Radiative transfer & line formation

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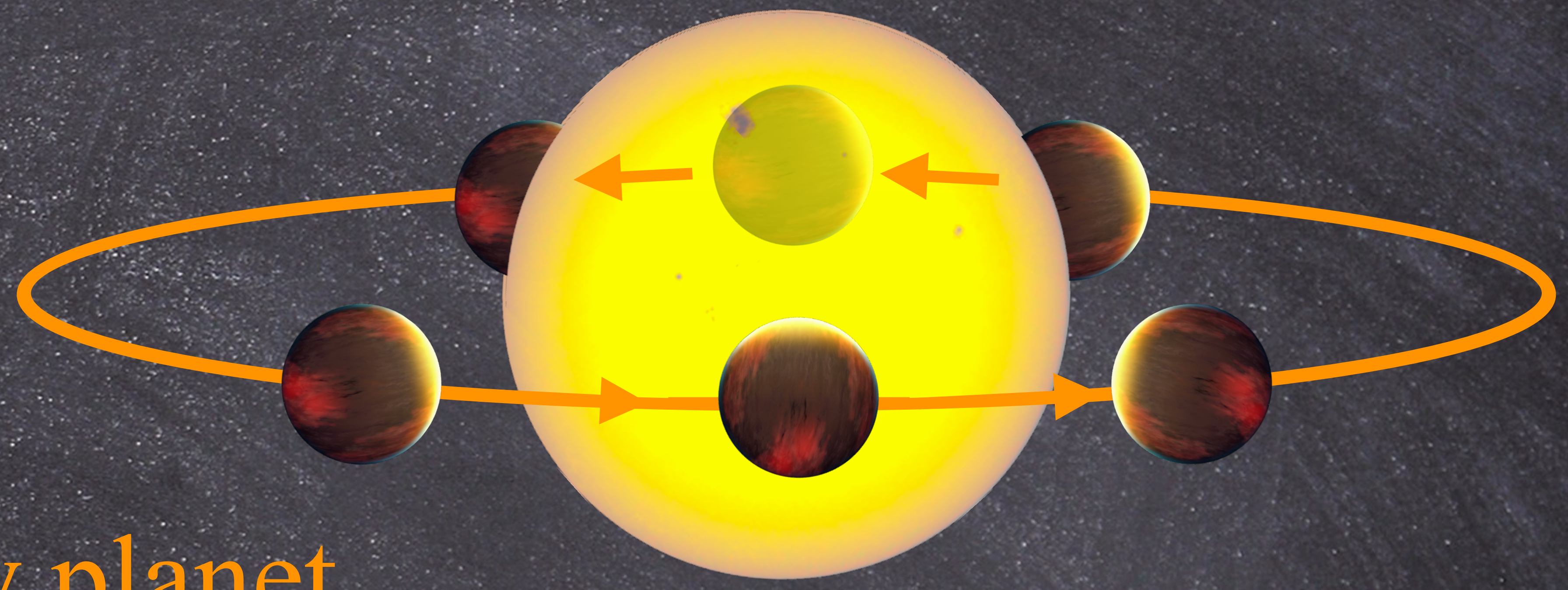
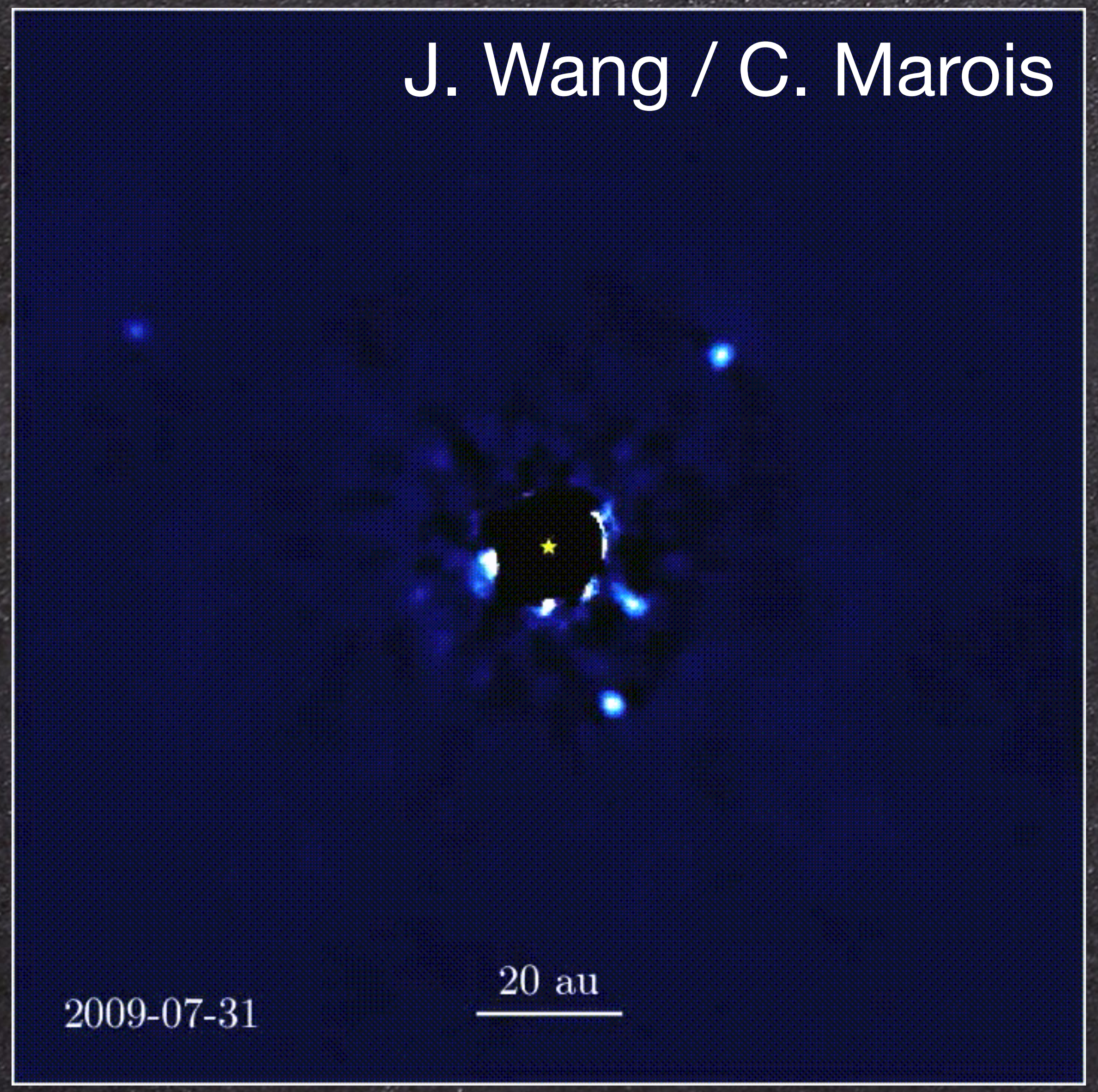
Why radiation and how to solve radiative transfer:

All exoplanets are studied remotely.



