The relativistic distorted-wave method for calculating cross sections for impact excitation and ionization by an electron beam

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In Memory of

Douglas H. Sampson

1925 -- 2002

(Penn State University)

Abstract

The main motivation for our work to obtain cross sections between magnetic sublevels by excitation and ionization by impact with an electron beam was to compare our results with the electron-beam ion-trap (EBIT) experiments at Livermore [1]. Often these experiments involve highly-charged ions of heavy elements for which a fully relativistic description is necessary. In this presentation, we will review the fully relativistic distorted-wave approach for calculating these cross sections. Then we will briefly describe the inclusion of the generalized Breit interaction, the resonance contribution, and a new ``top-up'' procedure for excitation. Finally, comparison with some EBIT experiments and other applications for these cross sections are given. We acknowledge contributions from M. Inal of University A. Belkaid.

Outline

- Relativistic distorted-wave method
- Collision strengths between magnetic sublevels
- Top-up – relativistic Coulomb-Bethe approximation
- New top-up – Kummer transformation
- Inclusion of generalized Breit interaction
- Resonance contributions
- Future work

Relativistic distorted-wave method

- Radial part: Dirac equations

$$[\frac{d}{dr}+\frac{\kappa}{r}]P(r) = \frac{\alpha}{2}[\epsilon - V + \frac{4}{\alpha^2}]Q(r)$$
$$[\frac{d}{dr}-\frac{\kappa}{r}]Q(r) = -\frac{\alpha}{2}[\epsilon - V]P(r).$$

where the relativistic quantum numbers are

$$\kappa = l,\ j = l - 1/2; \qquad \kappa = -l - 1,\ j = l + 1/2$$

- Angular part: using jj coupling, e.g.:

$$(1s_{1/2}2p_{1/2})_1 \sim 1s2p\,^3P_1$$

$$(1s_{1/2}2p_{3/2})_1 \sim 1s2p\,^1P_1$$

Potential

- Dirac-Fock-Slater (DFS) potential

$$V(r) = -\frac{2Z}{r} + V_c(r) + V_{\rm ex}$$

The classical potential: $$V_c(r) = \sum_{n'\kappa'} w_{n'\kappa'} \int_0^\infty \frac{2}{r_>}[P^2_{n'\kappa'}(r_2) + Q^2_{n'\kappa'}(r_2)]{\rm d}r_2\,,$$

The exchange potential: $$V_{\rm ex}(r) = -\left[\frac{24}{\pi}\rho(r)\right]^{1/3}$$

Electron number density: $$\rho(r) = \frac{1}{4\pi r^2}\sum_{n'\kappa'} w_{n'\kappa'}[P^2_{n'\kappa'}(r) + Q^2_{n'\kappa'}(r)]$$

- Semi-classical exchange (SCE)

$$V_{\rm sce}(r) = -\tfrac{1}{2}(E - V_c)\left\{\left[1 + \frac{4\rho}{r^2(E-V_c)}\right]^{1/2} - 1\right\}$$

Total excitation collision strength

- Collision strength is given by

$$\Omega(\Delta_t J_t - \Delta'_t J'_t) = 2 \sum_J (2J+1) \sum_{\substack{l,j \\ l',j'}} \mid R(\gamma,\gamma') \mid^2$$

- The coupled representation

$$\gamma = \Delta_t J_t \epsilon l j J; \quad \gamma' = \Delta'_t J'_t \epsilon' l' j' J$$

- R-matrix elements

$$R(\gamma,\gamma') = R_d(\gamma,\gamma') - R_e(\gamma,\gamma')$$

$$R_d(\gamma,\gamma') \sim \sum_\lambda A_d^\lambda D^\lambda, \quad R_e(\gamma,\gamma') \sim \sum_\lambda A_e^\lambda E^\lambda$$

Collision strength between magnetic sublevels by an electron beam

- First convert R-matrix elements to the uncoupled representation

$$R(\alpha,\alpha') = \sum_{J,M} C(J_t j M_t m; JM) C(J_t' j' M_t' m'; JM) R(\gamma,\gamma')$$

with

$$\alpha = \Delta_t J_t M_t k l j m, \quad \alpha' = \Delta_t' J_t' M_t' k' l' j' m'$$

