

Radiative Transfer

Lecture 04

The Physics of Star Formation

Les Houches School of Physics February 23, 2024

Lecturer: Dr. Stefan Reissl



Zentrum für Astronomie
der Universität Heidelberg

Line Radiative Transfer

Line RT equation

In contrast to dust, the opacities of gas are related to line transitions ruled by quantum mechanics.

⇒ Atoms or molecules have discrete energy states (level) to vibrate, rotate, and to occupy their electron shells.

1D RT equation without polarization:

$$\frac{I_{ij}}{dr} = J_{ij} - \alpha_{ij}I_{ij}$$

i = upper level
j = lower level

where each transition is related to a distinct frequency ν_{ij}

Line absorption and emission

For line transitions, the emissivity

$$j_{ij}(\Omega, \nu) = \frac{h\nu}{4\pi} N n_i A_{ij} \varphi_{ij}(\omega, \nu)$$

and absorption

$$\alpha_{ij}(\omega, \nu) = \frac{h\nu}{4\pi} N (n_j B_{ji} - n_i B_{ij}) \varphi_{ij}(\omega, \nu)$$

are linked to the type of atom/molecular via the Einstein coefficients for spontaneous emission A_{ij} , absorption B_{ji} , and stimulated emission B_{ij} .

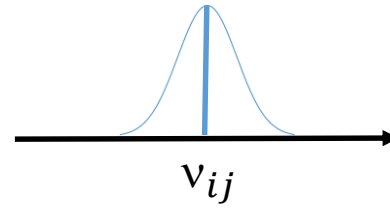
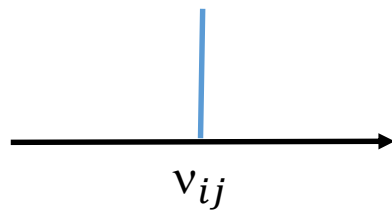
Note, these coefficients are not independent but obey

$$A_{ij} = \frac{2h\nu_{ij}^3}{c^2} B_{ij} \quad \text{and} \quad B_{ji} g_j = B_{ij} g_i \quad \text{where } g_i \text{ and } g_j$$

are statistical weights.

Line broadening

Each transition frequency ν_{ij} is exactly one sharp peak but the emission and absorption profile may become broadened by various effect.



Gaussian broadening profile:

$$\phi(\nu) = \frac{c}{\sqrt{\pi} a_D \nu_{ij}} \exp\left(-\frac{c^2(\nu - \nu_{ij})^2}{a_D^2 \nu_{ij}^2}\right)$$

Line width: $a_D = \sqrt{a_{th}^2 + a_{turb}^2} = \sqrt{\frac{2k_B T_g}{m_g} + a_{turb}^2}$
(thermal + microturbulence)

Lorentz profile (Cauchy profile, Breit-Wigner profile):

$$\phi(\nu) = \frac{1}{\pi} \frac{\gamma}{(\nu - \nu_{ij})^2 + \gamma^2}$$

Line width:

$$\gamma = \gamma_{nat} + \gamma_{coll}$$

(natural + collisional)

The total broadening profile

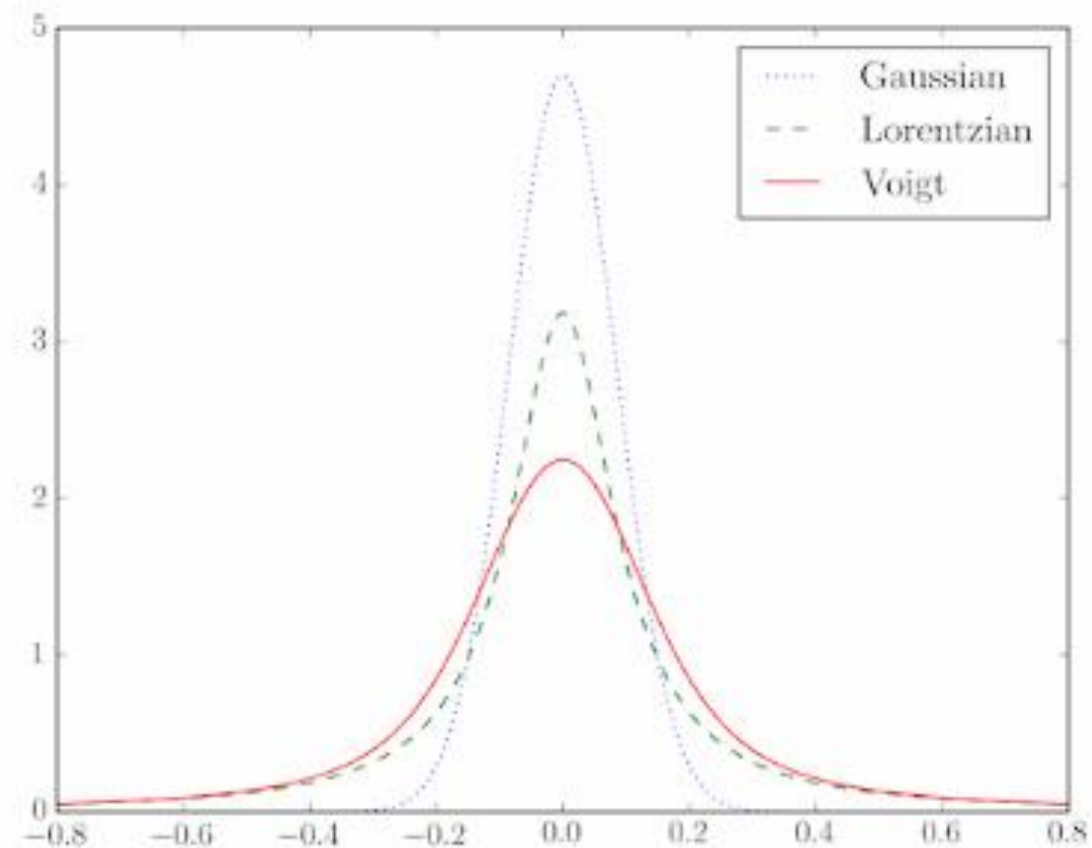
Combining all four effects of broadening (thermal, micro turbulent, natural, collisional) requires the convolution of the profiles:

$$F(\nu', a') = \int_0^\infty \phi(x) \phi(\nu_{ij} + \nu - x) dx$$

This defines the Voigt profile defined by the

$$\text{Parameters } \nu' = \frac{\nu - \nu_{ij}}{a_D} \text{ and } a' = \frac{\gamma}{a_D}$$

Note: For the 1D line RT problem, the Gaussian profile is a valid approximation; for line RT with the Zeeman effect, the side lobes of the profiles need to be exact.



Level population

- In local thermodynamic equilibrium (LTE), assume that the level population and gas are in equilibrium

$$\frac{n_j}{n_i} = \frac{g_j}{g_i} \exp\left(-\frac{E_j - E_i}{k_B T_g}\right)$$

- Non-LTE e.g. Large Velocity Gradient (LVG) method:

Statistical equilibrium equation including collisions

$$\sum_{j>i} \left[n_j A_{ji} + (n_j B_{ji} - n_i B_{ij}) J_{ji} \right] - \sum_{j<i} \left[n_i A_{ij} + (n_i B_{ij} - n_j B_{ji}) J_{ij} \right] + \sum_{j \neq i} [n_j C_{ji} - n_i C_{ij}] = 0$$

with probability to escape without further absorption

$$\beta_{ij} = \frac{1 - \exp(-\tau_{ij})}{\tau_{ij}} \quad \text{with optical depth} \quad \tau_{ij}^{\text{LVG}} = \frac{c^3}{8\pi\nu_{ij}^3} \frac{A_{ij} N_{\text{molec}}}{1.064 |\nabla \vec{v}|} \left[\frac{g_i}{g_j} n_j - n_i \right]$$

and radiation field

$$J_{ij} = (1 - \beta_{ij}) S_{ij} + \beta_{ij} J_{ij}^{\text{bg}}$$

Atomic and molecular data

LAMDA

Leiden Atomic and Molecular Database

[Data format](#) | [RADEX](#)

Atoms and ions		
C	O*	Si
Diatomic molecules		
AH*	CF*	CH
CH*	CN	CO
CS	HCl	HD
HF	NH	NO
NO*	NS*	OH
OH*	O ₂	PN
PO	SiO	Sis
SO		
Triatomic molecules		
C ₂ H	CH ₂	D ₂ H*
HCN	HCO*	HCS*
HDO	H ₂ O*	H ₂ O
H ₂ S	HNC	N ₂ H*
OCS	SiC ₂	SO ₂
Larger molecules		
CH ₃ OCHO	CH ₃ OH	CH ₃ CN
C ₂ H ₂	C ₂ H*	HC ₃ N
H ₂ CO	H ₂ CS	H ₂ O*

The aim of this project is to provide users of radiative transfer codes with the basic atomic and molecular data needed for the excitation calculation. Line data of a number of astrophysically interesting species are summarized, including energy levels, statistical weights, Einstein A-coefficients and collisional rate coefficients. Available collisional data from quantum chemical calculations and experiments are in some cases extrapolated to higher energies.

Currently the database contains data for 7 atomic / ionic and 49 molecular species. In addition, several isotopomers and deuterated versions are available, usually via the page for the main species. Work is permanently underway to add more datafiles. We encourage comments from the users in order to improve and extend the database.

