Theoretical Tools for Spectro-Polarimetry

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Polarized Radiative Transfer (PRT)  
Fundamental Requirements

1) Fully quantum-mechanical description
   - to treat atom+photon processes in complex atomic structures that have no 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 “atomic” and “radiation” parts
   - to enable recursive numerical schemes for the solution of the PRT in optically thick plasmas
The Numerical Problem of PRT

(e.g., Landi Degl'Innocenti & Landolfi 2004)
Atom-Photon Interaction

The interacting atom+photon system is described by a density operator \( \rho(t) \), evolving according to

\[
\rho(t) = U(t,t_0) \rho(t_0) U(t,t_0)^\dagger
\]

with formal solution

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

- Perturbation expansion leads to a *diagrammatic* treatment of atom+photon interaction
- Truncation order defines physical order of atom+photon processes
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 (flat-spectrum illumination and/or collision dominated plasma)
Atomic-Photon Processes (2)

2nd order: two-photon processes

- coherent scattering; two-photon absorption; two-photon cascade (via virtual state $r$)

- theory is still work in progress (e.g., Bommier 1997a,b; Casini et al., in preparation)

- applicable to the general case of Partial Redistribution regime of line formation
Evolution Equations

Solution separates into an atomic part (density matrix) and a radiation part (coherency matrix)

\[
\frac{d}{dt} \langle \mathcal{O}(t) \rangle + \frac{1}{i\hbar} \text{Tr}\left\{ \rho(t) [H_0, \mathcal{O}(t)] \right\} = \frac{1}{i\hbar} \text{Tr}\left\{ \mathcal{O}(t) [H_I(t), \rho(t)] \right\} \\
= -\frac{1}{i\hbar} \text{Tr}\left\{ \rho(t) [H_I(t), \mathcal{O}(t)] \right\}
\]

Atoms \quad \rightarrow \quad \mathcal{O}_A(t) = c_m^\dagger(t)c_n(t)

Photons \quad \rightarrow \quad \mathcal{O}_R(t) = a_l^\dagger(t)a_{l'}(t)

SEE \quad \rightarrow \quad \frac{d}{dt} \rho_{nm}(t) + i\omega_{nm} \rho_{nm}(t) = -\frac{1}{i\hbar} \text{Tr}\left\{ \rho(t) [H_I(t), c_m^\dagger(t)c_n(t)] \right\}

RTE \quad \rightarrow \quad \frac{d}{dt} I_{l'l}(t) + i\omega_{l'l} I_{l'l}(t) = -\frac{1}{i\hbar} \text{Tr}\left\{ \rho(t) [H_I(t), a_l^\dagger(t)a_{l'}(t)] \right\}
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 $\rightarrow$ depression of upper level population (exact cancellation when lower-term lifetime $\rightarrow \infty$)
- RTE acquire coherent scattering emission term
- absorption coefficient is unchanged; i.e., it provides the cross-section to both inelastic scattering (true absorption) and elastic scattering (from coherent term)
Partial Redistribution

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

\[
\frac{1}{c} \frac{d}{dt} S_i(\omega_{k'}, \hat{k}') = -\sum_j \kappa_{ij}(\omega_{k'}, \hat{k}') S_j(\omega_{k'}, \hat{k}') + \varepsilon^{(1)}_i(\omega_{k'}, \hat{k}') + \varepsilon^{(2)}_i(\omega_{k'}, \hat{k}'),
\]

\[
\varepsilon^{(2)}_i(\omega_{k'}, \hat{k}') = \frac{4}{3} \frac{e_0^4}{\hbar^2 c^4} N \omega^4 \sum_{l''} \sum_{ul''l'''} \sum_{qq'} \sum_{pp'} (-1)^{q'+p'} (r_q)_{ul}(r_q^*)_{u'l'}(r_p)_{ul'}(r_p^*)_{ul'},
\]

\[
\times \sum_{KQ} \sum_{K'Q'} \sqrt{(2K + 1)(2K' + 1)} \begin{pmatrix} 1 & 1 & K \\ -q & q' & -Q \end{pmatrix} \begin{pmatrix} 1 & 1 & K' \\ -p & p' & -Q' \end{pmatrix} T^{K'}_{Q'}(i, \hat{k}')
\]

\[
\times \int_0^\infty d\omega_k \left( \Psi_{ul,l'ul'}^{k,-k,-k} + \overline{\Psi}_{ul,l'ul'}^{k,-k,-k} \right) J^K_Q(\omega_k). \quad (i = 0, 1, 2, 3)
\]

\[
J^K_Q(\omega_k) = \int \frac{d\hat{k}}{4\pi} \sum_{j=0}^3 T^K_Q(j, \hat{k}) S_j(\omega_k, \hat{k})
\]

Redistribution Function
Application: Na I D$_1$ (no HFS)