- Collision strengths by impact with a polarized electron beam

$$\Omega^{m_s}(\Delta_t J_t M_t \to \Delta_t' J_t' M_t') = \frac{4}{k^2} \sum_{\substack{l,l_1,j,j_1 \\ l',j',m'}} \mathrm{i}^{l-l_1}[(2l+1)(2l_1+1)]^{1/2}$$
$$\times \exp[\mathrm{i}(\delta_\kappa - \delta_{\kappa_1})] C(l\tfrac{1}{2}0m_s; jm) C(l_1\tfrac{1}{2}0m_s; j_1 m) R(\alpha,\alpha') R(\alpha,\alpha_1')$$

- Collision strengths by impact with an unpolarized electron beam

$$\Omega(\Delta_t J_t M_t - \Delta_t' J_t' M_t') = \frac{1}{2} \sum_{m_s} \Omega^{m_s}(\Delta_t J_t M_t - \Delta_t' J_t' M_t')$$

Comparison with other calculations

Present collision strengths (first entries) from $1s^2$ to $(1s2p_{1/2})_1$ and $(1s2p_{3/2})_1$ in He-like Fe compared with those in Clark et al. (LANL Report No. LA-11436-M, 1988, second entries), and those in Inal and Dubau (J. Phys. Commu. **20**, 4221, 1987, third entries).

Excited			ϵ(Ry)				
Level	M_i'	ΔE(Ry)	550	700	900	1200	2000
$1s2p\ ^1P_1$	0	493.2	1.69[-3]	2.37[-3]	3.09[-3]	3.85[-3]	4.94[-3]
or		493.0	1.69[-3]	2.39[-3]	3.07[-3]	3.76[-3]	4.68[-3]
$(1s_{1/2}2p_{3/2})_1$			1.69[-3]	2.38[-3]	3.06[-3]	3.76[-3]	4.69[-3]
	1		4.19[-4]	6.12[-4]	8.84[-4]	1.30[-3]	2.32[-3]
			4.18[-4]	6.20[-4]	8.98[-4]	1.31[-3]	2.30[-3]
			4.06[-4]	5.84[-4]	8.87[-4]	1.35[-3]	2.39[-3]
$1s2p\ ^3P_1$	0	490.7	2.08[-4]	2.42[-4]	2.85[-4]	3.37[-4]	4.20[-4]
or		490.6	2.19[-4]	2.55[-4]	2.99[-4]	3.47[-4]	4.16[-4]
$(1s_{1/2}2p_{1/2})_1$							
	1		2.65[-4]	2.09[-4]	1.76[-4]	1.69[-4]	2.16[-4]
			2.66[-4]	2.09[-4]	1.78[-4]	1.72[-4]	2.20[-4]

Comparison with EBIT experiment

Table II from Beiersdorfer et al. (Phys. Rev. A 53, 3974 (1996)): Comparison of calculated and measured values of polarization of lines at E=6800eV for He-like Fe

Line	Shlyaptseva and co-workers	Inal and Dubau	Present calculations	Measurements
P_w	+0.82	+0.584	+0.599	$+0.56^{+0.17}_{-0.08}$
P_x	-0.75	-0.518	-0.515	$-0.53^{+0.05}_{-0.02}$
P_y	-0.23	-0.196	-0.192	$-0.22^{+0.05}_{-0.02}$
P_x (no cascades)	0.000	0.000	0.000	
P_z (with cascades)		-0.078	-0.074	$-0.076^{+0.007}_{-0.007}$

w: $1s2p\ ^1P_1 - 1s^2\ ^1S_0$ or $(1s2p_{3/2})_1 - (1s^2)_0$

x: $1s2p\ ^3P_2 - 1s^2\ ^1S_0$ or $(1s2p_{3/2})_2 - (1s^2)_0$

y: $1s2p\ ^3P_1 - 1s^2\ ^1S_0$ or $(1s2p_{1/2})_1 - (1s^2)_0$

z: $1s2s\ ^3S_1 - 1s^2\ ^1S_0$ or $(1s2s_{1/2})_1 - (1s^2)_0$

Comparison with EBIT experiment (2)

Table II from Beiersdorfer et al. (Phys. Rev. A 60, 4156 (1999)): Intensities and inferred linear polarization of He-like lines w, x, y, and z and of Li-like line q for Ti measured with Si(220) and Si(111) crystals.