This database should form an important tool in analyzing observations from current and future infrared and (sub)millimetre telescopes. Databases such as these rely heavily on the efforts by the chemical physics community to provide the relevant atomic and molecular data. We strongly encourage further efforts in this direction, so that data for more species become available and the current extrapolations of collisional rate coefficients can be replaced by actual calculations in future releases.

RADEX, a computer program for performing statistical equilibrium calculations is made publically available as part of the data base. The program comes in 2 versions: an on-line calculator for quick checks, and a stand-alone version for extensive calculations. **For publication-quality results, always use the stand-alone version.**

For new or changed datafiles, see the [update history](#) or follow us on [Twitter](#).

If you use the data files in your work please refer to the [publication](#) by [Schöier, F.L., van der Tak, F.F.S., van Dishoeck E.F., Black, J.H. 2005, A&A 432, 369-379](#) introducing this data base. Please mention the date when you accessed the database, in case questions arise about different versions of datafiles. When individual molecules are considered, we strongly suggest that you also refer to the original papers providing the spectroscopic and collisional data.

For a 2011 review of radiative transfer and molecular data for astrophysics and astrochemistry, see [this paper](#).

For a 2013 review of how to compute collisional cross-sections and rate coefficients for interstellar molecules, see [here](#).

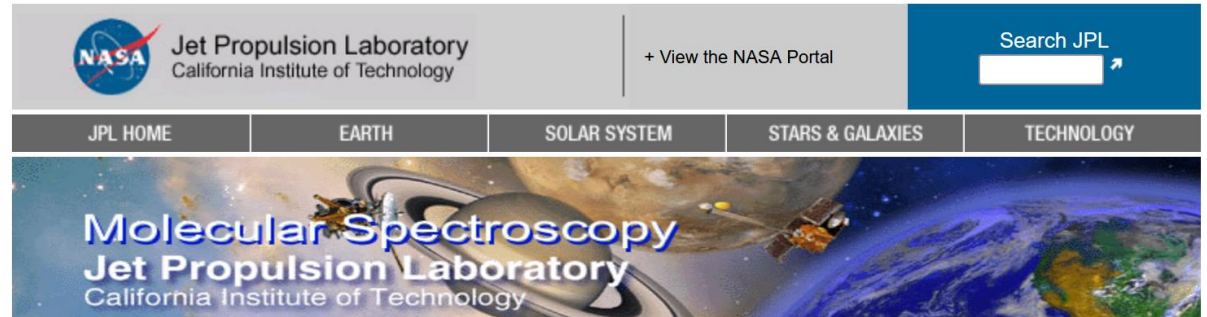
For a [Spring 2020 review of the current status and future plans of LAMDA](#), see [here](#).

This website is dedicated to Fredrik Schöier, who initiated this database. Unfortunately, Fredrik passed away on 14 January 2011, at the age of 41. We remember Fredrik as a dedicated and inspiring scientist. See also [this obituary](#).

Floris van der Tak, Ewine van Dishoeck, John Black

The LAMDA database is supported by the Netherlands Organization for Scientific Research (NWO), the Netherlands Research School for Astronomy (NOVA), and the Swedish Research Council.

<https://home.strw.leidenuniv.nl/~moldata/>



Molecular spectroscopy is the study of absorption of light by molecules. In the gas phase at low pressures, molecules exhibit absorption in narrow lines which are very characteristic of the molecule as well as the temperature and pressure of its environment. In the microwave and long-wavelength infrared regions of the spectrum, these lines are due to quantized rotational motion of the molecule. At shorter wavelengths similar lines are due to quantized vibration and electronic motion as well as rotational motion. The precise frequencies of these lines can be fit to quantum mechanical models which can be used both to determine the structure of the molecule and to predict the frequencies and intensities of other lines. Because this absorption is so characteristic, it is very valuable for detecting molecules in the Earth's stratosphere, planetary atmospheres, and even the interstellar medium. *This web site contains very specialized technical information. While the general user is welcome to browse its contents, the descriptions assume a knowledge of spectroscopy and quantum mechanics.*

