A New Formulation of Spectral Line Polarization with Partial Frequency Redistribution

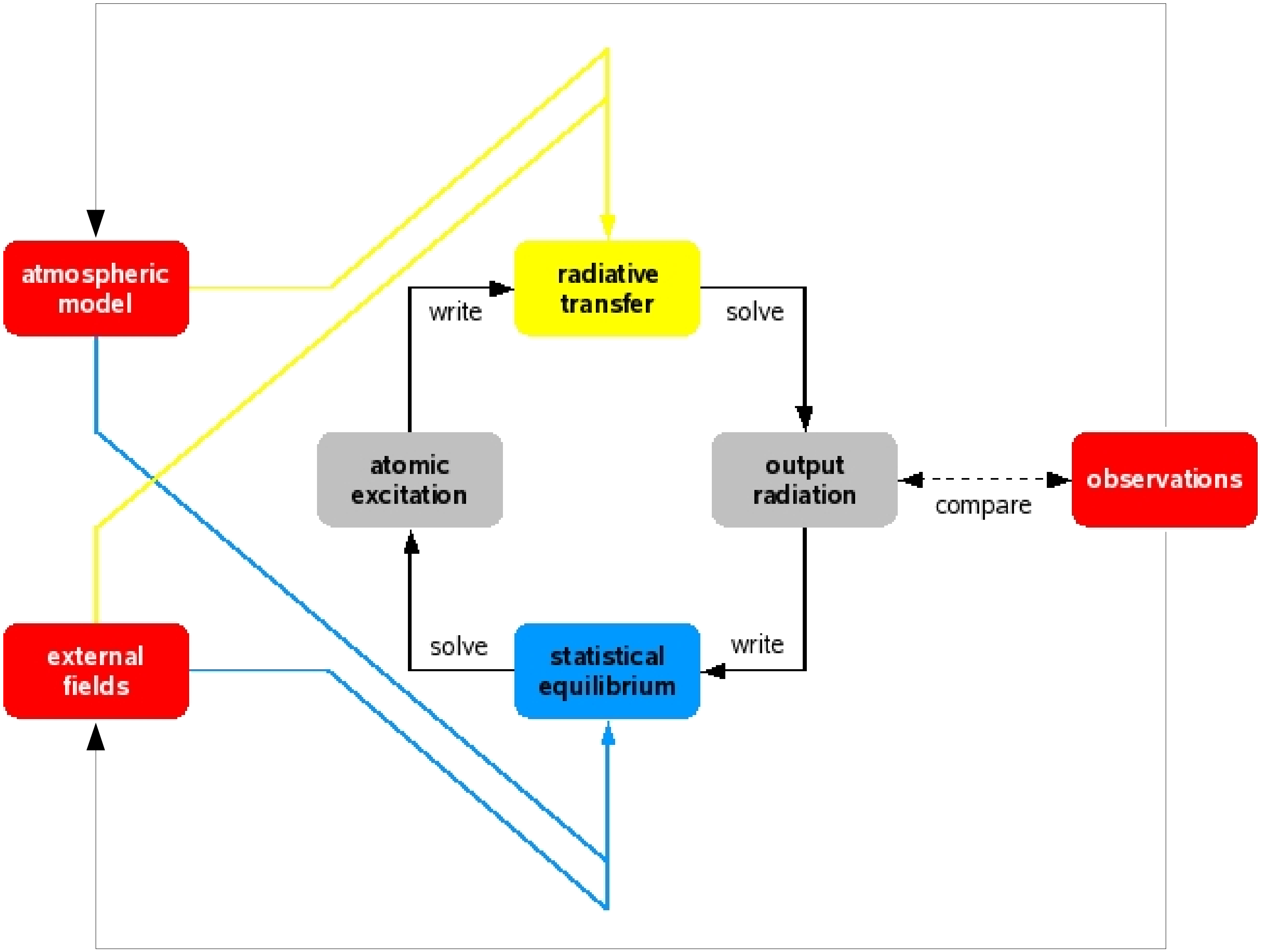
R. Casini
High Altitude Observatory

The High Altitude Observatory (HAO) at the National Center for Atmospheric Research (NCAR)
The National Center for Atmospheric Research is sponsored by the National Science Foundation. Any opinions, findings and conclusions or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