Line	Ion	Si(220) (counts)	Si(111) (counts)	Predicted polarization	Measured polarization
w	Ti^{20+}	18976	1820	+0.608	$+0.43^{+0.14}_{-0.12}$
x	Ti^{20+}	3628	185	-0.519	$-0.48^{+0.06}_{-0.06}$
y	Ti^{20+}	4468	268	-0.339	$-0.33^{+0.07}_{-0.07}$
z	Ti^{20+}	6511	470	-0.106	$-0.101^{+0.014}_{-0.013}$
q	Ti^{19+}	5999	569	+0.341	$+0.40^{+0.15}_{-0.10}$

q: $1s2s2p\ ^2P_{3/2} - 1s^2\ 2s\ ^2S_{1/2}$ or $[(1s2s)_1\ 2p_{1/2}]_{3/2} - (1s^2\ 2s)_{1/2}$

Top-up (1): Relativistic Coulom-Bethe Approximation

- Approximate Coulomb interaction

$$\frac{1}{\mid \mathbf{r}_N - \mathbf{r}_{N+1} \mid} = \sum_\lambda \frac{r_<^\lambda}{r_>^{\lambda+1}} C^\lambda(N) \cdot C^\lambda(N+1)$$
$$\simeq \frac{r_N}{r_{N+1}^2} C^{(1)}(N) \cdot C^{(1)}(N+1)$$

- Neglect exchange
- Use relativistic Coulomb functions in place of RDW functions

Top-up (1): Relativistic Coulom-Bethe Approximation

$$\Omega^{\mathrm{RCB}}_{m_s}(\beta_t J_t M_t \rightarrow \beta'_t J'_t M'_t) = 16 S(\beta_t J_t, \beta'_t J'_t) \sum_{\substack{l,l_1,j,j_1 \\ l',j',m'}} \mathrm{i}^{l-l_1}[(2l+1)(2l_1+1)]^{1/2}$$
$$\times \exp[\mathrm{i}(\delta_\kappa - \delta_{\kappa_1})] C(l\tfrac{1}{2}0m_s; jm) C(l_1\tfrac{1}{2}0m_s; j_1 m)$$
$$\times \sum_k \begin{pmatrix} j & 1 & j' \\ -m_s & k & m' \end{pmatrix} \begin{pmatrix} j_1 & 1 & j' \\ -m_s & k & m' \end{pmatrix} \begin{pmatrix} J_t & 1 & J'_t \\ -M_t & k & M'_t \end{pmatrix}^2$$
$$\times (-1)^{j+j'-2m_s} I(klj, k'l'j') I(kl_1 j, k'l'j')$$
$$\times \langle j \parallel C^{(1)} \parallel j' \rangle \langle j_1 \parallel C^{(1)} \parallel j' \rangle$$

where

$$\langle j_1 \parallel C^{(1)} \parallel j_2 \rangle = (-1)^{j_1+1/2}[(2j_1+1)(2j_2+1)]^{1/2} \begin{pmatrix} j_1 & \lambda & j_2 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$$

Top-up (1): Relativistic Coulom-Bethe Approximation

- Results with top-up

$$\Omega = \sum_{l=0}^{l_1} \Omega_l^{\mathrm{RDW}} + \sum_{l=l_1+1}^{l_2} \Omega_l^{\mathrm{RCB}} + \Omega_{l_2}^{\mathrm{RCB}} \frac{R}{1-R}, \qquad R = \Omega_{l_2}^{\mathrm{RCB}} / \Omega_{l_2-1}^{\mathrm{RCB}}$$

- No simple form – still have to get partial-wave results up to l_2
- Not always converging, especially on machines other than the Cray
- Still is time consuming, although faster than RDW

