Density matrix approach to the recombination and electron capture of high–Z ions

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- Motivation: Processes in collisions of high–Z ions with electrons and target atoms
- Another view: Density matrix theory
- Total and angular–differential capture cross sections
- Photon polarization
- Summary and outlook: Two–step processes

Radiative recombination studies

So far:

- Total radiative recombination cross sections $\sigma^{RR}(E)$
- Photon angular distributions $\frac{d\sigma^{RR}}{d\Omega}(E, \theta)$
- Alignment $\mathcal{A}_2$ of the ion following the electron capture.
  A first step towards polarization studies.

Less studied phenomena:

- RR photon polarization characteristics
- Polarization of subsequently emitted photons
- Influence of nuclear and electron spins

- Multi–step processes: coincidence studies

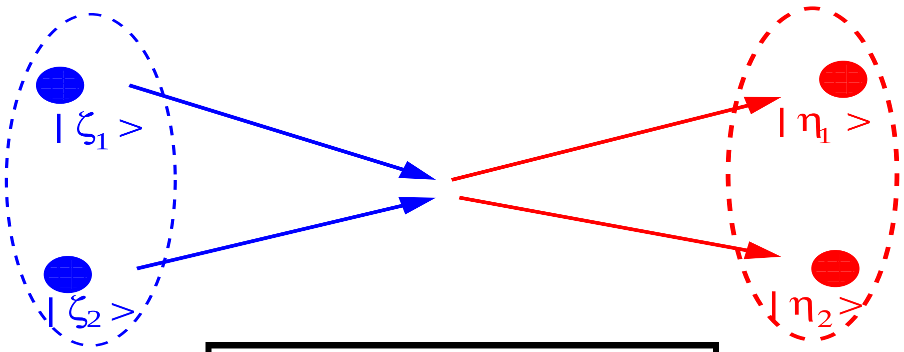
Density matrix theory: Atomic collisions

Two–particle collisions: time–independent description.

Initial state

$(t \to -\infty)$

$\hat{\rho}_i$



Final state

$(t \to +\infty)$

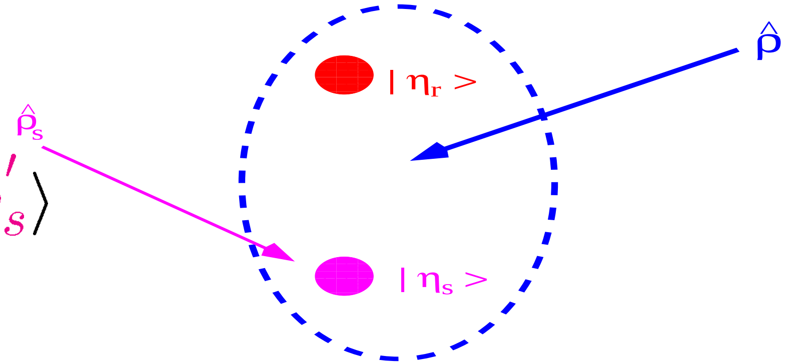
$\hat{\rho}_f$

$$\boxed{\hat{\rho}_f = \hat{S}\,\hat{\rho}_i\,\hat{S}^+}$$

$\hat{S}$ ... scattering operator.

Subsystem density matrix.

$$\langle \eta_s | \hat{\rho}_s | \eta_s^{'} \rangle = Tr_{(r)}(\hat{\rho}) = \sum_{\eta_r} \langle \eta_r \eta_s | \, \hat{\rho} \, | \eta_r \eta_s^{'} \rangle$$



Measurement of the physical properties.

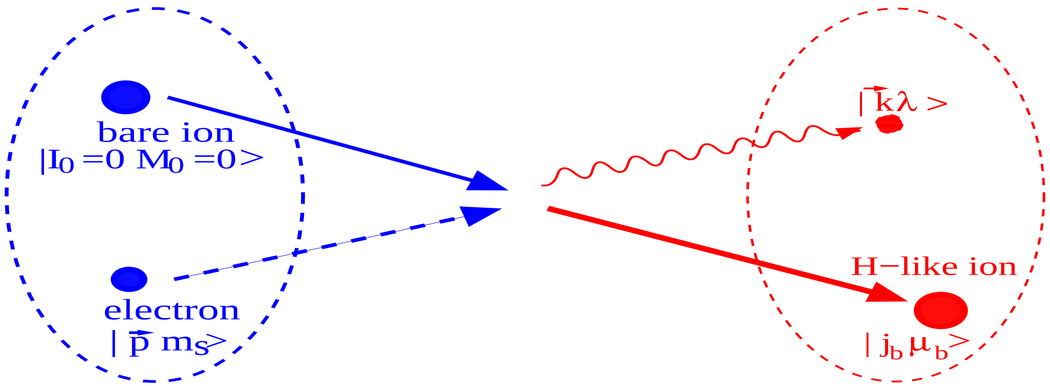
$\hat{P} = |\epsilon\rangle\langle\epsilon|$ ... 'detector operator' describes experimental setup.