Requirements of the Theory

1) Fully quantum-mechanical derivation
   - to treat atom+photon processes in complex atomic structures without classical analog
   - to provide a unified scheme for the description of radiation and atomic polarization
   - to model the creation, modification, and “circulation” of atomic polarization (Hanle effect, level-crossing physics)
2) Separable into its “atomic” and “radiation” parts
   - to enable recursive numerical schemes for the solution of the PRT in optically thick plasmas

The Numerical Problem of PRT



Polarization of Light and Matter (1)

- monochromatic radiation, propagating along z, oscillating on the (x,y) plane:

$$E_x = E_x(\boldsymbol{r},t,\omega)\ , \qquad E_y = E_y(\boldsymbol{r},t,\omega)$$

  - infinite wave train ($\Delta\omega \to 0$ implies $\Delta t \to \infty$)
  - stationary, 100% polarized (like a *pure state* in QM)

- needs **four** parameters to be fully specified (two amplitudes and two phases, i.e., E_x and E_y are complex)

  - *Jones vector* (like a *ket* in QM)

$$\mathbf{J} \equiv \begin{pmatrix} E_x \\ E_y \end{pmatrix}$$

  - *coherency matrix* (like a *density matrix* in QM)

$$\mathbf{C} \equiv \begin{pmatrix} E_x^* E_x & E_x^* E_y \\ E_y^* E_x & E_y^* E_y \end{pmatrix}$$

Polarization of Light and Matter (2)

- non-monochromatic radiation:
  - representable as a wave packet (i.e., with finite Δt)
  - can be *partially* (<100%) polarized (a “mixture” in QM)
- needs **four** parameters to be fully specified (e.g., Stokes parameters I, Q, U, V)
  - no Jones vector (that's only for 100% polarized light!)
  - coherency matrix

$$\mathbf{C} \equiv \begin{pmatrix} \langle E_x^* E_x \rangle & \langle E_x^* E_y \rangle \\ \langle E_y^* E_x \rangle & \langle E_y^* E_y \rangle \end{pmatrix}$$

where $\langle \cdots \rangle$ is an average over the spectral and temporal bandwidths of the measurement

Polarization of Light and Matter (3)

A quantum statistical ensemble of *non-interacting* atoms (e.g., a gas where atom-atom correlations are negligible; not a Bose-Einstein condensation!) is represented by the "single atom" density matrix, i.e., a (real) linear combination of *pure, single-atom state projectors*

$$\rho^{\mathrm{A}} = \Sigma_\alpha \, p_\alpha \, |\alpha\rangle\langle\alpha|$$

- *incoherent* superposition of quantum states ("mixture"), instead of a *coherent* superposition (new pure state)
- problem analogous to representing partially polarized radiation by the coherency matrix (not a Jones vector)

Polarization of Light and Matter (4)

The density matrix of an ensemble of atoms describes the statistical distribution of the atomic-level *population* and *coherence* → ***atomic polarization***

$$\langle m|\rho^{\mathrm{A}}|m\rangle = \Sigma_\alpha\, p_\alpha \langle m|\alpha\rangle\langle\alpha|m\rangle$$

$$= \Sigma_\alpha\, p_\alpha \Sigma_{n'n}\; c^\alpha{}_{n'}\,(c^\alpha{}_n)^*\; \langle m|n'\rangle\langle n|m\rangle$$

$$= \Sigma_\alpha\, p_\alpha |c^\alpha{}_m|^2$$

(compound probability)

$$\langle m'|\rho^{\mathrm{A}}|m\rangle = \Sigma_\alpha\, p_\alpha \langle m'|\alpha\rangle\langle\alpha|m\rangle$$

$$= \Sigma_\alpha\, p_\alpha \Sigma_{n'n}\; c^\alpha{}_{n'}\,(c^\alpha{}_n)^*\; \langle m'|n'\rangle\langle n|m\rangle$$

$$= \Sigma_\alpha\, p_\alpha\, c^\alpha{}_{m'}\,(c^\alpha{}_m)^*$$

Some History of QM PRD...