Top-up (2): Kummer transformation

- Complete relativistic distorted-wave results

$$\Omega = \sum_{l=0}^{l_1} \Omega_l^{\mathrm{RDW}} + \sum_{l=l_1+1}^{\infty} \Omega_l^{\mathrm{RDW}}$$

- Plane-wave Born (PWB) results

$$\Omega^{\mathrm{PWB}} = \sum_{l=0}^{l_1} \Omega_l^{\mathrm{PWB}} + \sum_{l=l_1+1}^{\infty} \Omega_l^{\mathrm{PWB}}$$

- Kummer transformation

Let $$\sum_{l=l_1+1}^{\infty} \Omega_l^{\mathrm{RDW}} \approx \sum_{l=l_1+1}^{\infty} \Omega_l^{\mathrm{PWB}}$$

then $$\Omega = \sum_{l=0}^{l_1} \Omega_l^{\mathrm{RDW}} + (\Omega^{\mathrm{PWB}} - \sum_{l=0}^{l_1} \Omega_l^{\mathrm{PWB}})$$

Plane-Wave Born (PWB) collision strength

- Partial-wave Ω_l^{PWB}: using spherical Bessel functions in place of distorted-wave functions
- Total PWB collision strength Ω^{PWB} can be computed numerically

$$\Omega_{J_t M_t, J_t' M_t'} = \frac{8}{\Delta E} \int_{K_{\min}}^{K_{\max}} f_{\mathrm{rel}}\, g f_{aa'}(K) \mathrm{d}(\ln K)$$

where the generalized oscillator strength is

$$f_{aa'}(K) = \frac{2\Delta E}{K^2} \sum_{\substack{tt' \\ (t-t')\mathrm{even}}} i^{t-t'} \sqrt{(2t+1)(2t'+1)}\, \mathcal{P}_t^{(M'-M)}(\cos\theta_K)\, \mathcal{P}_{t'}^{(M'-M)}(\cos\theta_K)$$

$$\times \begin{pmatrix} J & t & J' \\ -M & (M-M') & M' \end{pmatrix} \begin{pmatrix} J & t' & J' \\ -M & (M-M') & M' \end{pmatrix}$$

$$\times \langle \gamma J || \textstyle\sum_{m=1}^{N} j_t(K r_m) C_m^{(t)} || \gamma' J' \rangle \langle \gamma J || \textstyle\sum_{m=1}^{N} j_{t'}(K r_m) C_m^{(t')} || \gamma' J' \rangle$$

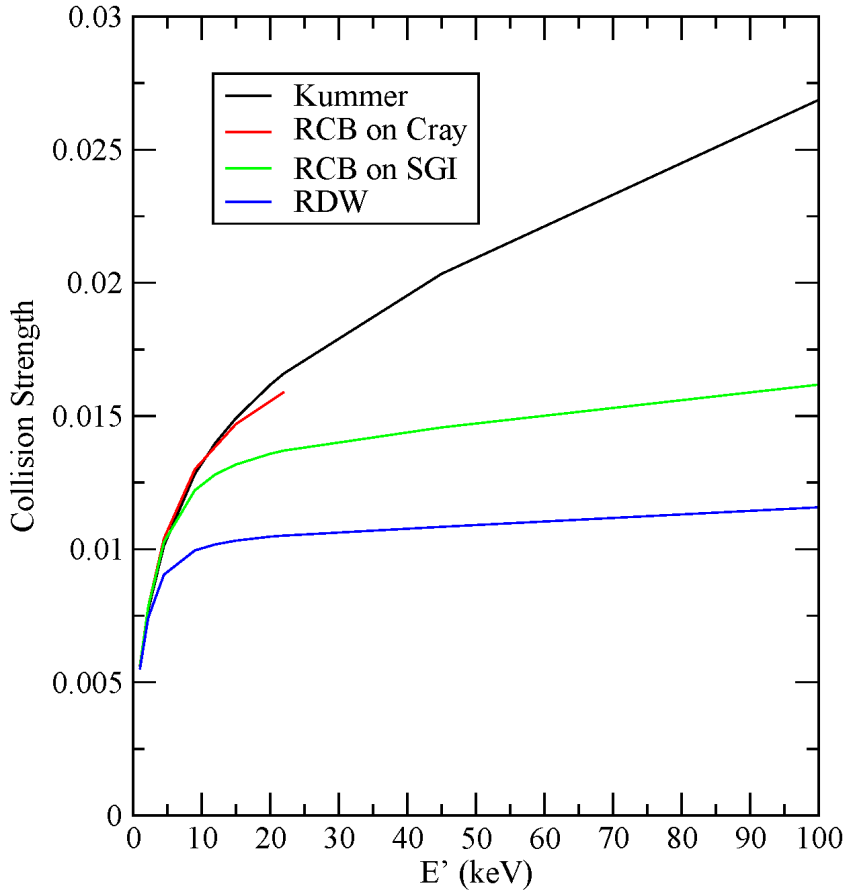
Comparison between RCB and Kummer transformation