Transiting planet

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



Directly imaged planets

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

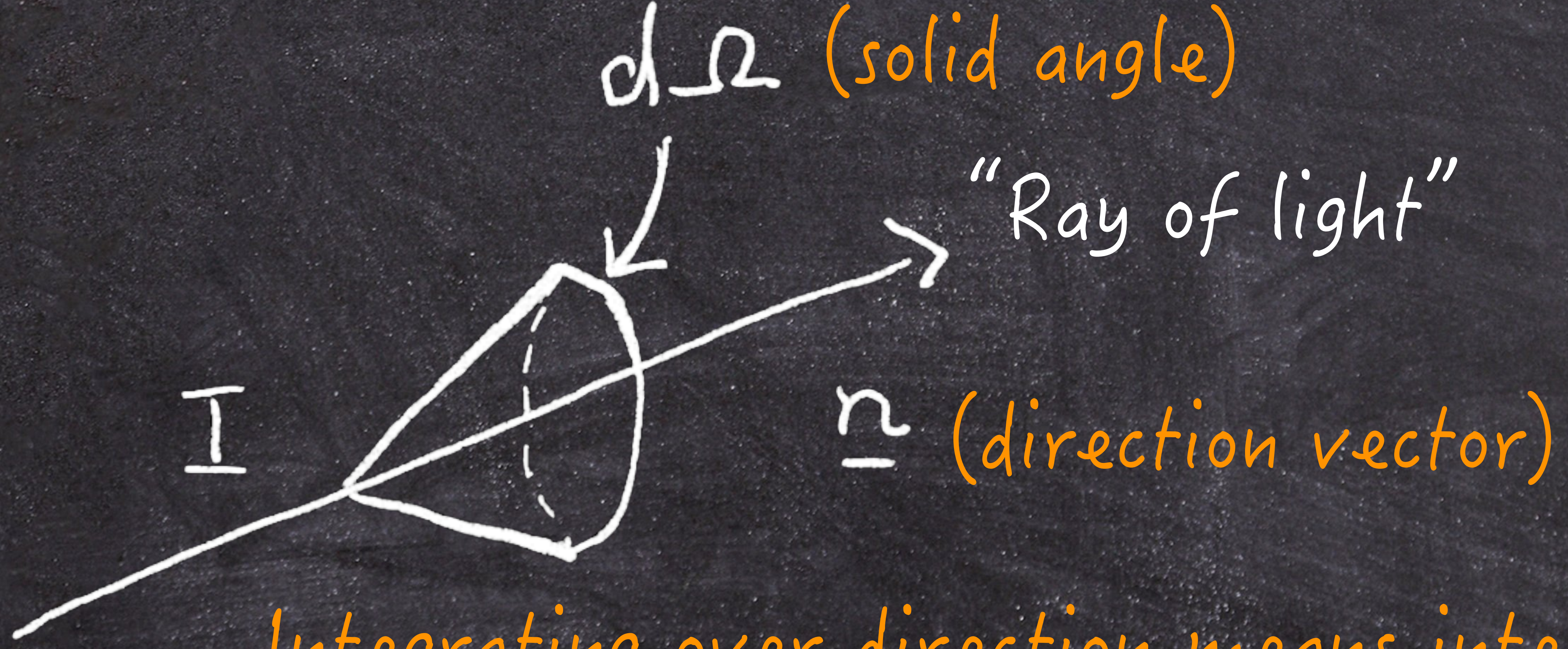
We need to describe the interaction between electromagnetic radiation and the atmosphere.

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!)

$$\text{Intensity} = \frac{\text{Energy}}{\text{Area} \times \text{time} \times \text{frequency} \times \text{direction (solid angle)}} \quad \text{or} \quad I = \frac{dE}{dA\ dt\ d\nu\ d\Omega}$$



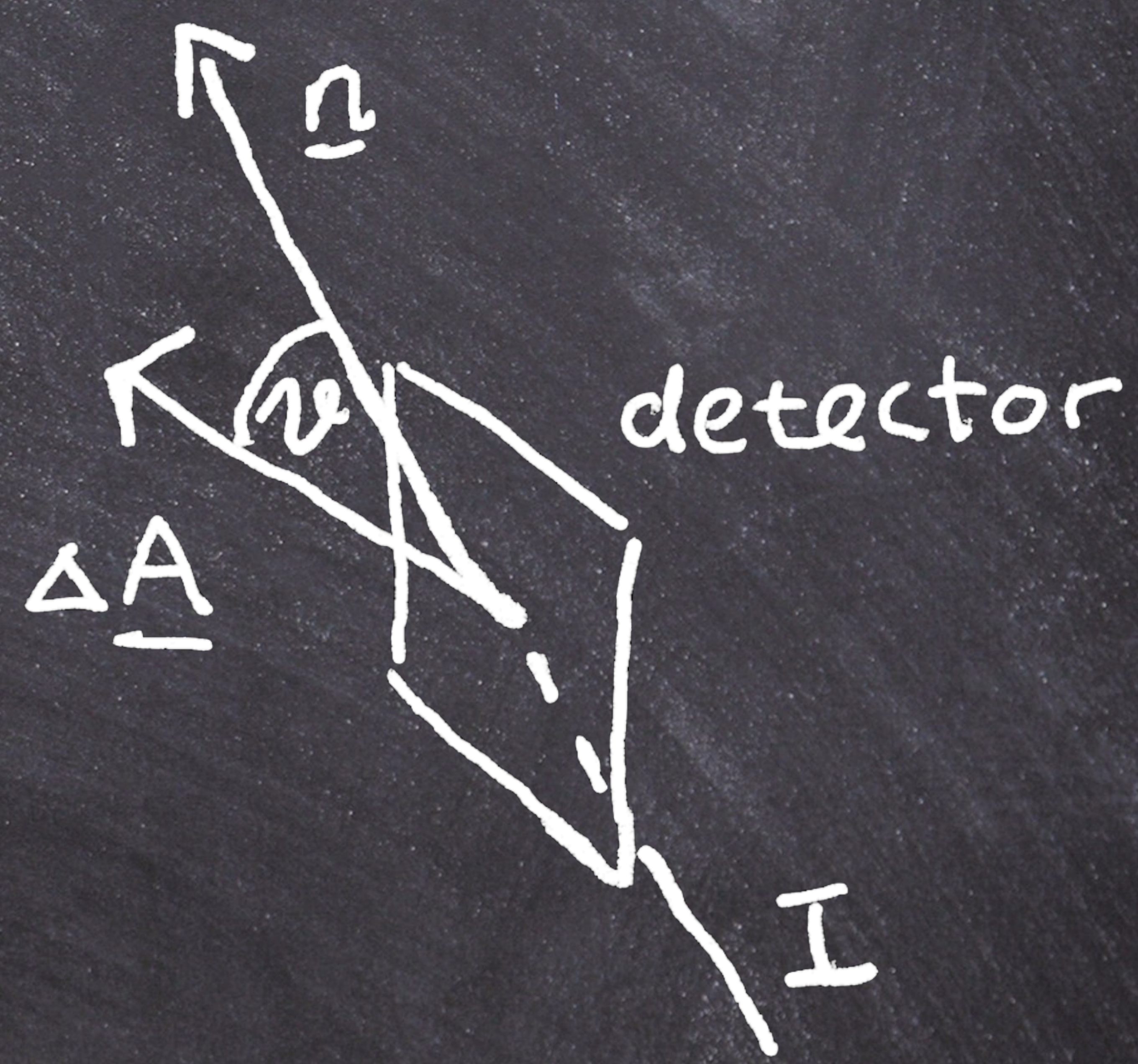
Integrating over direction means integrating over Ω.

Flux 1

Flux = direction-integrated intensity perpendicularly passing through detector

$$I = \frac{dE}{dA\ dt\ d\nu\ d\Omega} \quad \Rightarrow \quad F = \frac{dE}{dA\ dt\ d\nu}$$