Several lines of development:

- Fiutak & Van Kranendonk (1962): expanded *impact theory* formalism of Anderson (1949) to 2^{nd} order to treat molecular Raman scattering
  - assume *non-coherent* initial state (i.e., diagonal density matrix)
  - Omont & collabs.; Heinzel & collabs.
- Lamb & Ter Haar (1971): applied formalism of Heitler (1954) to the evolution of the atom+photon system to 2^{nd} order
- Stenflo (1976, 1994): semi-classical theory built upon Kramers-Heisenberg scattering amplitude
  - assumes *non-coherent* initial state
- Bommier & Sahal-Bréchot (1978), Landi Degl'Innocenti (1983): evolution ("master") equations for the atomic and radiation systems
  - Bommier (1997a,b) formulated extension to higher orders
- Landi Degl'Innocenti et al (1997): *metalevel theory* of polarized line formation (building upon an idea of Woolley & Stibbs 1953)

Atom-Photon Interaction (1)

- ensemble of atoms (A) interacting with the radiation (R); described by the Hamiltonian operator

$$H = H_{\mathrm{A}} + H_{\mathrm{R}} + H_{\mathrm{I}}$$

where H_{I} is the *atom-photon interaction* Hamiltonian

- in the electric-dipole approximation

$$H_{\mathrm{I}} = -\boldsymbol{d} \cdot \boldsymbol{E}_{\mathrm{R}}(0)$$

where $\boldsymbol{E}_{\mathrm{R}}(0)$ is the radiation field at the atom

NO COLLISIONS

Atom-Photon Interaction (2)

The atom+photon system is described by a statistical operator $\rho(t)$ evolving according to the quantum-mechanical Liouville equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\rho(t) = \frac{1}{\mathrm{i}\hbar}\,[H(t),\rho(t)]$$

with formal solution

$$\rho(t) = \rho(t_0) + \sum_{n=1}^{\infty} \frac{1}{(\mathrm{i}\hbar)^n} \int_{t_0}^{t} \mathrm{d}t_n \int_{t_0}^{t_n} \mathrm{d}t_{n-1} \cdots \int_{t_0}^{t_2} \mathrm{d}t_1 \times \Big[H(t_n), \big[H(t_{n-1}), \cdots, [H(t_1), \rho(t_0)] \cdots \big] \Big]$$

Atom-Photon Interaction (3)

Alternatively, the operator $\rho(t)$ evolves according to

$$\rho(t) = U(t,t_0)\rho(t_0)U^\dagger(t,t_0)$$

with formal solution

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{(\mathrm{i}\hbar)^{-n}}{n!} \int_{t_0}^{t} \cdots \int_{t_0}^{t} d\tau_n \cdots d\tau_1 \, T\{H(\tau_n)\cdots H(\tau_1)\}$$

- This approach allows a *diagrammatic* treatment of atom+photon interaction, **after** a formal procedure of second quantization of the atomic system

Atom-Photon Interaction (4)

With either approach:

- truncation order of solution expansion sets physical order of atom+photon processes
- system density matrix satisfies the initial condition of factorization