Comparison of collision strengths for the transition $(1s2s)_1$ M=-1 to $(1s2p_{1/2})_1$ M'=0 in He-like Ba (Z = 56).

RCB on the Cray I_2 = 190

RCB on the SGI I_2 = 78

The Kummer transformation gives converged results and takes fully relativistic effects into account.



Inclusion of generalized Breit interaction

$$g(1,2) = \frac{1}{r_{12}} - (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2)\frac{\exp(i\omega r_{12})}{r_{12}} + (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\nabla}_1)(\boldsymbol{\alpha}_2 \cdot \boldsymbol{\nabla}_2)\frac{\exp(i\omega r_{12}) - 1}{\omega^2 r_{12}}$$

Table 3 from K. Widmann, P. Beiersdorfer et al. (X-Ray and Inner-shell Processes, p.444, 2000)

line	σ_{EE} barn	$\sigma_{non-rel}$ barn	σ_{rel} barn	σ_{GBI} barn
Ly-α_1	8.6 ± 1.5		8.256	8.109
Ly-$\alpha_{2,3}$	8.2 ± 3.4		6.541	6.787
w	7.0 ± 2.0	21.64	17.45	8.364
y	3.9 ± 1.5	0.127	7.313	3.842
z	1.08 ± 0.48	0.123	0.172	0.152

Comparison between measured and calculated cross sections for H- and He-like Xe:

σ_{EE}: Experiment

$\sigma_{non\text{-}rel}$: Non-relativistic

σ_{rel}: Relativistic

σ_{GBI}: with generalized Breit interaction

Resonance contributions

- Resonance transition

$$\mathrm{e} + (i_M = |J_i M_i\rangle) \rightarrow (j_M = |J_j M_j\rangle) \rightarrow \mathrm{e}' + (i'_M = |J'_i M'_i\rangle)$$

- Resonance contribution to the collision strength

$$\Omega^{\mathrm{res}}(i_M \rightarrow i'_M) = \sum_{j_M} \Omega^{\mathrm{cap}}(i_M \rightarrow j_M) B_{ji'} \delta(\epsilon - E_{ii'})$$

- Branching ratio

$$B_{ji'} = \frac{A^{\mathrm{a}}(j_M \rightarrow i'_M)}{\sum_m A^{\mathrm{a}}(j \rightarrow m) + \sum_k A^{\mathrm{r}}(j \rightarrow k)}$$

Capture collision strength and autoionization rate

- Collision strength between magnetic sublevels -- capturing a **directive** electron

$$\Omega^{\rm cap}(i_M \rightarrow j_M) = 2\pi \sum_{\substack{l,l_1,j,j_1 \\ m_s}} {\rm i}^{l-l_1}[(2l+1)(2l_1+1)]^{1/2} \exp[{\rm i}(\delta_\kappa - \delta_{\kappa_1})]$$
$$\times C(l\tfrac{1}{2}0m_s; jm) C(l_1\tfrac{1}{2}0m_s; j_1 m) R(\alpha, \alpha'') R(\alpha_1, \alpha'') \delta(\epsilon - \epsilon_{ij})$$

- Autoionization rate between magnetic sublevels -- releasing an electron in **any** direction

