Radiative transfer & line formation

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Why radiation and how to solve radiative transfer:

All exoplanets are studied remotely.

Their atmospheres can only be studied by radiation: Emitted light, and scattered light or stellar light blocked by planet. (transmission spectra)

We will only discuss emitted/scattered light here! See Hannah Wakeford’s talk for transmission spectra!

We need to describe the interaction between electromagnetic radiation and the atmosphere.

Instead of solving Maxwell’s equations it is customary to work in the limit of geometric optics.
**Geometric optics and the intensity**

*Geometric optics*: wavelengths smaller than structure which photons interacts with. Radiation propagates along **straight rays**. Refraction cannot be treated.

*but scattering can, also off small particles!*

\[
I = \frac{\text{Energy}}{\text{Area} \times \text{time} \times \text{frequency} \times \text{direction} \times (\text{solid angle})}
\]

or

\[
I = \frac{dE}{dA \, dt \, d\nu \, d\Omega}
\]

Integrating over direction means integrating over \(\Omega\).
Flux = direction-integrated intensity perpendicularly passing through detector

\[ I = \frac{dE}{dA \, dt \, d\nu \, d\Omega} \quad \Rightarrow \quad F = \frac{dE}{dA \, dt \, d\nu} \]

\[ F = \frac{1}{|\Delta A|} \int (\mathbf{n} \cdot \Delta \mathbf{A}) \, I(\mathbf{n}) d\Omega \]
Flux 2

Measuring flux emitted by planet far away:

\[ F = \frac{1}{|\Delta A|} \int \left( \mathbf{n} \cdot \Delta A \right) I(\mathbf{n}) dΩ \]

\[ \Rightarrow F = \pi I \left( \frac{R_p}{r} \right)^2 \text{, if } I \text{ is isotropic and the same everywhere on the planet.} \]

So flux depends on distance to target \( F \propto r^{-2} \).

But it holds that \( dI/dr = 0 \) in the absence of extinction, emission, scattering.

So in the simplest case, intensity is constant!
Radiative transfer equation: considering extinction

\[ \mathbf{n} \cdot \nabla I = 0 \]

In the absence of extinction, emission, scattering.

Spatial derivative along the ray

\[ \mathbf{n} \cdot \nabla I = -\alpha_{\text{tot}} I \]

, where \( \alpha_{\text{tot}} \) is the extinction coefficient.

Sources of extinction:

- **Absorption** (the photon is destroyed)
- **Scattering** (the photon changes direction)

Thus we can write:

\[ \alpha_{\text{tot}} = \alpha_{\text{abs}} + \alpha_{\text{scat}} \]
Radiative transfer equation: adding emission

\[ \mathbf{n} \cdot \nabla I = - \alpha_{\text{tot}} I + j, \] where \( j \) is the emissivity.

Relation between emissivity and blackbody emission (Planck function):

A blackbody emits with intensity \( I = B(T) \).

If light passes through a non-scattering medium in local thermal equilibrium (LTE), which has the same temperature as the emitting blackbody:

\[ I = \text{cst} \Rightarrow \mathbf{n} \cdot \nabla I = 0 \Rightarrow j = \alpha_{\text{abs}} B \] in LTE.

This is Kirchhoff’s law.
Radiative transfer equation: adding scattering

\[ \mathbf{n} \cdot \nabla I = -\alpha_{\text{tot}} I + j + \alpha_{\text{scat}} \int I(\mathbf{n}') p(\mathbf{n}, \mathbf{n}') d\Omega' \]

where \( p \) is the scattering phase function which answers this question:

“Coming from direction \( \mathbf{n}' \), how likely is it to be scattered in direction \( \mathbf{n} \)?”

\( p \) is a property of the scattering partner of the photon (e.g., molecule or cloud particle).

Isotropic scattering, so \( p = 1/(4\pi) \):

\[ \mathbf{n} \cdot \nabla I = -\alpha_{\text{tot}} I + j + \alpha_{\text{scat}} J, \]

where \( J \) is the mean intensity:

\[ J = \frac{1}{4\pi} \int I(\mathbf{n}) d\Omega \]

Scattering makes radiative transfer hard: we need to know \( I \) to solve for \( I \).

(usually solved iteratively on a computer)
Radiative transfer equation: full beauty

\[ \mathbf{n} \cdot \nabla I(x, n, \nu) = -\alpha_{\text{tot}}(x, \nu)I(x, n, \nu) + j(x, \nu) + \alpha_{\text{scat}}(x, \nu) \oint I(x, n', \nu)p(x, n, n', \nu)d\Omega' \]

We have dropped a couple of implicit dependencies before:

To make things more digestible we drop them again (only in notation).
Also we now move to a coordinate system parallel to the ray we investigate.

\[ \frac{dI}{ds} = -\alpha_{\text{tot}}I + j + \alpha_{\text{scat}} \oint I(n')p(n, n')d\Omega' \]
Radiative transfer equation: optical depth

The extinction coefficient $\alpha_{\text{tot}}$ is the inverse mean free path of a photon

\[\lambda^{-1} = k \rho \lambda = 1\]

Therefore:

$\alpha_{\text{tot}} = \lambda^{-1} = k \rho$

The optical depth $\tau$ is distance in units of mean free paths:

\[d\tau = \alpha_{\text{tot}} \, ds\]
Radiative transfer equation: source function