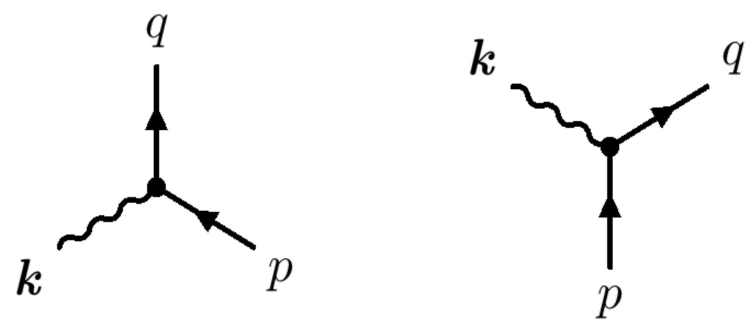
$$\rho(t_0) = \rho^{\mathrm{A}}(t_0) \otimes \rho^{\mathrm{R}}(t_0)$$

i.e., matter and radiation are initially uncorrelated

Atom-Photon Processes (1)

1st order: single-photon processes

– absorption; emission



– theory is well established (e.g., *Landi Degl'Innocenti & Landolfi 2004*)

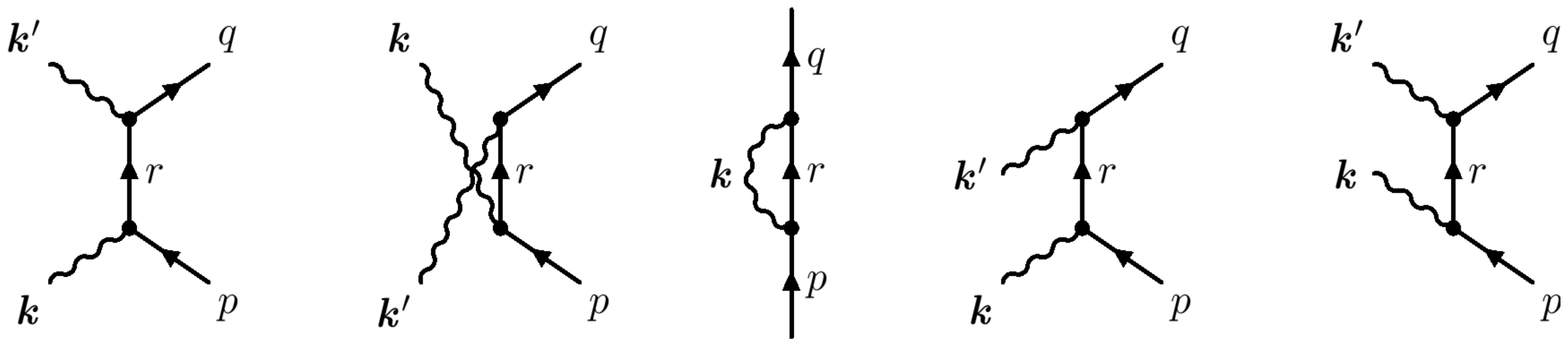
– applicable only in the Complete Redistribution regime of line formation

- **incoherent** scattering (collision dominated and/or flat-spectrum radiation)

Atom-Photon Processes (2)

2nd order: two-photon processes

– **coherent** scattering; two-photon absorption (non-linear term!); two-photon cascade

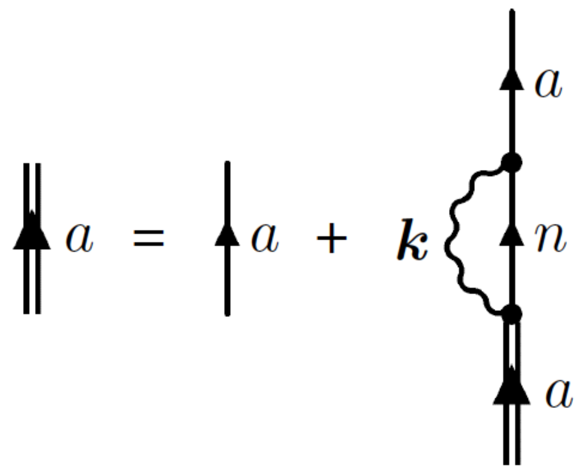


– theory is work in progress (e.g., *Bommier 1997a,b; Bommier, this workshop; Casini et al., in preparation*)

– applicable to the general case of Partial Redistribution regime of line formation

Atom-Photon Processes (3)