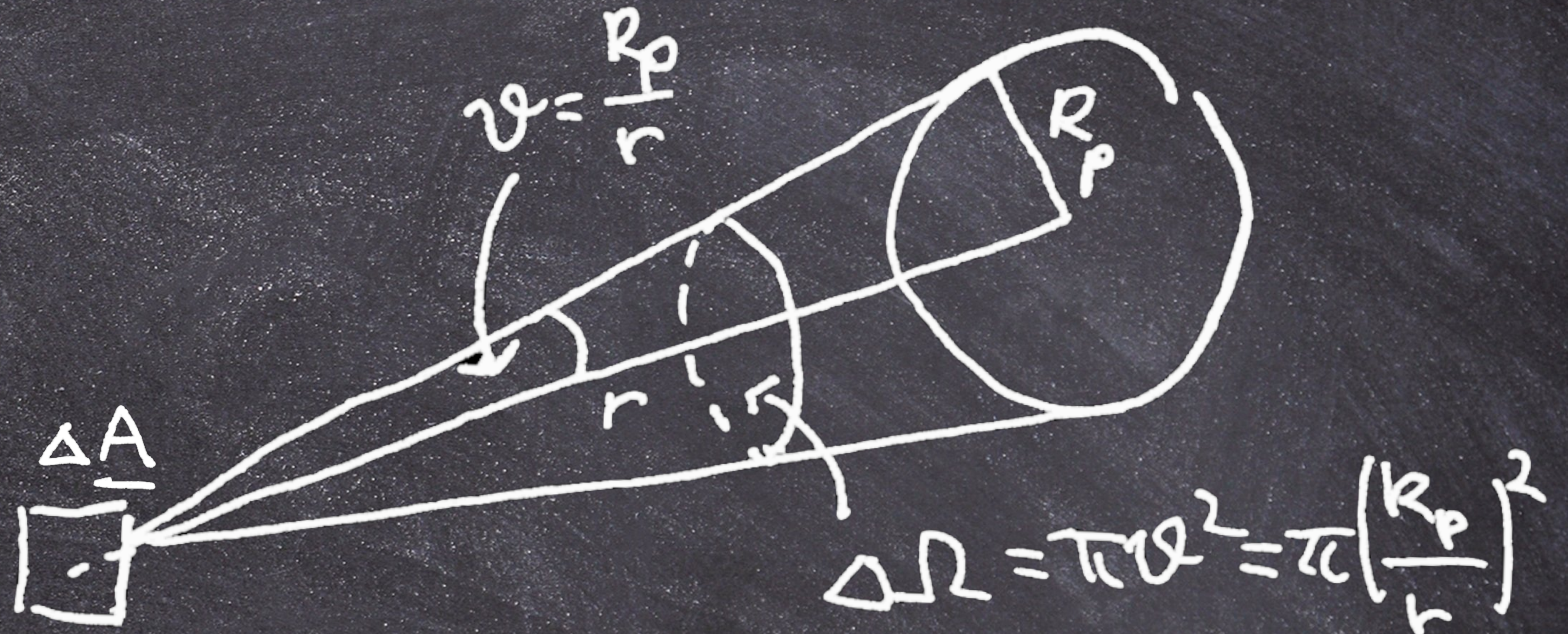
$$F = \frac{1}{|\mathbf{\Delta A}|} \int (\mathbf{n} \cdot \mathbf{\Delta A})\ I(\mathbf{n}) d\Omega$$



Flux 2

Measuring flux emitted by planet far away:

$$F = \frac{1}{|\mathbf{\Delta A}|} \int \underbrace{(\mathbf{n} \cdot \mathbf{\Delta A})}_{\sim\text{parallel}} \, I(\mathbf{n}) d\Omega$$



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

(not necessarily a good assumption!)

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

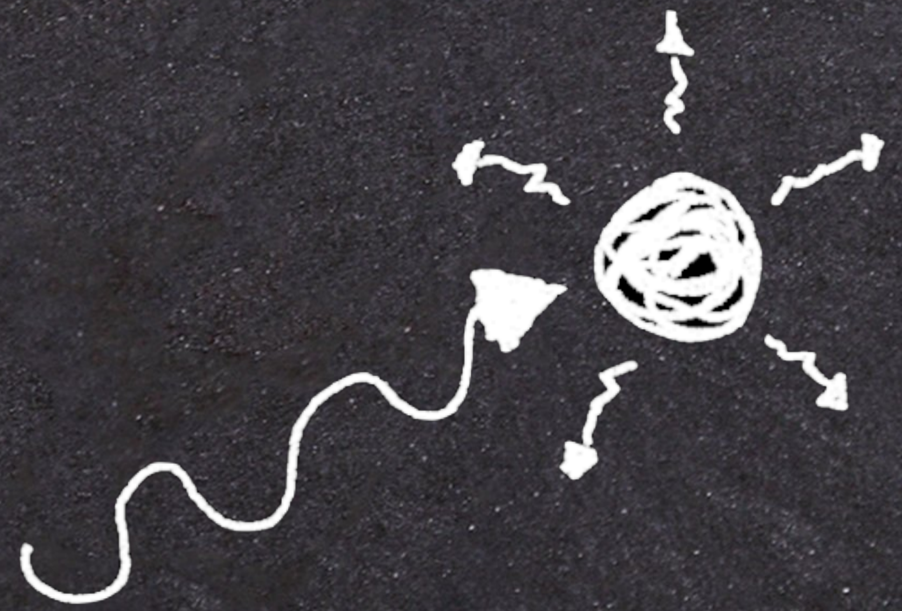
$\mathbf{n} \cdot \nabla I = 0$ In the absence of extinction, emission, scattering.

Spatial derivative along the ray

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

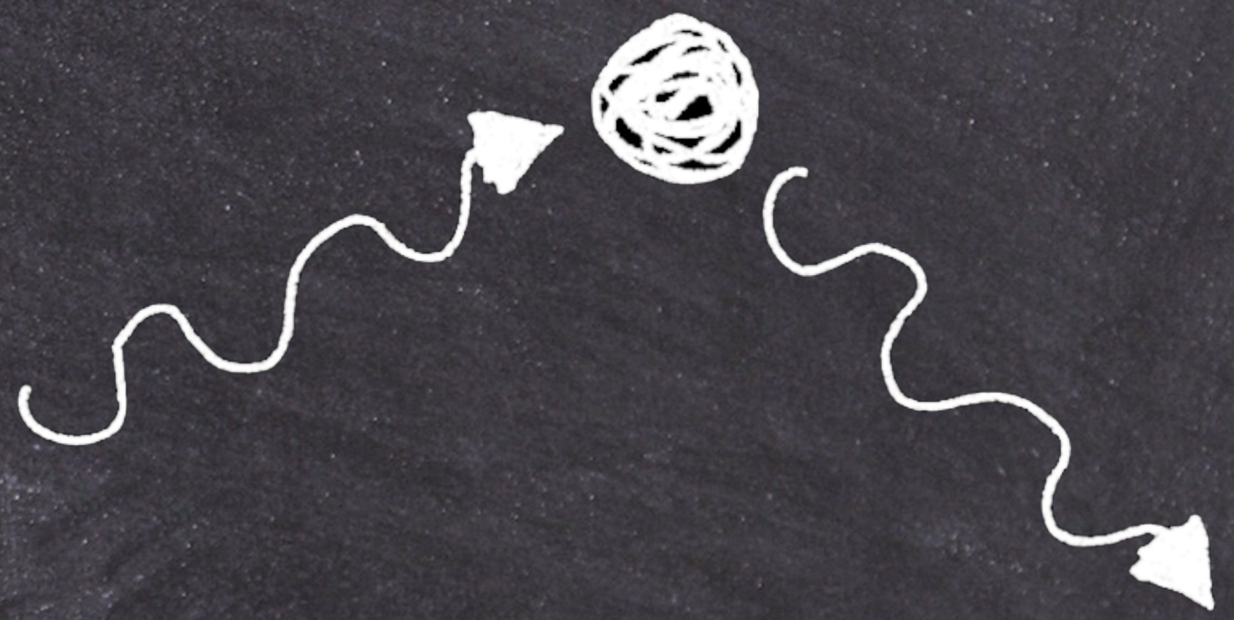
, where α_{tot} is the extinction coefficient.

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

$\mathbf{n} \cdot \nabla I = -\alpha_{\text{tot}} I + \boxed{j}$, where j is the emissivity.

Relation between emissivity and blackbody emission (Planck function):

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

Blackbody temperature

Planck function

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

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

This is Kirchhoff's law.