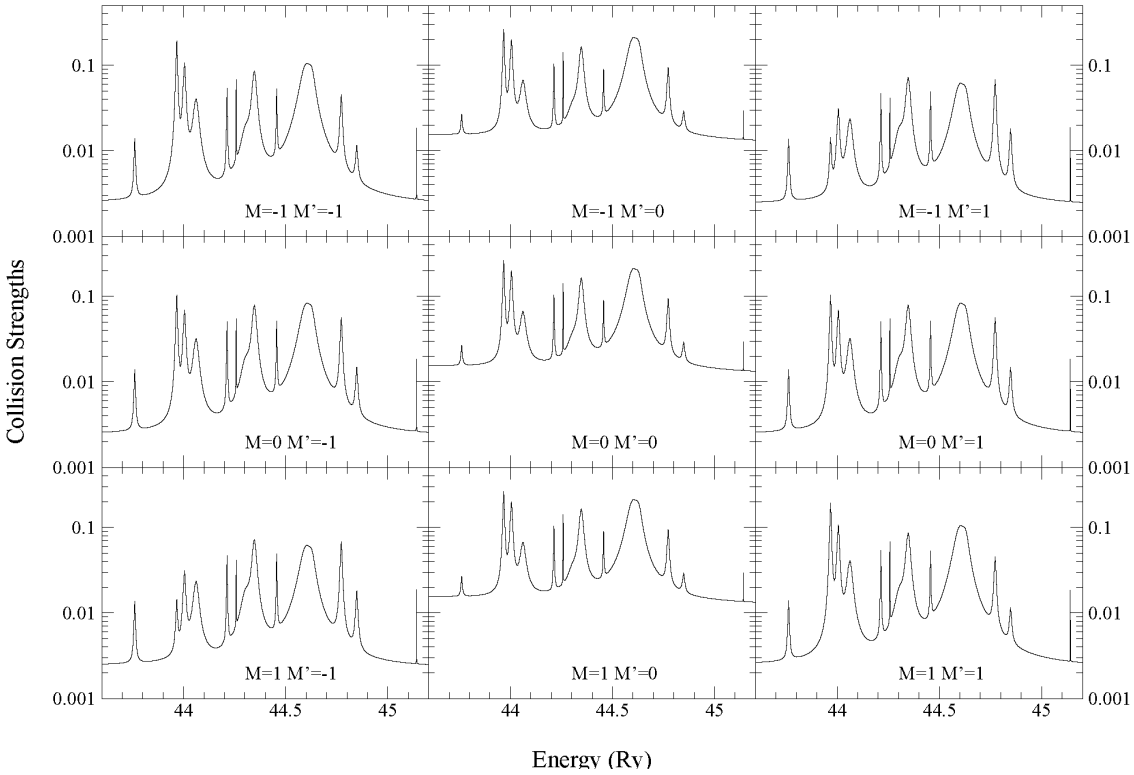
$$A^a(j_M \rightarrow i'_M) = \frac{2}{\hbar} \sum_{l',j',m'} C(J'j'M'm'; J''M'')^2 \mid R(\gamma', \gamma'') \mid^2$$

- Autoionization rate between fine-structurelevels

$$A^a(j \rightarrow i') = \frac{2}{\hbar} \sum_{l',j'} \mid R(\gamma', \gamma'') \mid^2$$

Resonance contributions

Complete RDW collision strengths for transtion between magnetic sublevels of $(1s2s)_1$ -- $(1s2p_{3/2})_1$ in He-like oxygen. Shown here are the contributions from the KMM complex.



Ionization

Ionization to specific magnetic sublevels by an electron beam: Application to the effect of inner-shell ionization on the polarization of Se^{24+} lines

Phys. Rev. A, **63**, 052713 (2001)

Conclusion

- Relativistic distorted-wave method for calculating collision strengths between magnetic sublevels
- Relativistic Kummer transformation is compared to the relativistic Coulomb-Bethe approximation as top-up
- Inclusion of generalized Breit interaction gives better agreement to experiment
- Resonance contributions are added to obtain complete collision strengths
- Electron-impact ionization between magnetic sublevels has also been implemented

Future work

- Implement these methods in the LANL suite of codes
- Obtain method for computing angular differential cross sections
- Carry out non-LTE kinetic calculations with these data for relevant appications