Formal procedure of “dressing” of the atomic propagator (*Dyson equation*) yields lifetimes of excited atomic states for spontaneous emission, and corresponding level widths



Risk of “double counting” of terms is avoided, relying on Wick's theorem and diagram topology

Evolution Equations

the solution separates into an **atomic** part (density matrix) and a **radiation** part (coherency matrix)

$$\frac{d}{dt}\langle\mathcal{O}(t)\rangle + \frac{1}{\mathrm{i}\hbar}\,\mathrm{Tr}\{\rho(t)\,[H_0,\mathcal{O}(t)]\} = \frac{1}{\mathrm{i}\hbar}\,\mathrm{Tr}\{\mathcal{O}(t)\,[H_\mathrm{I}(t),\rho(t)]\}$$

$$= -\frac{1}{\mathrm{i}\hbar}\,\mathrm{Tr}\{\rho(t)\,[H_\mathrm{I}(t),\mathcal{O}(t)]\}$$

Atoms → $\mathcal{O}_\mathrm{A}(t) = c_m^\dagger(t)c_n(t)$

Photons → $\mathcal{O}_\mathrm{R}(t) = a_{\boldsymbol{l}}^\dagger(t)a_{\boldsymbol{l}'}(t)$

substitute recursive solution here

SEE → $$\frac{d}{dt}\rho_{nm}(t) + \mathrm{i}\omega_{nm}\,\rho_{nm}(t) = -\frac{1}{\mathrm{i}\hbar}\,\mathrm{Tr}\left\{\boxed{\rho(t)}\,[H_\mathrm{I}(t), c_m^\dagger(t)c_n(t)]\right\}$$

RTE → $$\frac{d}{dt}I_{\boldsymbol{l}'\boldsymbol{l}}(t) + \mathrm{i}\omega_{l'l}\,I_{\boldsymbol{l}'\boldsymbol{l}}(t) = -\frac{1}{\mathrm{i}\hbar}\,\mathrm{Tr}\left\{\boxed{\rho(t)}\,[H_\mathrm{I}(t), a_{\boldsymbol{l}}^\dagger(t)a_{\boldsymbol{l}'}(t)]\right\}$$

Assumptions

- highly diluted radiation field
  - only retain 1st order terms in the radiation field intensity (i.e., neglects non-linear radiation effects)
- handling of the initial conditions (**very critical**)
  - "evolving" observable $\mathcal{O}(t)$ is subject to the condition

$$\partial_t \langle \mathcal{O}(t) \rangle (t, \rho(t_0)) \approx \partial_t \langle \mathcal{O}(t) \rangle (t, \rho(t))$$

    (essentially, the Markov approximation)
  - "thermal bath" observable is frozen at initial condition

NOTE: this effectively extends the factorization of $\rho(t)$ in the atomic and radiation parts beyond t_0

Main Results
(two-term atom; no stimulation)

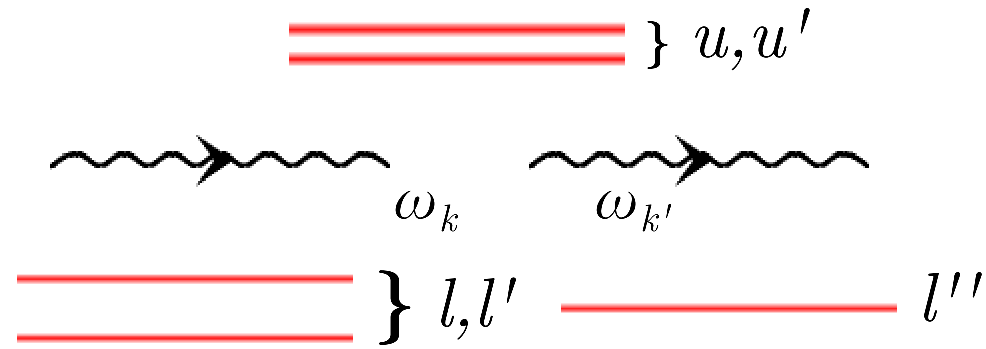
- Both SEE and RTE are modified to 2nd order of atom+photon interaction
- SEE acquire a term that partially compensates the absorption rate → depression of upper level population (exact cancellation when lower-term lifetime $\to \infty$)
- RTE acquire coherent scattering emission term
- absorption coefficient in RTE is unchanged