Radiative transfer equation: adding scattering

$$\mathbf{n} \cdot \nabla\, I = -\,\alpha_{\mathrm{tot}} I + j + \boxed{\alpha_{\mathrm{scat}} \oint I(\mathbf{n}') p(\mathbf{n}, \mathbf{n}') d\Omega'}$$

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 $p = 1/(4\pi)$: $\mathbf{n} \cdot \nabla\, I = -\,\alpha_{\mathrm{tot}} I + j + \alpha_{\mathrm{scat}} J$,

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

We have dropped a couple of implicit dependencies before:

Frequency

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

Location

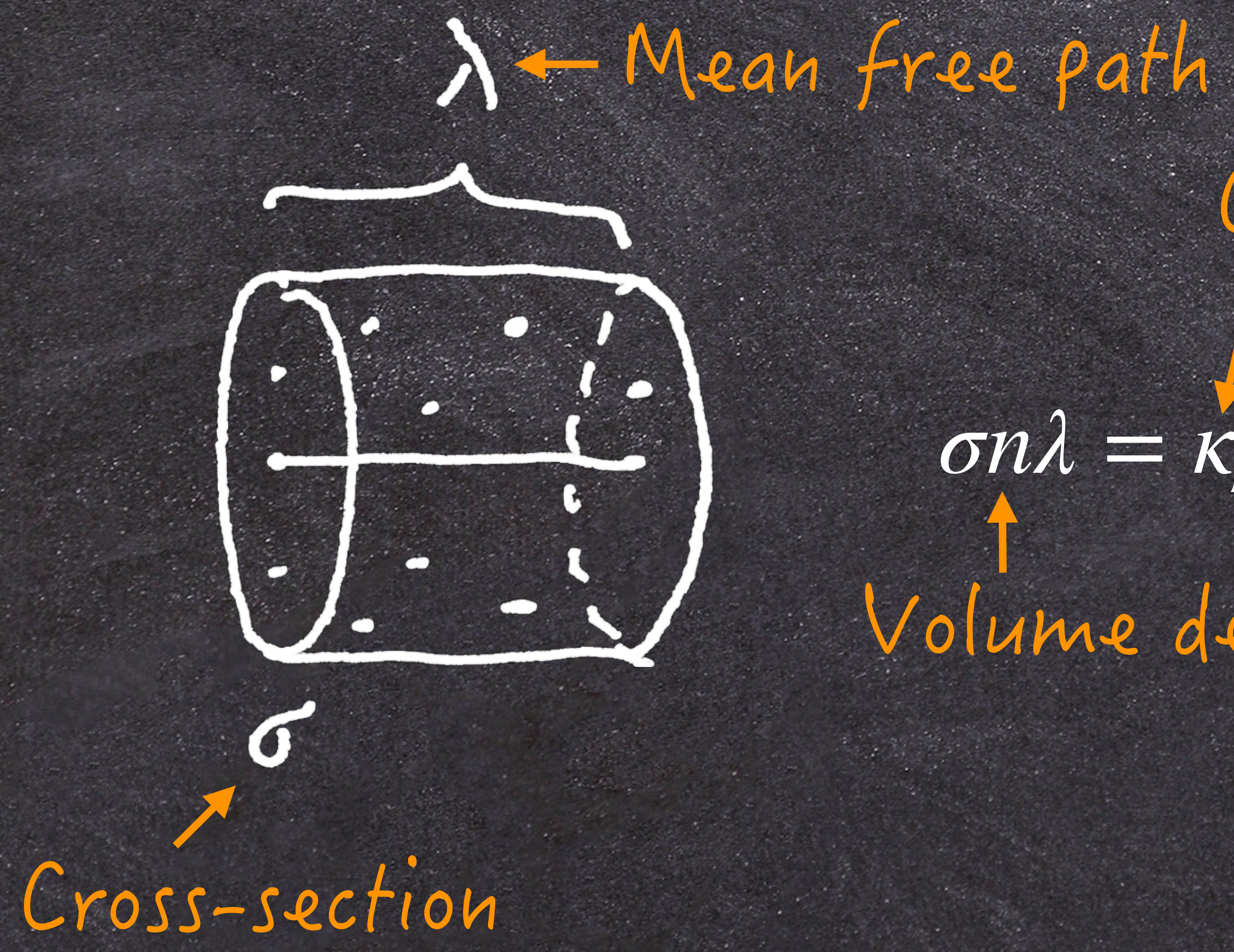
To make things more digestible we drop them again (only in notation).
Also we now move to a coordinate system parallel to the ray we investigate.

$$\frac{dI}{ds} = -\,\alpha_{\text{tot}} I + j + \alpha_{\text{scat}} \oint I(\mathbf{n}') p(\mathbf{n}, \mathbf{n}') d\Omega'$$

Distance in ray direction

Radiative transfer equation: optical depth

The extinction coefficient α_{tot} is the inverse mean free path of a photon



Cross section per unit mass ("opacity")

Mass density

$$\sigma n \lambda = \kappa \rho \lambda = 1$$

Volume density

Therefore: $\alpha_{\text{tot}} = \lambda^{-1} = \kappa\rho$

The optical depth τ is distance in units of mean free paths:

$$d\tau = \alpha_{\text{tot}} ds$$

Radiative transfer equation: source function

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

Now we define the source function S: $$S = \frac{j}{\alpha_{\text{tot}}} + \frac{\alpha_{\text{scat}}}{\alpha_{\text{tot}}} \oint I(\mathbf{n}')p(\mathbf{n},\mathbf{n}')d\Omega'$$

Then: $$\boxed{\frac{dI}{d\tau} = -I + S}$$

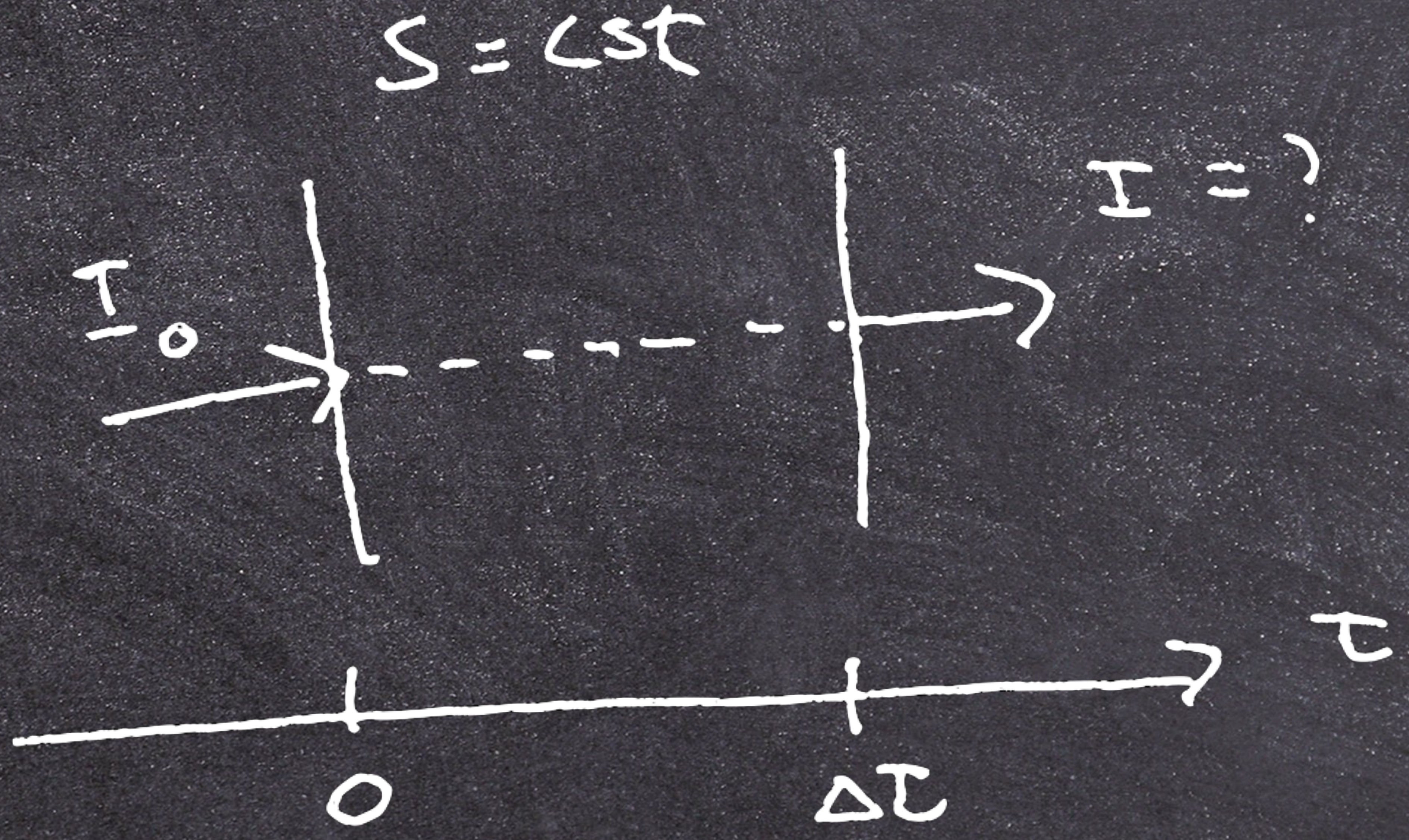
In LTE and for isotropic scattering it holds that