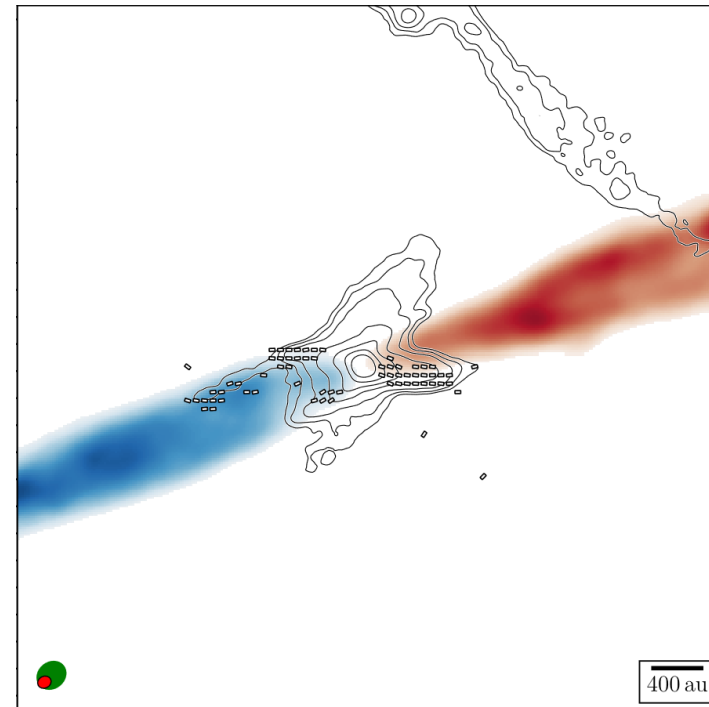
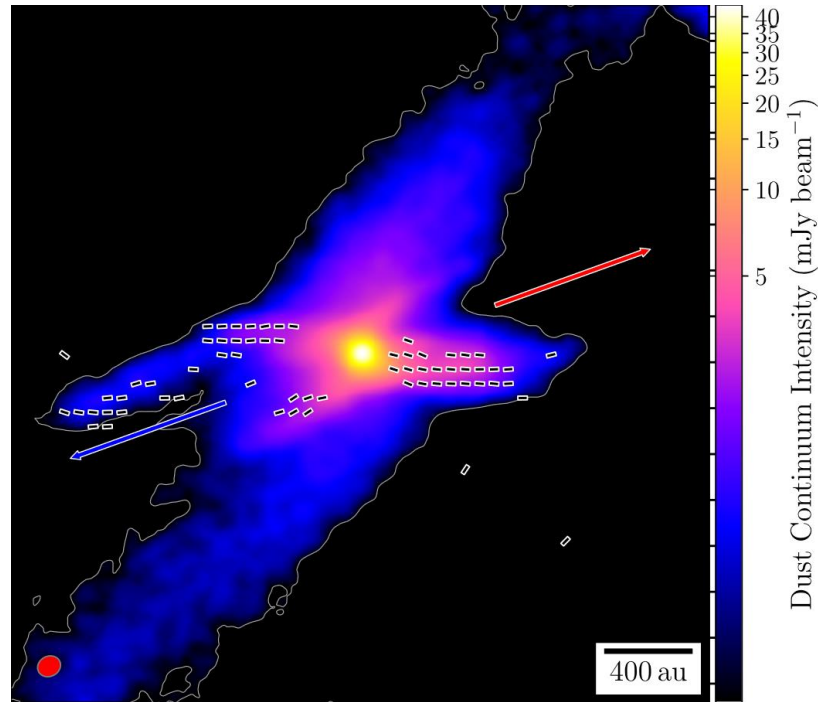
The JPL Molecular Spectroscopy Team supports NASA programs in Astrophysics, Atmospheric Science, and Planetary Science. Its activities include measurement of rotational lines, fitting the lines, and preparing a catalog of line positions and intensities. The members of the team include [Pin Chen](#), [Timothy J. Crawford](#), [Brian J. Drouin](#), [John C. Pearson](#), [Shanshan Yu](#), and [Keeyoon Sung](#), and [Deacon Nemchick](#).

Quick Links

- [Spectroscopy Laboratory](#)
- [Catalog Directory with links](#)
- [Catalog Browser Form](#)
- [New Catalog Additions](#)
- [What's New with Fitting Programs](#)