NOTE: last result agrees with Optical Theorem

– absorption coefficient gives the cross-section to **both** inelastic scattering (i.e., true absorption) **and** elastic scattering (from coherent term)

Partial Redistribution (1)

Polarized Radiative Transfer
Two-Term Atom
(no stimulated emission;
no collisions)



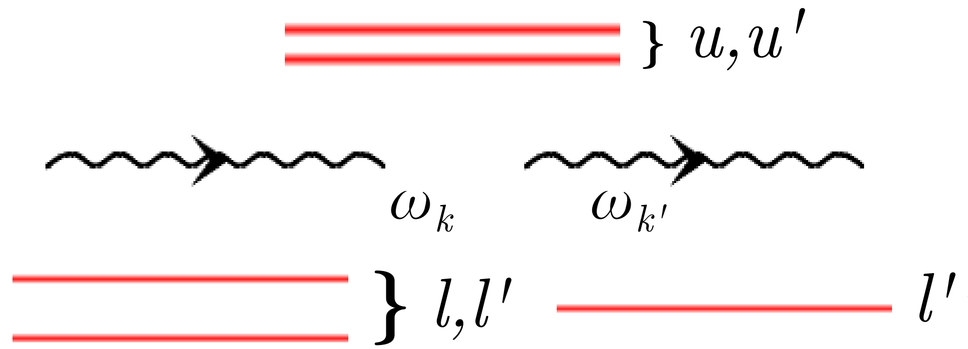
$$\frac{1}{c}\frac{d}{dt}S_i(\omega_{k'},\hat{\boldsymbol{k}}') = -\sum_j \kappa_{ij}(\omega_{k'},\boldsymbol{k}')\,S_j(\omega_{k'},\hat{\boldsymbol{k}}') + \varepsilon_i^{(1)}(\omega_{k'},\hat{\boldsymbol{k}}') + \boxed{\varepsilon_i^{(2)}(\omega_{k'},\hat{\boldsymbol{k}}')}$$

$$\varepsilon_i^{(2)}(\omega_{k'},\hat{\boldsymbol{k}}') \equiv \frac{4}{3}\frac{e_0^4}{\hbar^2 c^4}\,\mathcal{N}\omega_{k'}^4 \sum_{ll'}\rho_{ll'} \sum_{uu'l''}\sum_{qq'}\sum_{pp'}(-1)^{q'+p'}\,(r_q)_{ul}(r_{q'})^*_{u'l'}(r_p)_{u'l''}(r_{p'})^*_{ul''}$$
$$\times \sum_{KQ}\sum_{K'Q'}\sqrt{(2K+1)(2K'+1)}\begin{pmatrix}1 & 1 & K\\ -q & q' & -Q\end{pmatrix}\begin{pmatrix}1 & 1 & K'\\ -p & p' & -Q'\end{pmatrix} T_{Q'}^{K'}(i,\hat{\boldsymbol{k}}')$$
$$\times \int_0^\infty d\omega_k \boxed{\left(\Psi_{u'l',l''ul}^{-k,+k'-k} + \bar{\Psi}_{ul,l''u'l'}^{-k,+k'-k}\right)} J_Q^K(\omega_k)\,. \qquad (i=0,1,2,3)$$

$$J_Q^K(\omega_k) = \oint \frac{d\hat{\boldsymbol{k}}}{4\pi}\sum_{j=0}^{3} T_Q^K(j,\hat{\boldsymbol{k}})\,S_j(\omega_k,\hat{\boldsymbol{k}})$$

Redistribution Function

Partial Redistribution (2)