$\boxed{S = \epsilon B + \omega J,}$ with the photon destruction probability: $\epsilon = \alpha_{\text{abs}}/\alpha_{\text{tot}}$

and single-scattering albedo: $\omega = \alpha_{\text{scat}}/\alpha_{\text{tot}} = 1 - \epsilon$

Radiative transfer equation: solution for constant S

Exercise :)



Derive that for a constant source function S it holds that: $I(\Delta\tau) = I_0 e^{-\Delta\tau} + S(1 - e^{-\Delta\tau})$

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

In LTE all intensities of rays passing through an optically thick, non-scattering medium with temperature T will have $I = B(T)$.

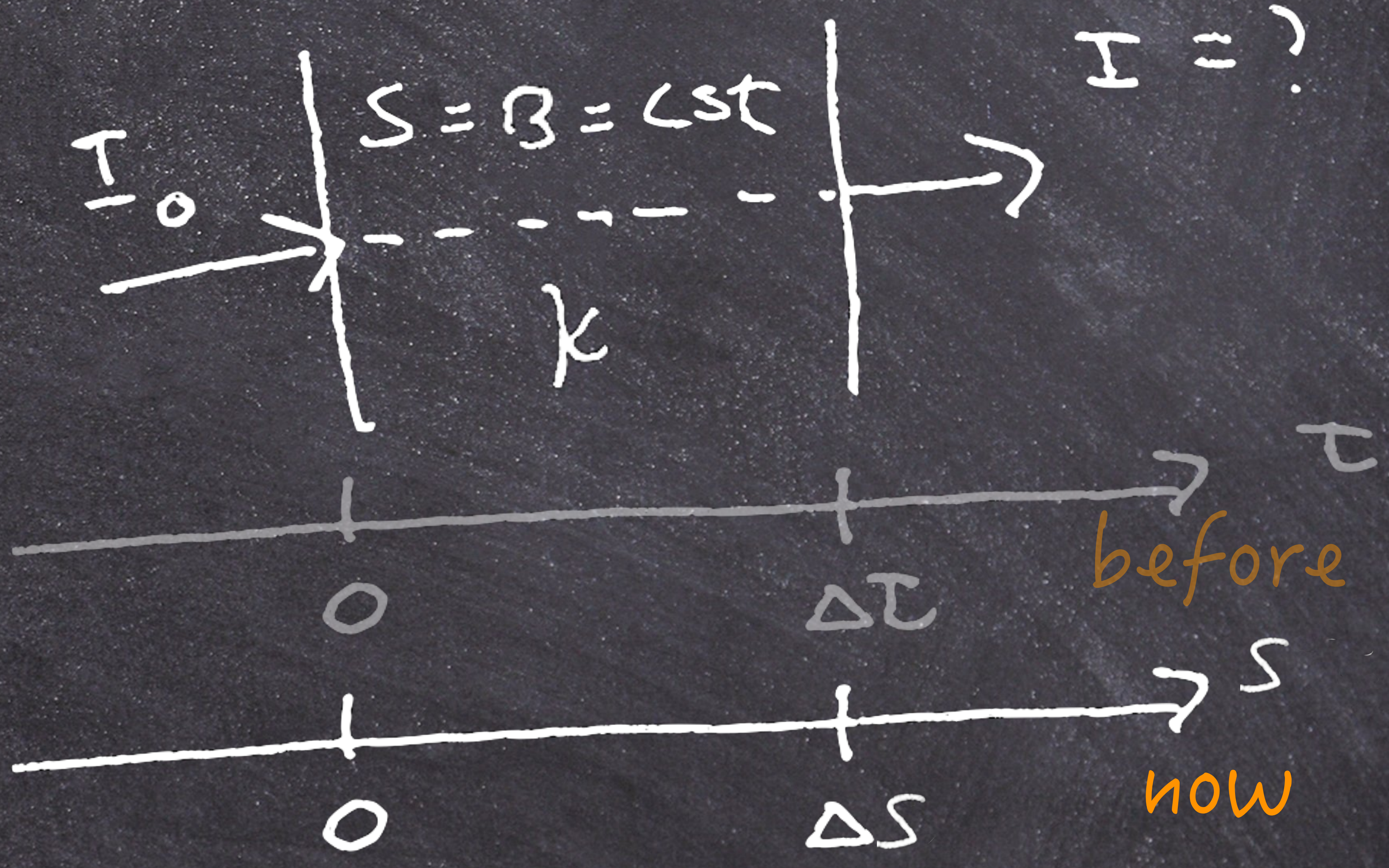
Large Δτ

Line formation 1

Imagine you have a line-shaped opacity κ:

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

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



So $\Delta\tau = \Delta\tau(s, \nu)$, and we can use

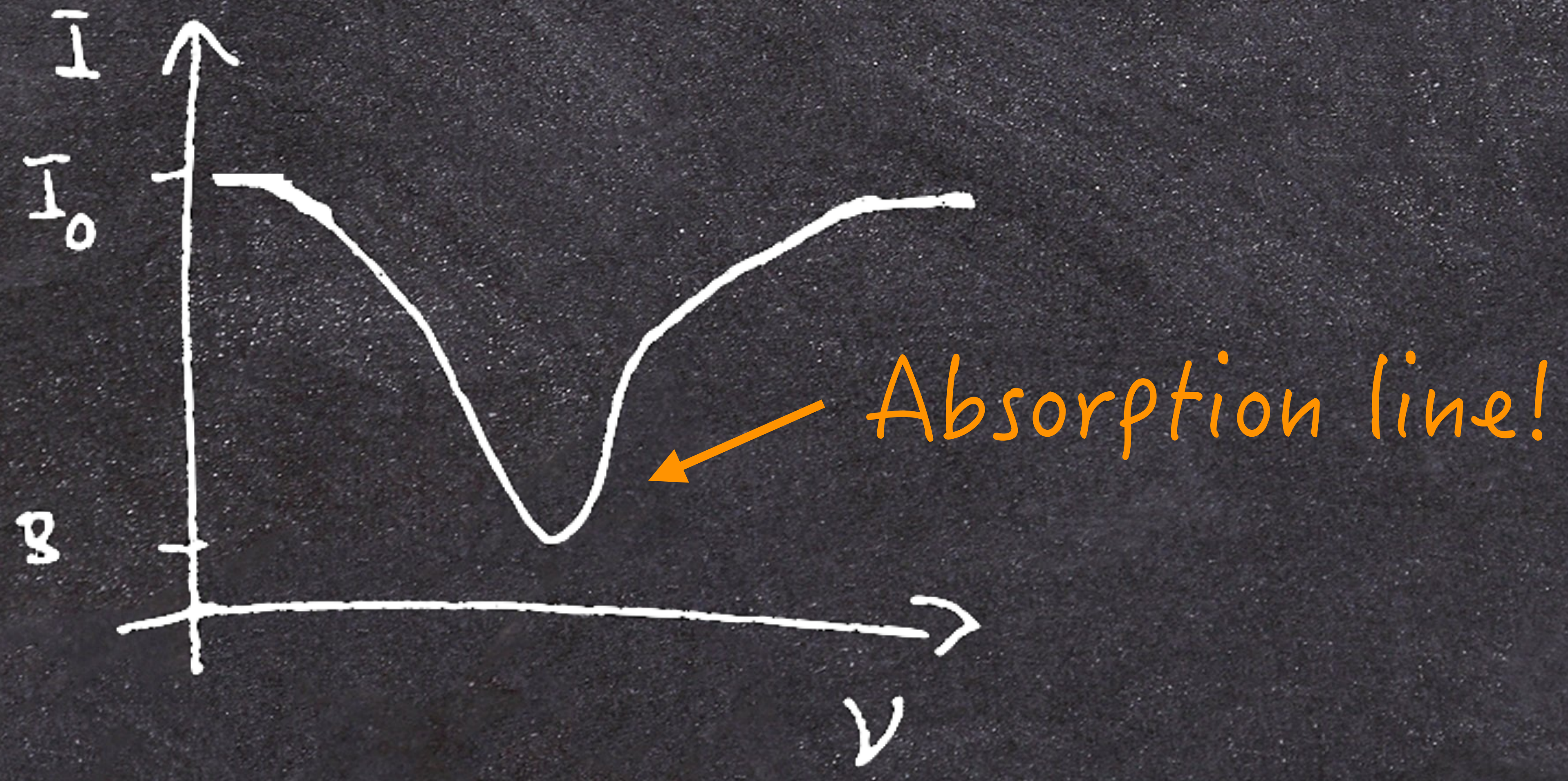
$$I(\Delta s, \nu) = I[\Delta\tau(\Delta s, \nu)] = I_0 e^{-\Delta\tau(\Delta s,\nu)} + B(1 - e^{-\Delta\tau(\Delta s,\nu)})$$