We had: \[
\frac{dI}{ds} = -\alpha_{\text{tot}} I + j + \alpha_{\text{scat}} \int I(n') p(n, n') d\Omega'
\]

Now we define the source function \( S \):

\[
S = \frac{j}{\alpha_{\text{tot}}} + \frac{\alpha_{\text{scat}}}{\alpha_{\text{tot}}} \int I(n') p(n, n') d\Omega'
\]

Then:

\[
\frac{dI}{d\tau} = -I + S
\]

In LTE and for isotropic scattering it holds that

\[
S = \epsilon B + \omega J,
\]

with the photon destruction probability: \( \epsilon = \frac{\alpha_{\text{abs}}}{\alpha_{\text{tot}}} \)

and single-scattering albedo: \( \omega = \frac{\alpha_{\text{scat}}}{\alpha_{\text{tot}}} = 1 - \epsilon \)
Radiative transfer equation: solution for constant $S$

Exercise :) 

$$I(\Delta \tau) = I_0 e^{-\Delta \tau} + S(1 - e^{-\Delta \tau})$$

This has the following limits: $$\lim_{\Delta \tau \to 0} I(\Delta \tau) = I_0 \quad \text{and} \quad \lim_{\Delta \tau \to \infty} I(\Delta \tau) = S$$

In LTE all intensities of rays passing through an optically thick, non-scattering medium with temperature $T$ will have $I = B(T)$. Large $\Delta \tau$
Imagine you have a line-shaped opacity $\kappa$:

$$\Delta\tau = \kappa \rho \Delta s$$

Let's solve for $I(s, \nu)$, so as function of distance, not $I(\tau, \nu)$:

$$I(\Delta s, \nu) = I[\Delta\tau(\Delta s, \nu)] = I_0 e^{-\Delta\tau(\Delta s, \nu)} + B(1 - e^{-\Delta\tau(\Delta s, \nu)})$$

to calculate $I(\Delta s, \nu)$. 
Line formation 2

Now use $I(\Delta s, \nu) = I[\Delta \tau(\Delta s, \nu)] = I_0 e^{-\Delta \tau(\Delta s, \nu)} + B(1 - e^{-\Delta \tau(\Delta s, \nu)})$ and

Case 1: $B < I_0$

If $B = B(T)$ and $I_0 \approx B(T_0)$:

Absorption lines form if $T < T_0$.

Case 2: $B > I_0$

Emission lines form if $T > T_0$.

The sign of the temperature gradient $dT/ds$ determines whether absorption or emission lines form.
Lines arise from the quantization (discrete value restriction) of energy states in molecules, atoms, and ions.

Absorption of light is being used to change the electronic, vibrational or rotational state of the absorber.

Vibrational modes of H$_2$O:

Absorption strength is calculated using Einstein coefficients (+absorption−stimulated emission).
Lines are broadened (so not infinitely narrow)!

Two effects dominate, with different functional forms:

1. Lifetime-related broadening \((\Delta E \Delta t \geq \hbar/2)\)
   - Natural broadening: \(\gamma \propto \text{vacuum fluctuations!}\)
   - Excited states decay spontaneously.
   - Pressure broadening: \(\gamma \propto PT^{-1/2}\).

2. Doppler broadening
   - Due to velocity distribution of absorbers (e.g., Maxwell-Boltzmann in LTE)
   - Broadening \(\gamma \propto \sqrt{T/m}\).
Line broadening 2

No broadening → Natural broadening → Pressure broadening → Pressure broadening

Thermal broadening

Higher temperature thermal broadening

\[ \phi_{\text{Lorentz}}(\nu) = \frac{1}{\pi \gamma^2 + (\nu - \nu_{\text{line}})^2} \]

\[ \phi_{\text{thermal}}(\nu) = \frac{1}{\gamma \sqrt{\pi}} e^{-(\nu - \nu_{\text{line}})^2 / \gamma^2} \]

(for Maxwell-Boltzmann)
Line broadening 3

Pressure broadening and Doppler broadening are usually active at the same time.

Core: Doppler dominates!
Wings: Lorentz dominates!

The effective Voigt profile arises from convolution:

\[ \phi_{\text{Voigt}}(\nu) = \int_{0}^{\infty} \phi_{\text{Lorentz}}(\nu') \phi_{\text{Doppler}}(\nu - \nu') d\nu' \]
Lines and spectrograph resolution

Actual data is often not at high enough resolution to resolve lines.

Model resolution ($\lambda/\Delta\lambda$):

- $R=100,000$
- $R=30,000$
- $R=5,000$
- $R=300$
- $R=30$

Line strengths and shapes still determine the shape of a spectrum, also at low resolution!
Summary

• In the absence of absorption, emission and scattering, the intensity $I$ is constant.

• This is a useful form of the equation of radiative transfer:
\[
\frac{dl}{d\tau} = -I + S
\]

• A useful solution for $S = \text{cst}$ is:
\[
I(\Delta \tau) = I_0 e^{-\Delta \tau} + S(1 - e^{-\Delta \tau})
\]

We are talking about emitted flux, not transmission spectra here!

• Absorption lines form in the planetary spectrum if $dT/dr < 0$.
• Emission lines form in the planetary spectrum if $dT/dr > 0$.

• Lines are caused from the quantization of energy states in molecules, atoms and ions.

• Lines a broadened, pressure broadening and thermal broadening usually dominate.

Radial coordinate of atmosphere