$W = Tr(\hat{P}\,\hat{\rho}_f) = \sum_{\eta_1 \eta_2} \langle \eta_1 \eta_2 | \, \hat{P}\,\hat{\rho}_f \, | \eta_1 \eta_2 \rangle$ ... probability to get a 'click'.

Density matrix theory: Radiative recombination

Radiative recombination: time–independent description.

$$\hat{\rho}_i = \hat{\rho}_e \otimes \hat{\rho}_{ion}$$



$$\hat{\rho}_f = \hat{R}\ \hat{\rho}_i\ \hat{R}^+$$

$$\langle j_b\mu_b, \mathbf{k}\lambda|\hat{\rho}_f|j_b\mu_b', \mathbf{k}\lambda'\rangle = \sum_{m_s m_s'} \langle j_b\mu_b, \mathbf{k}\lambda|\hat{R}|\mathbf{p}m_s\rangle\, \langle \mathbf{p}m_s|\hat{\rho}_e|\mathbf{p}m_s'\rangle\, \langle \mathbf{p}m_s'|\hat{R}^+|j_b\mu_b', \mathbf{k}\lambda'\rangle$$

$$\langle j_b\mu_b, \mathbf{k}\lambda|\hat{R}|\mathbf{p}m_s\rangle \equiv c\, M^{RR}_{\mathbf{p},b}(m_s,\ \lambda,\ \mu_b)$$

. . . electron–photon interaction.

√ **Photon angular distribution $W(\mathbf{n})_{j_b}$:**

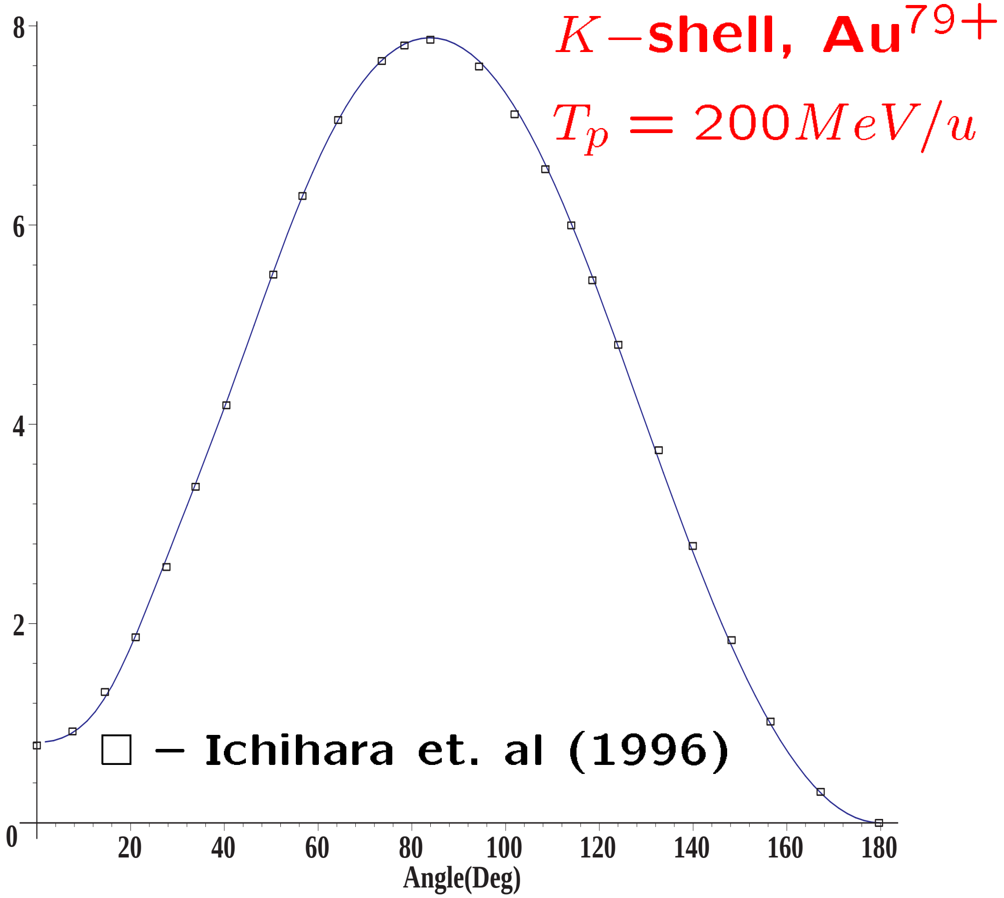
$$\hat{P}_{\mathrm{k}} = \sum_{\lambda\mu_b} |j_b\mu_b\rangle|\mathbf{k}\lambda\rangle\langle\mathbf{k}\lambda|\langle j_b\mu_b| \implies W(\mathbf{n})_{j_b} = Tr(\hat{P}_{\mathrm{k}}\,\hat{\rho}_f) = c \sum_{\lambda\ \mu_b\ m_s} |M^{RR}_{\mathbf{p},b}(m_s,\ \lambda,\ \mu_b)|^2$$