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

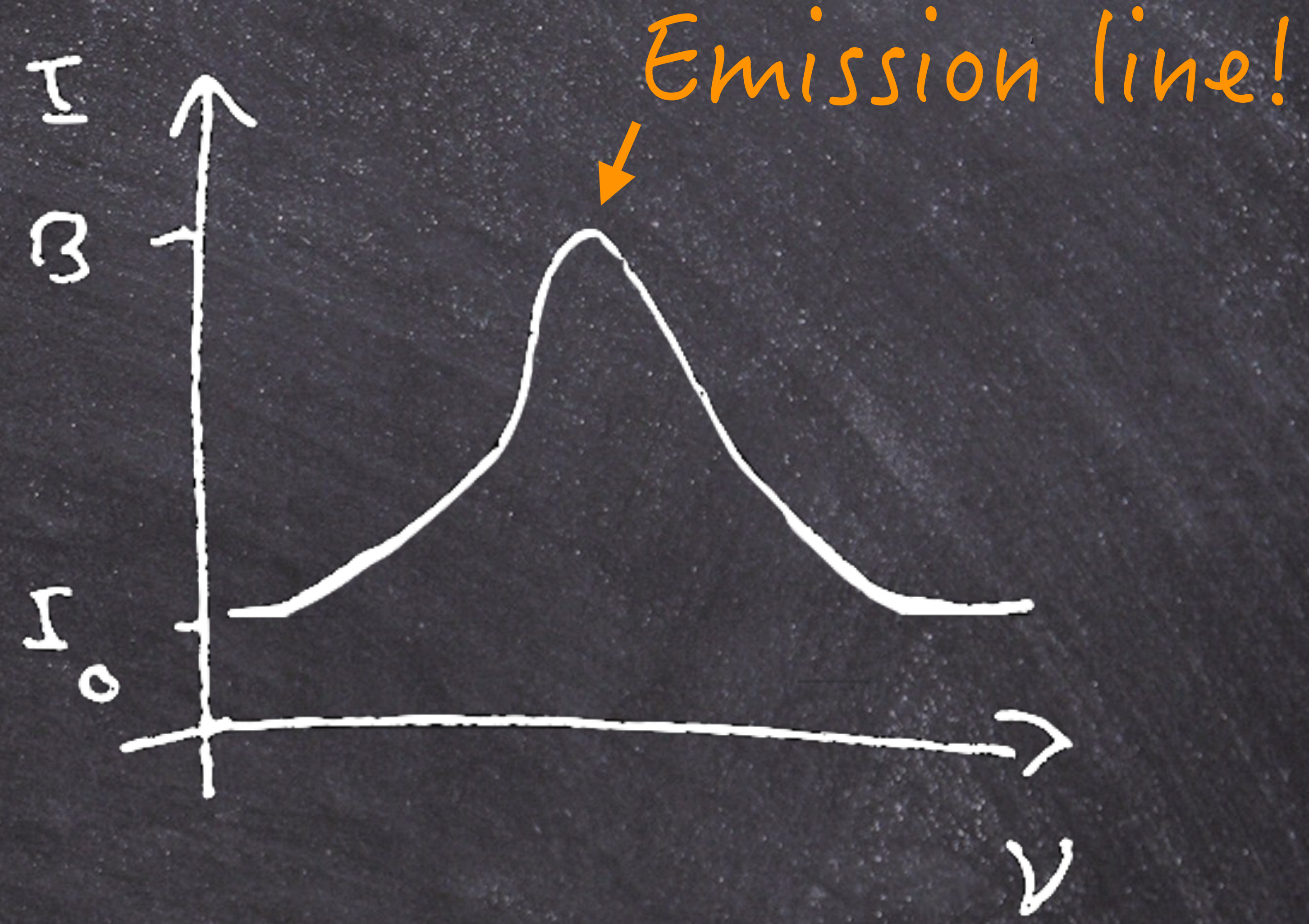
Case 1: $B < I_0$



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

Absorption lines form if $T < T_0$.