Redistribution Function
(atomic rest frame)

$$
\begin{aligned}
\mathcal{R}(\Omega_u, \Omega_{u'}; \Omega_l, \Omega_{l'}, \Omega_{l''}; \omega_k, \omega_{k'}) &\equiv (\epsilon_{uu'} + \mathrm{i}\omega_{uu'}) \left(\Psi^{-k,+k'-k}_{u'l',l''ul} + \bar{\Psi}^{-k,+k'-k}_{ul,l''u'l'} \right) \\
&= \frac{2\epsilon_{l''}(\epsilon_{ll'} + \mathrm{i}\omega_{ll'})}{(\omega_k - \omega_{ul'} + \mathrm{i}\epsilon_{ul'})(\omega_k - \omega_{u'l} - \mathrm{i}\epsilon_{u'l})(\omega_{k'} - \omega_{ul''} + \mathrm{i}\epsilon_{ul''})(\omega_{k'} - \omega_{u'l''} - \mathrm{i}\epsilon_{u'l''})} \\
&+ \frac{2\epsilon_{l''}(\epsilon_{uu'} + \mathrm{i}\omega_{uu'})}{(\omega_k - \omega_{ul'} + \mathrm{i}\epsilon_{ul'})(\omega_k - \omega_{u'l} - \mathrm{i}\epsilon_{u'l})(\omega_k - \omega_{k'} + \omega_{l'l''} + \mathrm{i}\epsilon_{l'l''})(\omega_k - \omega_{k'} + \omega_{ll''} - \mathrm{i}\epsilon_{ll''})} \\
&+ \frac{(\epsilon_{ll'} + \mathrm{i}\omega_{ll'})(\epsilon_{uu'} + \mathrm{i}\omega_{uu'})}{(\omega_{k'} - \omega_{ul''} + \mathrm{i}\epsilon_{ul''})(\omega_{k'} - \omega_{u'l''} - \mathrm{i}\epsilon_{u'l''})(\omega_k - \omega_{k'} + \omega_{l'l''} + \mathrm{i}\epsilon_{l'l''})(\omega_k - \omega_{k'} + \omega_{ll''} - \mathrm{i}\epsilon_{ll''})} \\
&+ \frac{2\epsilon_{l''}(\epsilon_{ll'} + \mathrm{i}\omega_{ll'})(\epsilon_{uu'} + \mathrm{i}\omega_{uu'})}{(\omega_k - \omega_{ul'} + \mathrm{i}\epsilon_{ul'})(\omega_k - \omega_{u'l} - \mathrm{i}\epsilon_{u'l})(\omega_{k'} - \omega_{ul''} + \mathrm{i}\epsilon_{ul''})(\omega_{k'} - \omega_{u'l''} - \mathrm{i}\epsilon_{u'l''})} \\
&\qquad \times \frac{2\epsilon_{l''} + \epsilon_{ll'} + \epsilon_{uu'} + \mathrm{i}(\omega_{ll'} + \omega_{uu'})}{(\omega_k - \omega_{k'} + \omega_{l'l''} + \mathrm{i}\epsilon_{l'l''})(\omega_k - \omega_{k'} + \omega_{ll''} - \mathrm{i}\epsilon_{ll''})} \,,
\end{aligned}
$$

$$
\Omega_a \equiv \omega_a - \mathrm{i}\epsilon_a \,, \qquad \omega_{ab} \equiv \omega_a - \omega_b \,, \quad \epsilon_{ab} \equiv \epsilon_a + \epsilon_b
$$

Results

- derived redistribution function encompasses all prior results found in the literature (in the atomic rest frame, assuming no collisions), e.g., for the radiation scattering in a two- and three-level atom (Omont et al. 1972, Heinzel 1981, Hubeny 1982)
- extends those prior results to the generally polarized two-term atom
- found to be identical to a (never cited) result of Lamb & Ter Haar (1971)

Ongoing and Future Plans

- implement more rigorous treatment of initial conditions
- develop parallel diagrammatic formalism for collisions