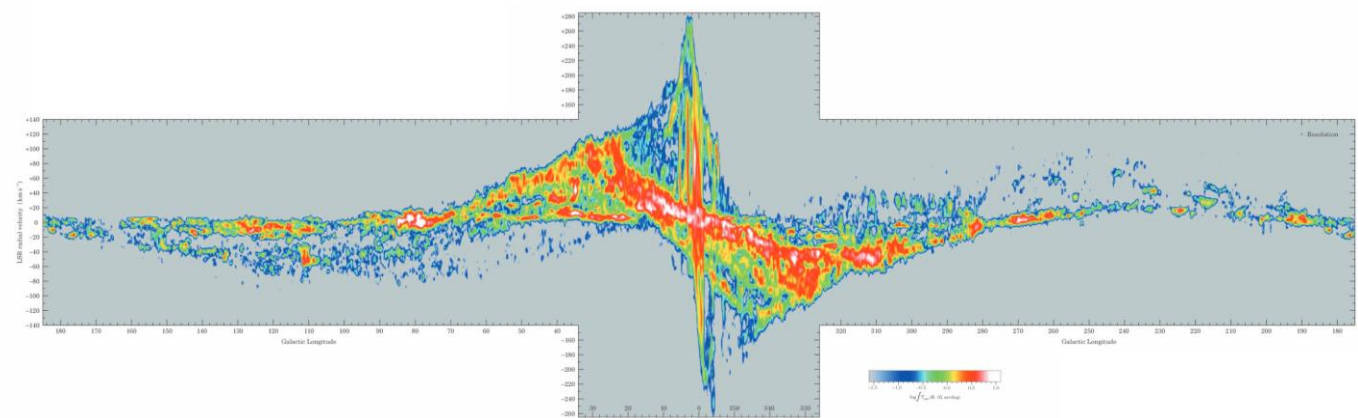
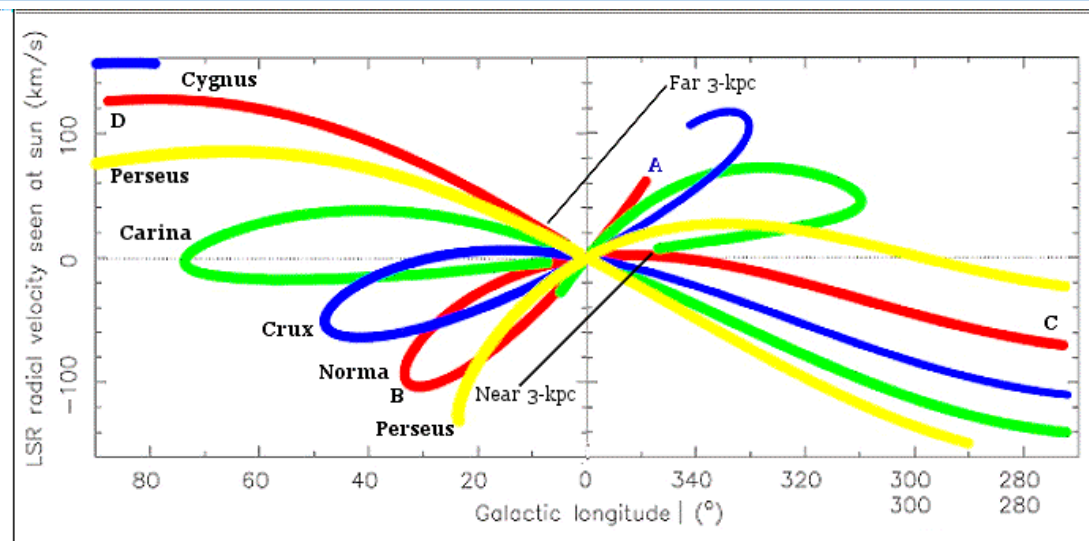
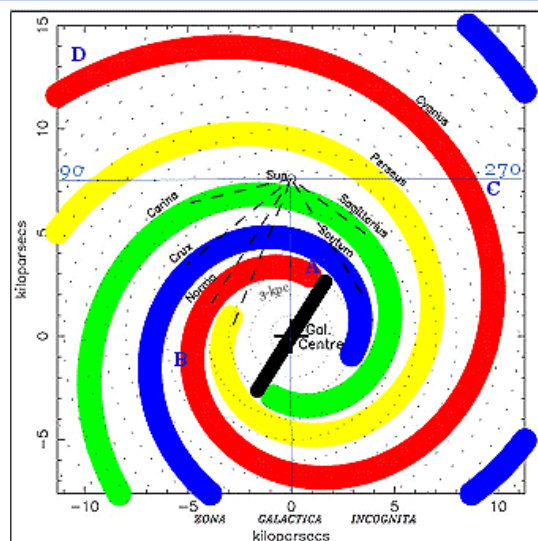
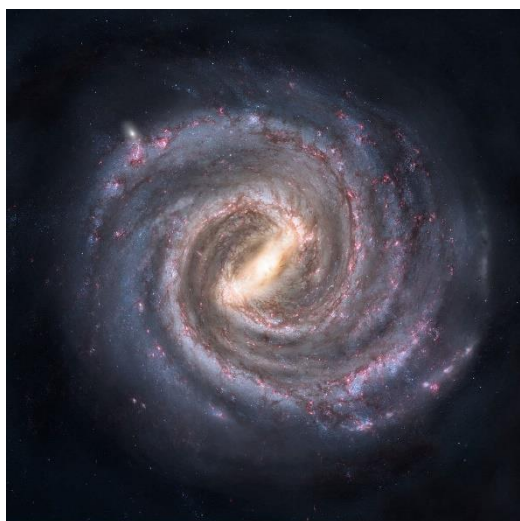
<https://spec.jpl.nasa.gov/>

