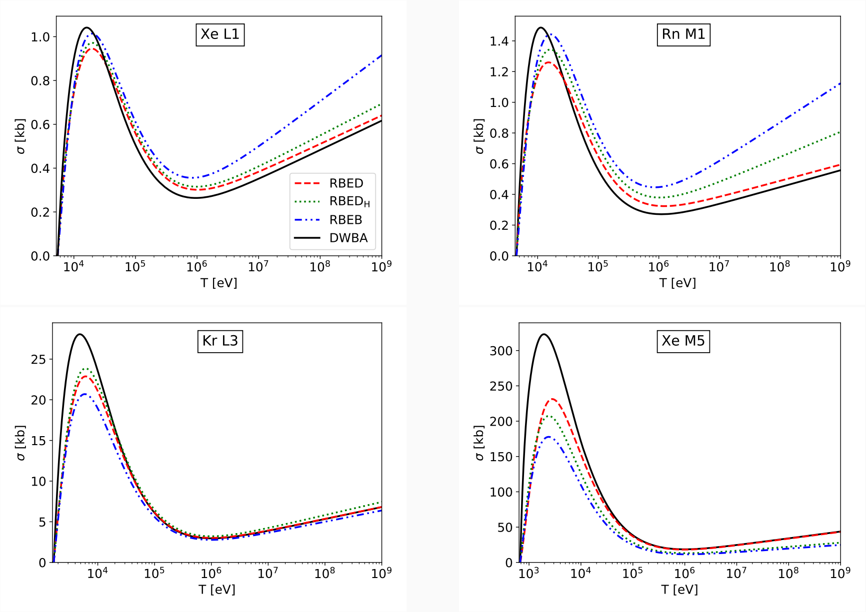
Agreement is good for the K-shell of low-Z elements



But for high Z the relativistic asymptotic behaviour is wrong!



Results: TCSs, L and M subshells



Asymptotic mismatch

Relativistic Bethe equation for ionization in the high-energy limit:

$$\sigma_{\mathrm{Bethe}} = \frac{4\pi a_0^2 \alpha^4 N}{\beta_t^2 \, 2b'} \, b_i \left[\underbrace{\ln \frac{1}{1-\beta_t^2} - \beta_t^2}_{\text{trans}} \underbrace{- \ln \frac{2b'}{c_i \beta_t^2}}_{\text{long}} \right]$$

b_i and c_i are parameters determined from Fano plots

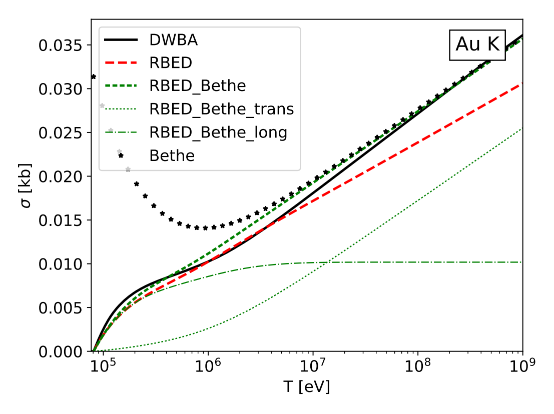
RBED high-energy asymptotic limit:

$$\sigma_{\mathrm{RBED}} = \frac{4\pi a_0^2 \alpha^4 N}{(\beta_t^2 + \beta_u^2 + \beta_b^2) \, 2b'} \left\{ b_i \left[\ln \frac{1}{1-\beta_t^2} - \beta_t^2 - \ln \frac{2b'}{\beta_t^2} \right] + \left(2 - \frac{N_i}{N} \right) \right\}$$

Prefactors are different $\Longrightarrow$ RBED cannot reproduce the Bethe limit!

Results: asymptotic behaviour

We can restore the PWBA prefactor to the distant (longitudinal and transverse) part of RBED



Can recover correct asymptotic limit, but intermediate region is worse

Highlights limitations of combining two disparate models semi-empirically

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