$\delta(\lambda)$-illumination

90° scattering; maximum anisotropy

$B = 100$ G, $\theta_B = 90^\circ$, $\varphi_B = 45^\circ$

$T = 4000$ K
Application: He I 1083 nm

\(\delta(\lambda)\)-illumination

90° scattering; maximum anisotropy

\[ B = 100 \, \text{G}, \, \theta_B = 90^\circ, \, \phi_B = 45^\circ \]

\[ T = 10000 \, \text{K} \]
Ongoing and Future Work

- improve treatment of initial conditions of the evolution equation (ongoing)
- develop a parallel, diagrammatic formalism for collisions (barely started... many years ago...)
- more applications...
Additional Slides
Some History of QM PRT

Several lines of development:

- Fiutak & Van Kranendonk (1962): expanded *impact theory* formalism of Anderson (1949) to 2nd 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 2nd order

  - assumes *non-coherent* initial state

  - Bommier (1997a,b) formulated extension to higher orders

Atom-Photon Interaction (1)

- Ensemble of atoms (A) interacting with the radiation (R); described by the Hamiltonian operator
  \[ H = H_A + H_R + H_I \]
  
  where \( H_I \) is the \textit{atom-photon interaction} Hamiltonian

- In the electric-dipole approximation
  \[ H_I = \mathbf{d} \cdot \mathbf{E}_R(0) \]
  
  where \( \mathbf{E}_R(0) \) is the radiation field at the atom

NO COLLISIONS
Atom-Photon Interaction (3)

- The system's density operator satisfies an initial condition of factorization
  
  $\rho(t_0) = \rho^A(t_0) \otimes \rho^R(t_0)$

  i.e., matter and radiation are initially uncorrelated
- Truncation order of perturbation expansion sets physical order of atom+photon processes
Formal procedure of “dressing” of the atomic propagator (Dyson counting" of terms is avoided, relying on Wick's theorem and diagrammatic techniques.)
Assumptions

- **highly diluted radiation field**
  - only retain 1st-order terms in the radiation field (e.g., neglects multi-photon absorption)

- **handling of the initial conditions** (very critical)
  - "evolving" observable $O(t)$ is subject to the condition
    \[
    \partial_t \langle O(t) \rangle(t, \rho(t_0)) \approx \partial_t \langle O(t) \rangle(t, \rho(t))
    \]
  - (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 $t_0$
Partial Redistribution (2)

Redistribution Function
(atomic rest frame; Casini et al. 2014)

\[
\mathcal{R}(\Omega_{ul}, \Omega_{u' l'; l', uu'}; \omega_k, \omega_{k'}) \approx (\epsilon_{uu'} + i\omega_{uu'}) \left( \Psi_{u' l', uu'}^{k,-} + \overline{\Psi}_{ul', uu'}^{k,-} \right)
\]

\[
= \frac{2\epsilon_{uu'}(\epsilon_{uu'} + i\omega_{uu'})}{(\omega_k - \omega_{ul'} + i\epsilon_{ul'})(\omega_k - \omega_{ul'} - i\epsilon_{ul'})(\omega_{k'} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{k'} - \omega_{ul'} - i\epsilon_{ul'})}
\]

\[
+ \frac{2\epsilon_{uu'}(\epsilon_{uu'} + i\omega_{uu'})}{(\omega_k - \omega_{ul'} + i\epsilon_{ul'})(\omega_k - \omega_{ul'} - i\epsilon_{ul'})(\omega_{k'} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{k'} - \omega_{ul'} - i\epsilon_{ul'})}
\]

\[
+ \frac{2\epsilon_{uu'}(\epsilon_{uu'} + i\omega_{uu'})}{(\omega_k - \omega_{ul'} + i\epsilon_{ul'})(\omega_k - \omega_{ul'} - i\epsilon_{ul'})(\omega_{k'} - \omega_{ul'} + i\epsilon_{ul'})(\omega_{k'} - \omega_{ul'} - i\epsilon_{ul'})}
\]

\[
\Omega_a \equiv \omega_a - i\epsilon_a, \quad \Omega_{ab} \equiv \omega_a - \omega_b, \quad \epsilon_{ab} \equiv \epsilon_a + \epsilon_b
\]
Partial Redistribution (3)

Redistribution Function
(laboratory rest frame; lower levels; incoherent lower term)

\[
R_{II}(\Omega_u, \Omega_{u'}; \Omega_l, \Omega_{l'}, \Omega_{l''}; \hat{\omega}_k, \hat{\omega}_{k'}; \Theta) = \frac{\pi}{4\Delta\omega_T^2 C_2 S_2} \exp \left[ -\frac{(\hat{\omega}_{k'} - \hat{\omega}_k - \omega_{l''})^2}{4S_2^2 \Delta\omega_T^2} \right] \\
\times \left[ W\left(\frac{1}{2}(v_{ul} + w_{ul''})/C_2, a_u/C_2\right) + \overline{W}\left(\frac{1}{2}(v_{u'l'} + w_{u'l''})/C_2, a_u/C_2\right) \right]
\]

\[
W(v, a) = \frac{1}{\pi} \int_{-\infty}^{\infty} dp \frac{e^{-p^2}}{a + i(p - v)} = H(v, a) + i L(v, a)
\]