Outflow observations



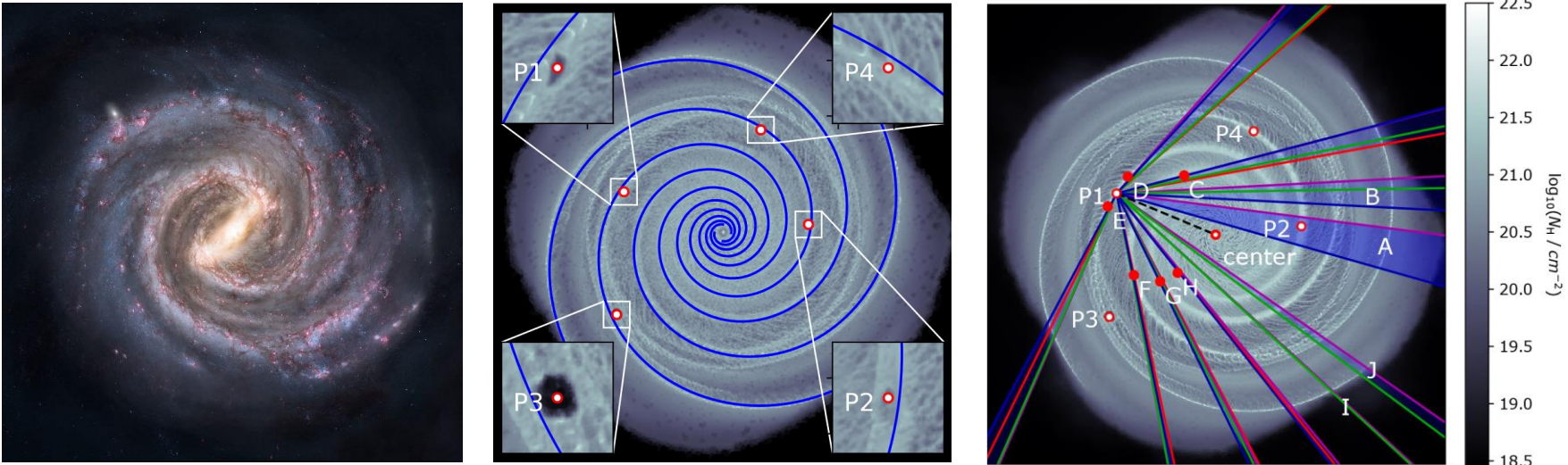
Le Gouellec+ 2019

MW spiral arms

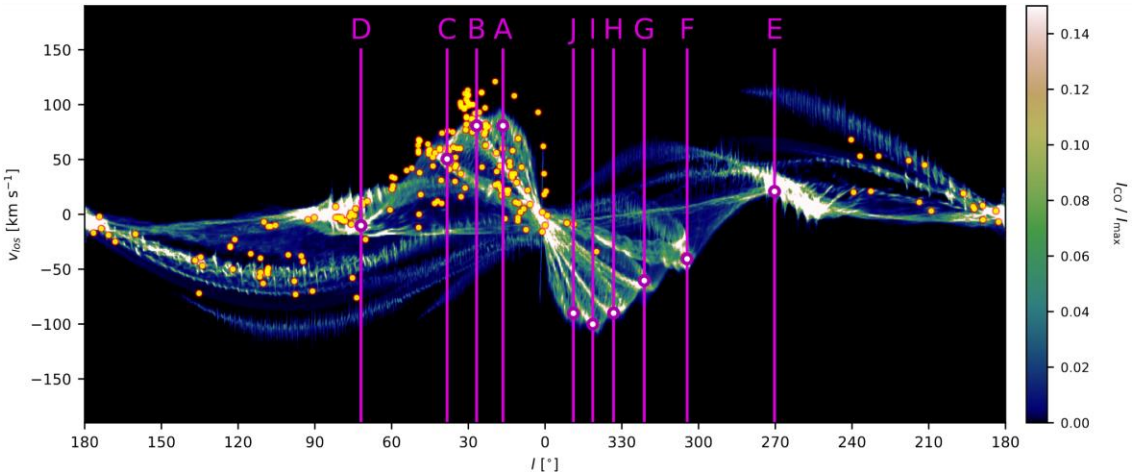


Velocity map of 21 cm neutral hydrogen emission in the Milky Way