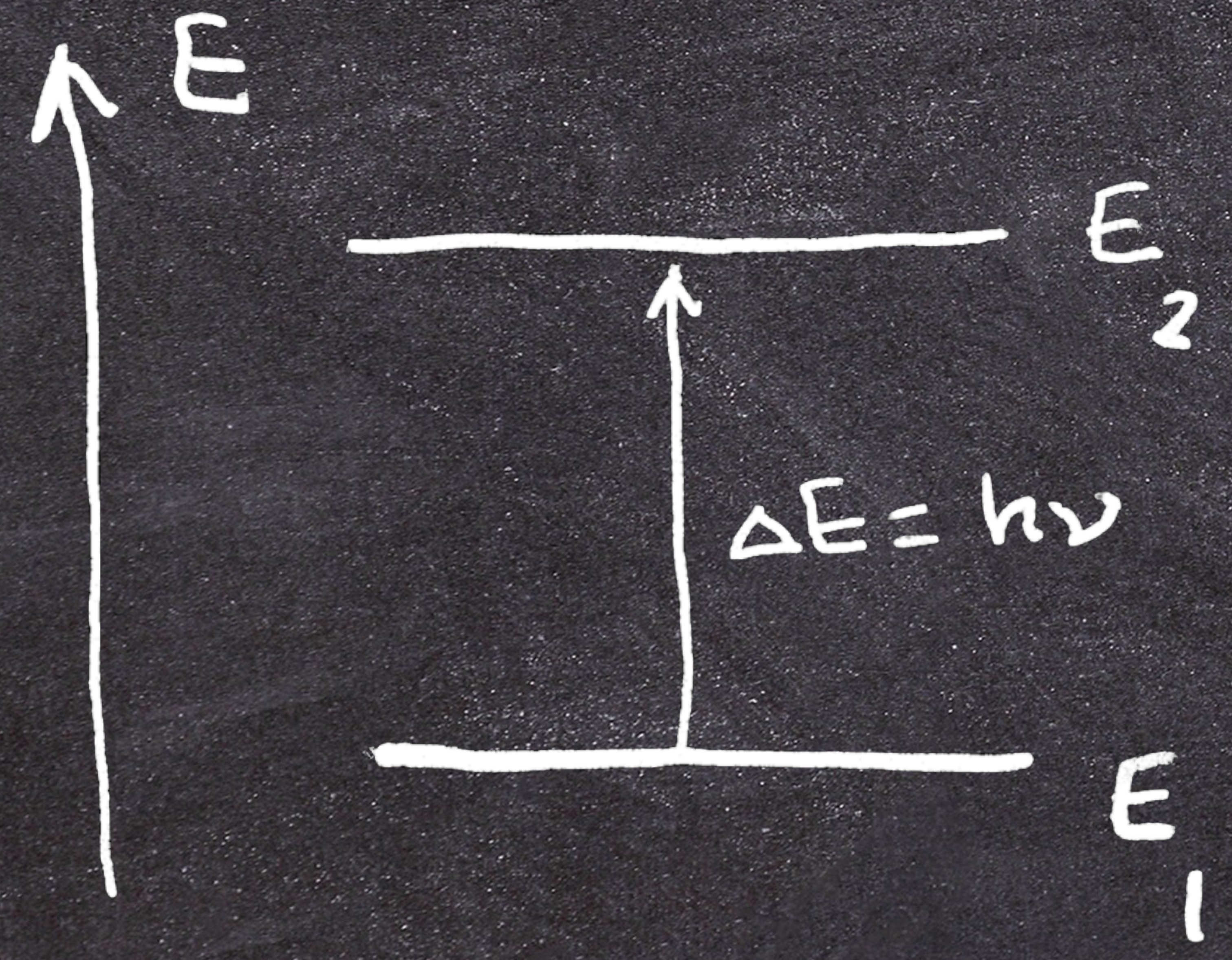
Case 2: $B > I_0$



Emission lines form if $T > T_0$.

The sign of the temperature gradient dT/ds determines whether absorption or emission lines form.

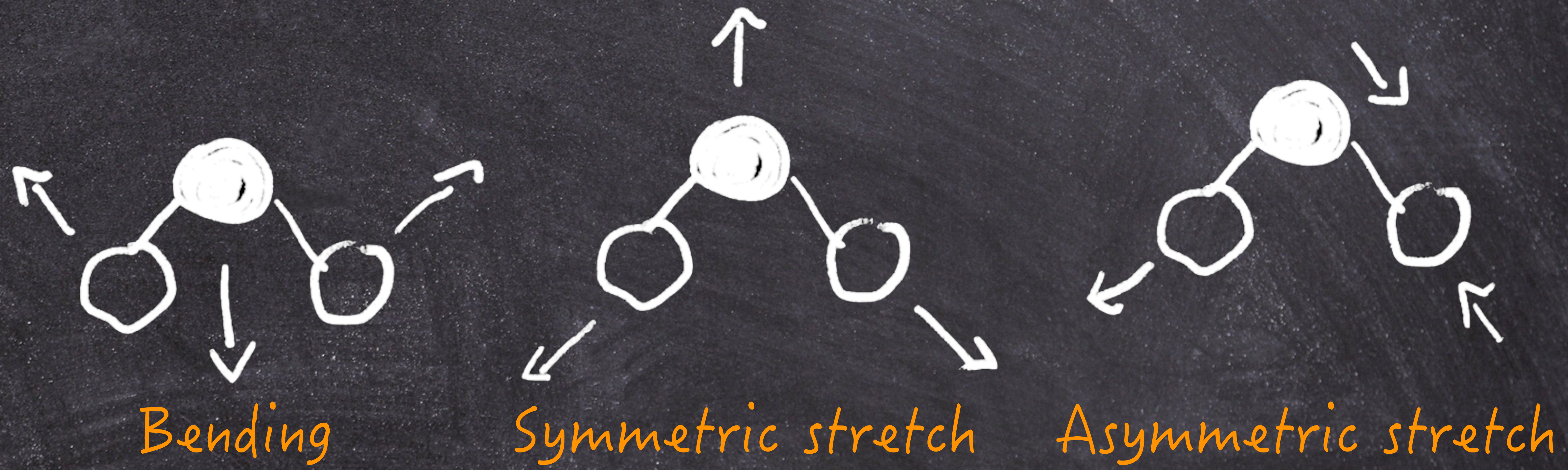
Quantum-mechanical origin of lines



Lines arise from the quantization (discrete value restriction) of energy states in molecules, atoms, and ions.

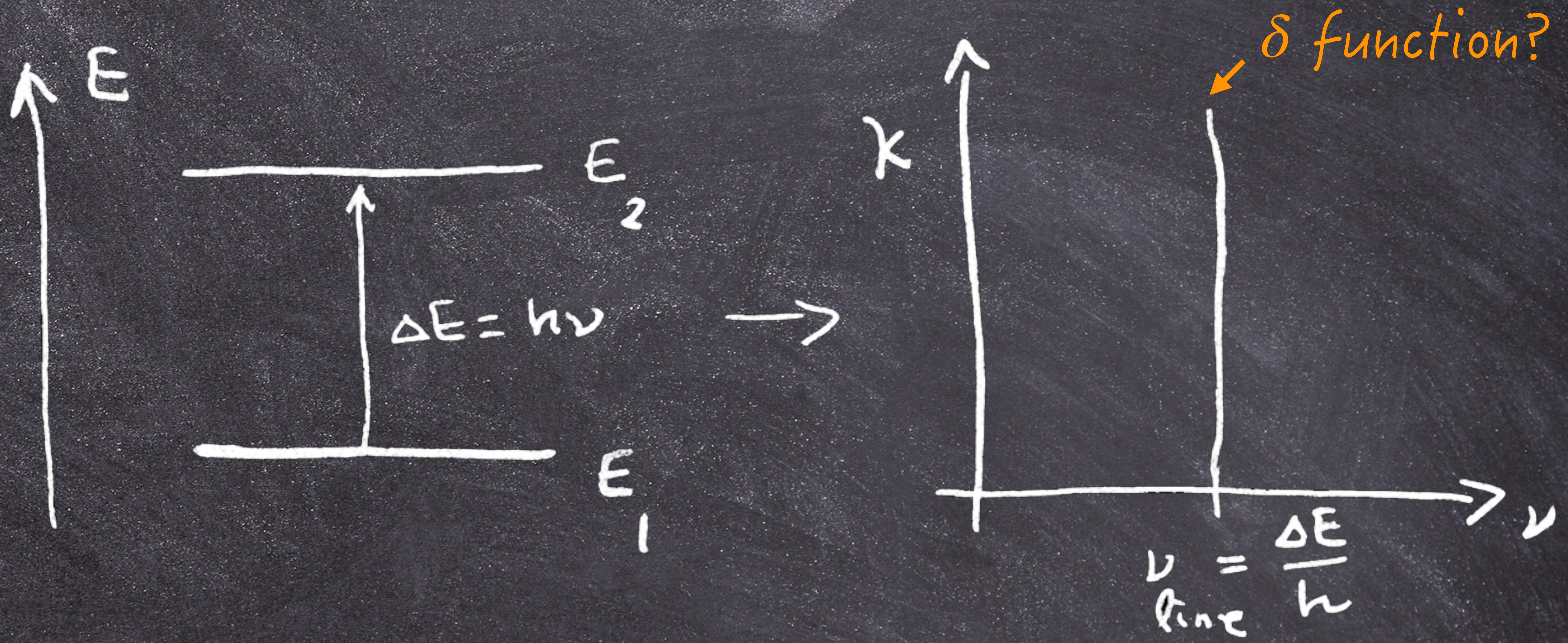
Absorption of light is being used to change the electronic, vibrational or rotational state of the absorber.

Vibrational modes of H_2O:



Absorption strength is calculated using Einstein coefficients (+absorption−stimulated emission).

Line broadening 1



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:
Excited states decay spontaneously. (Vacuum fluctuations!)

Pressure broadening:
Collisional de-excitation, broadening $\gamma \propto P T^{-1/2}$.