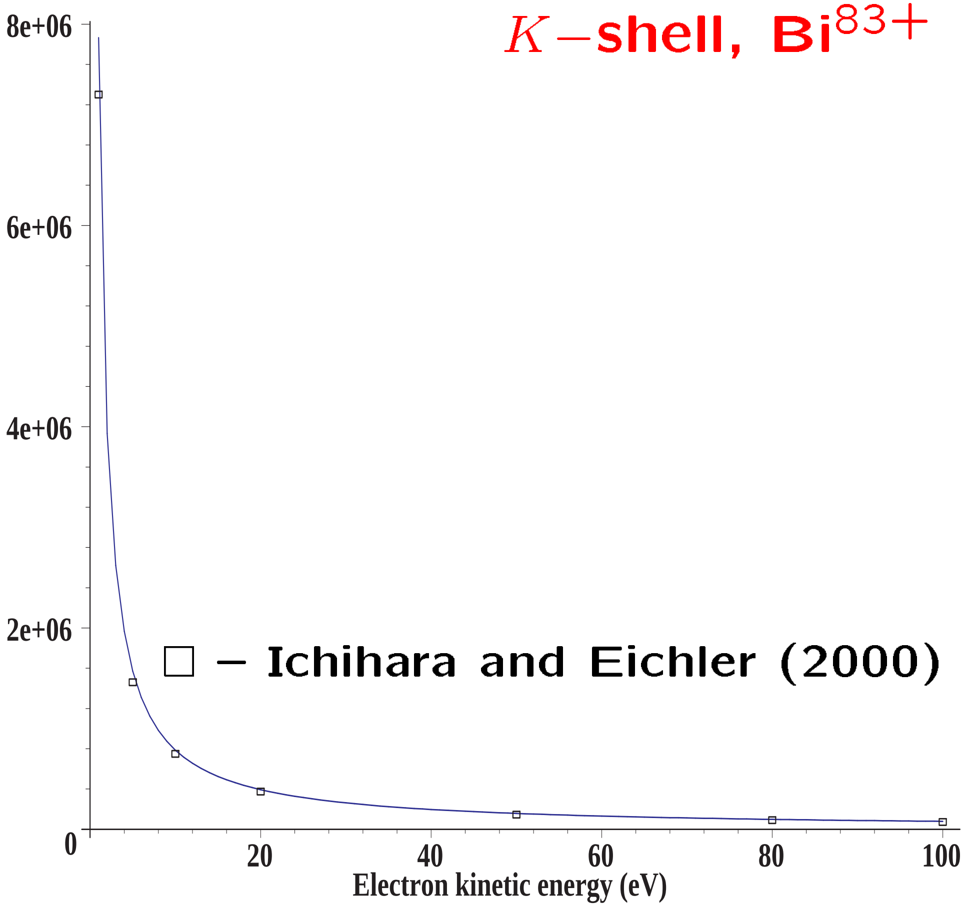
√ **Partial total cross section for RR into substate $|j_b\mu_b\rangle$:**

$$\hat{P}_{\mu_b} = \sum_{\lambda} \int d\mathbf{\Omega}_{\mathrm{k}}\, |j_b\mu_b\rangle|\mathbf{k}\lambda\rangle\langle\mathbf{k}\lambda|\langle j_b\mu_b| \implies \sigma_{\mu_b} = c \sum_{\lambda\ m_s} \int d\mathbf{\Omega}_{\mathrm{k}}\, |M^{RR}_{\mathbf{p},b}(m_s,\ \lambda,\ \mu_b)|^2$$