Detecting the MW spiral arms

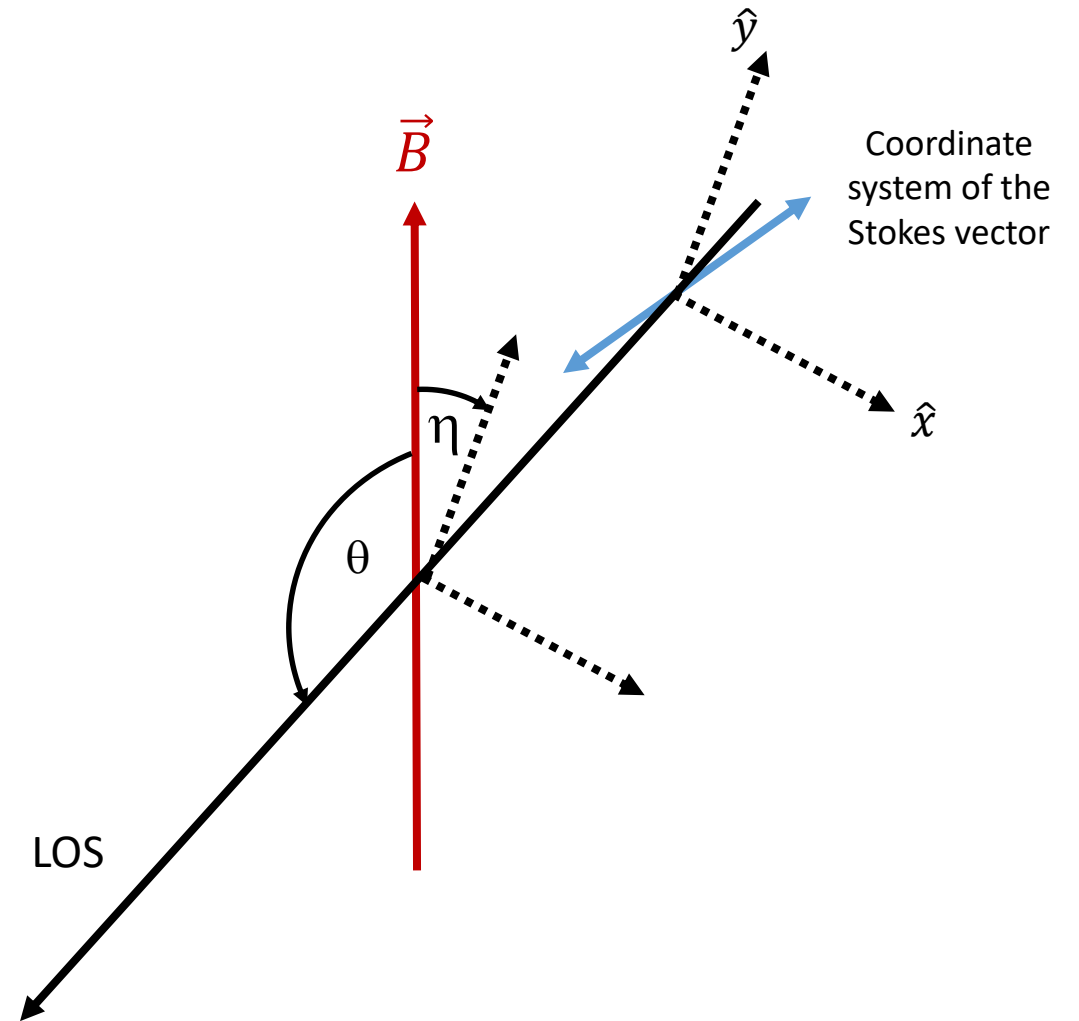
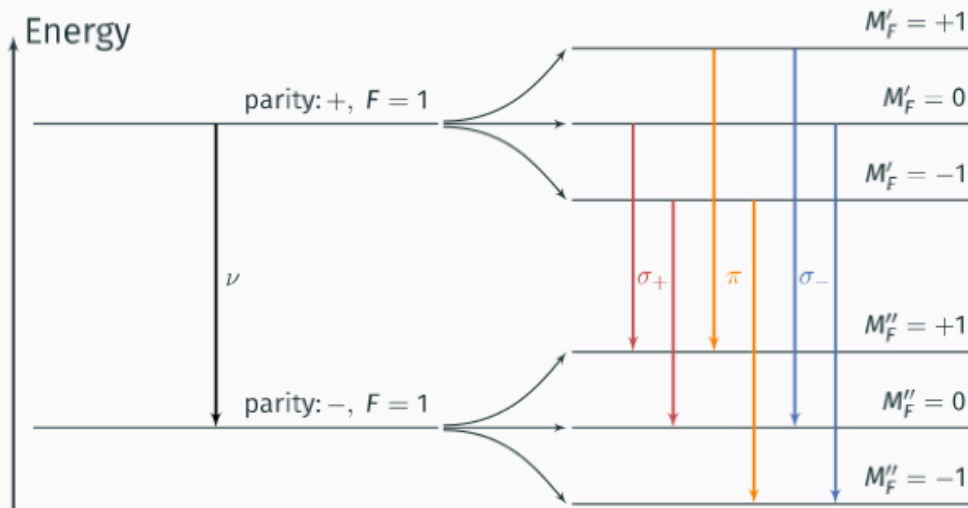
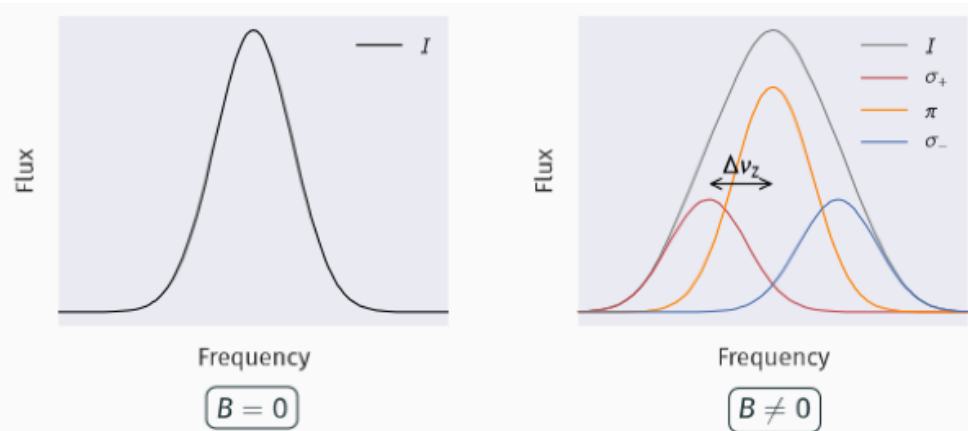