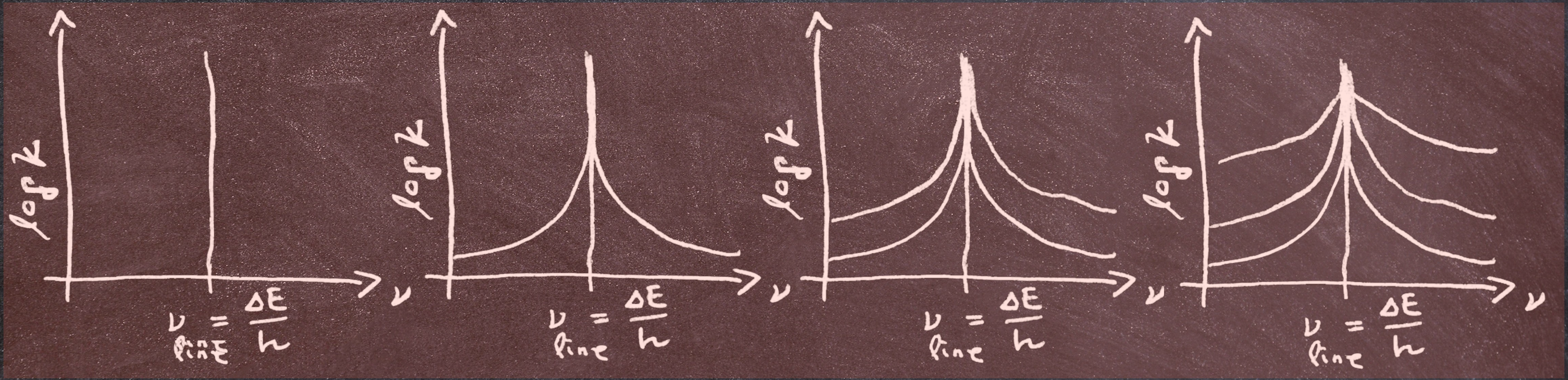
2. Doppler broadening

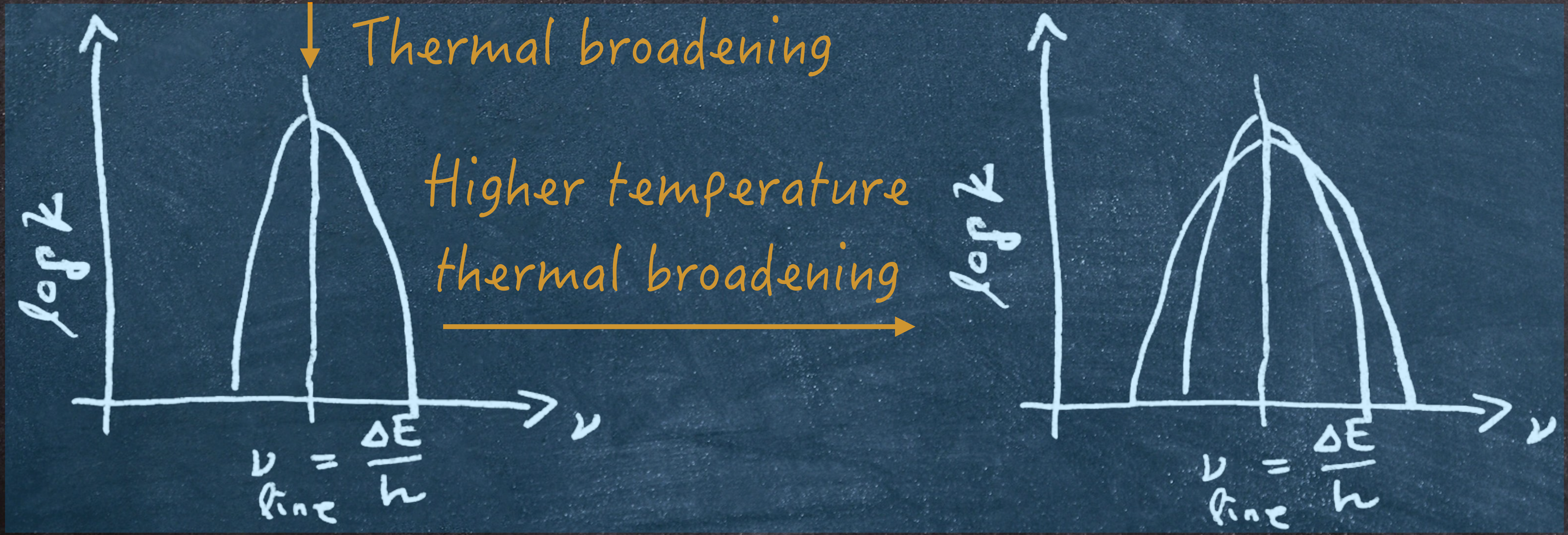
Due to velocity distribution of absorbers (e.g., Maxwell-Boltzmann in LTE)

Broadening $\gamma \propto \sqrt{T/m}$. (Absorber mass)

Line broadening 2

No broadening → Natural broadening → Pressure broadening → Higher pressure broadening





Line shapes:

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

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

(for Maxwell-Boltzmann)

Line broadening 3

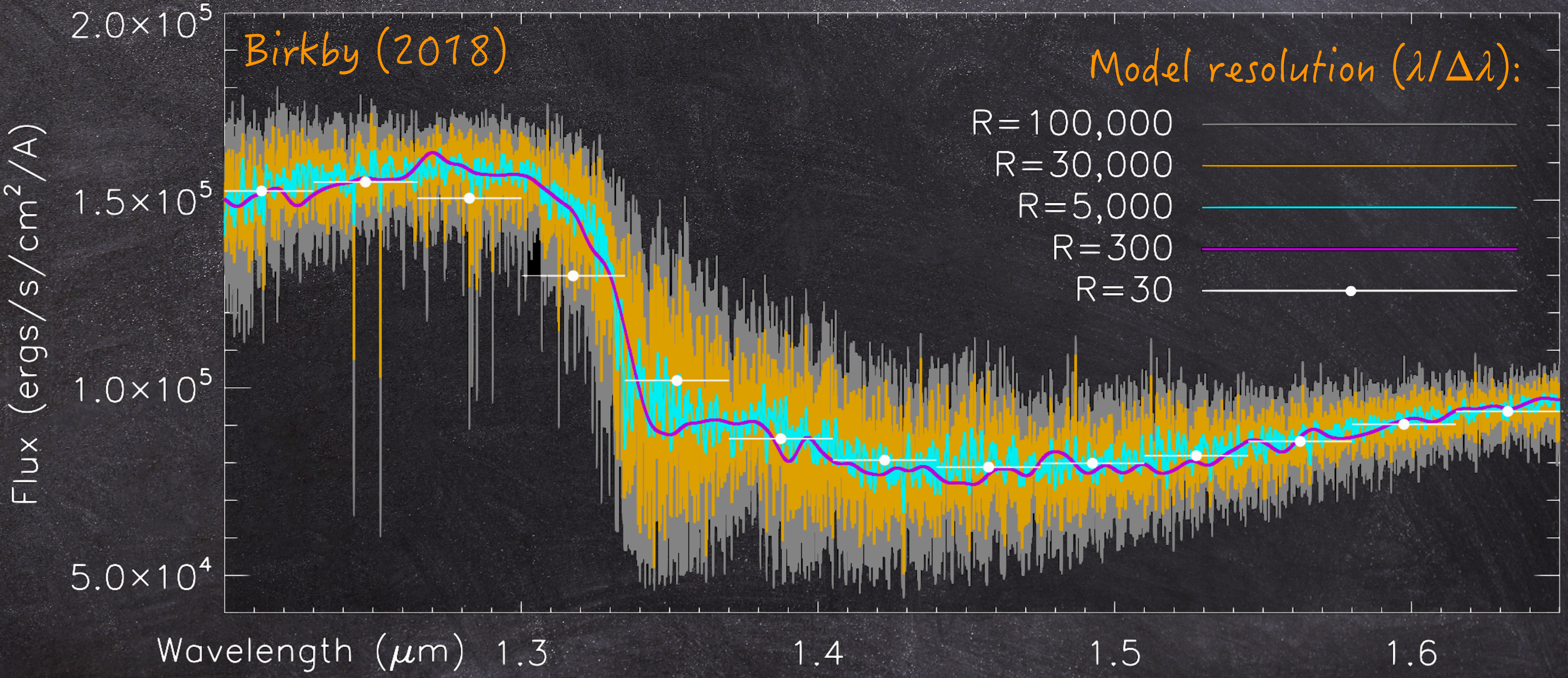
Pressure broadening and Doppler broadening are usually active at the same time.

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.



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:

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

- 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!

Radial coordinate of atmosphere

- 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.