Photon angular distribution

Total RR cross section





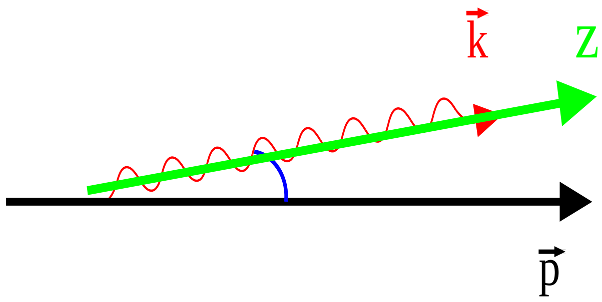
$$W(\hat{\mathbf{n}})_{j_b} = c \sum_{\lambda \mu_b m_s} |M^{RR}_{\mathbf{p},b}(m_s,\, \lambda,\, \mu_b)|^2$$

$$\sigma^{RR}_{j_b} = c \sum_{\lambda \mu_b m_s} \int d\Omega_k\, |M^{RR}_{\mathbf{p},b}(m_s,\, \lambda,\, \mu_b)|^2$$

Photon polarization and Stokes parameters

Helicity representation

$$\langle\, \mathbf{k}\lambda \,|\, \hat{\rho}_\gamma \,|\, \mathbf{k}\lambda' \,\rangle_{\lambda,\,\lambda'=\pm 1} = Tr_{(\mu_b)}(\hat{\rho}_f) = \frac{1}{2}\begin{pmatrix} 1+P_3 & -P_1+iP_2 \\ -P_1-iP_2 & 1-P_3 \end{pmatrix}$$

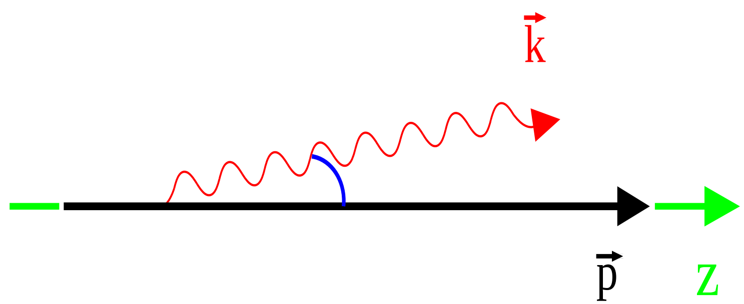


Degree of polarization:

- **linear:** $P_L = \sqrt{P_1^2 + P_2^2}$
- **circular:** $P_C = P_3$

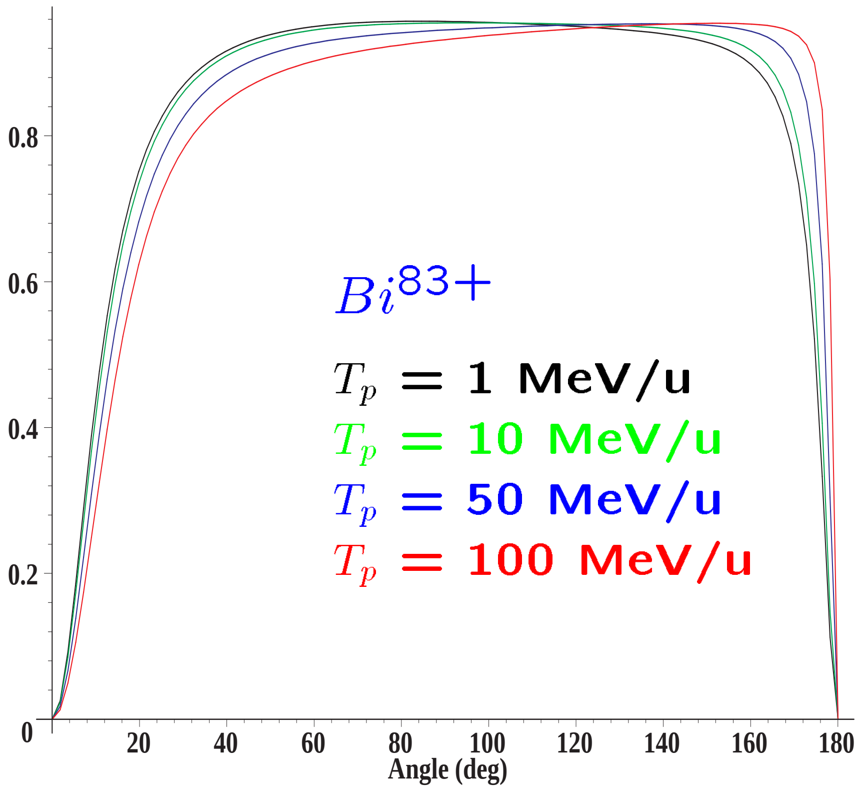
Rotation:

$$\hat{\mathbf{u}}_\lambda\, e^{i\mathbf{kr}} = \sqrt{2\pi}\sum_{L=1}^{\infty}\sum_{M=-L}^{M=+L} i^L\sqrt{2L+1}\,\mathcal{A}_{LM}^{\lambda}\; D_{M\lambda}^{L}(\mathbf{k}\to\mathbf{z})$$

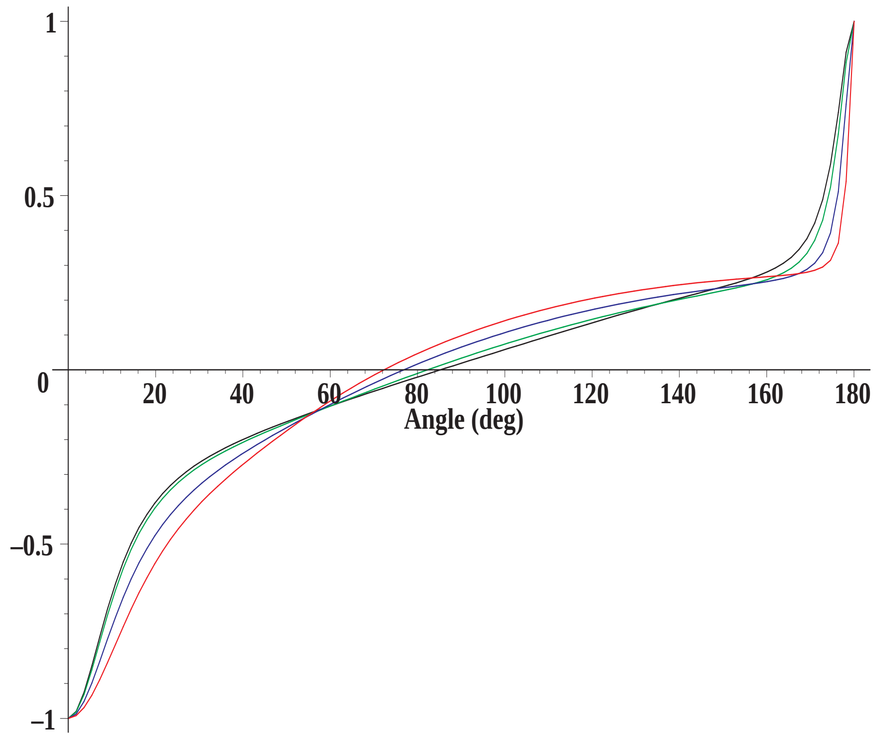


Angular dependence of the Stokes parameters

Linear polarization P_L



Circular polarization P_C



- Electron is unpolarized
- No circular polarization occurs
- Helicity frame

- For completely polarized electrons
- Collision frame

Summary

- Density matrix theory provides a successful and widely–applicable framework for studying electron–ion and ion–atom collision processes.
- For the RR of high–Z ions, this theory help understand a large variety of properties including total and angular–dependent cross section but also different polarization effects.
- Dirac toolbox "answers" many experimental FAQ's on the properties and dynamics of high–Z ions.

➥ basis for studying few–particle ions

RR of completely polarized electrons $m_s = +1/2$ into polarized Bi^{83+} $(I_o = 9/2)$ ions with $M_o = 1/2$, $M_o = 5/2$, and $M_o = 9/2$.