Reissl+ 2020

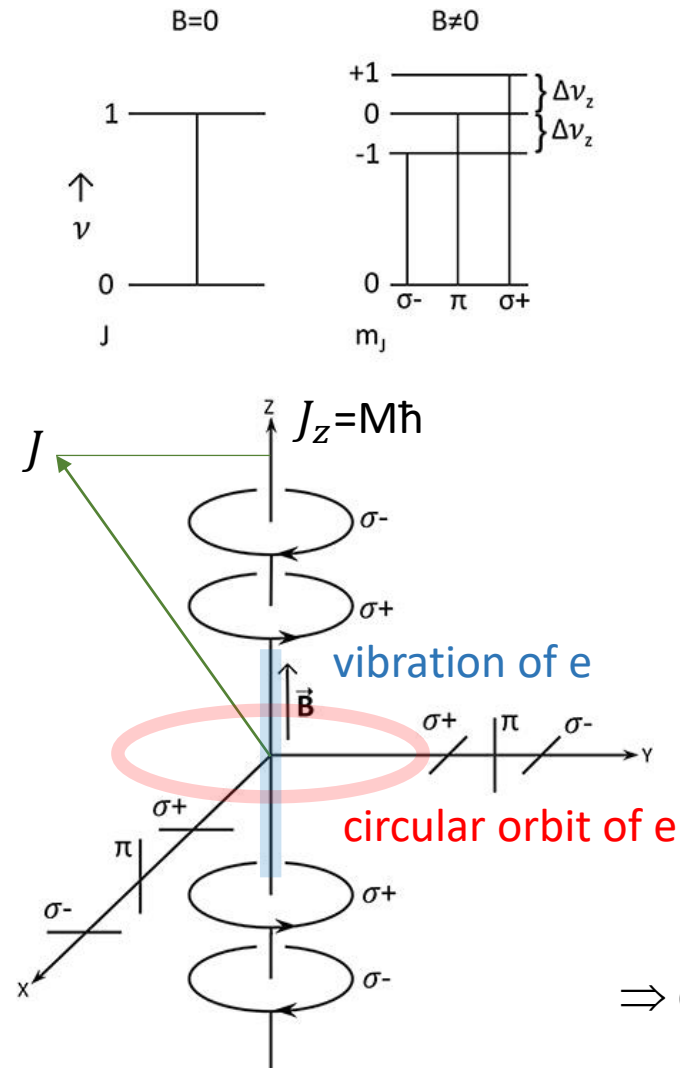


Reid+ 2019, Reissl+ 2020

The Zeeman effect



The Zeeman Effect



The Zeeman RT problem

The line RT equation including polarization:

$$\frac{d\vec{S}_V}{dr} = -\hat{K}\vec{S}_V + \vec{J}_V$$

with the transfer matrix for the Zeeman effect

$$\hat{K} = \frac{N}{2} S_0 \sum_{M', M''} S_{M', M''} F(v', a') \hat{A}_{M', M}$$

Line strength between sub-level:

$$\Delta M_F = 0: \quad S_{M', M''} = \frac{3M_F^2}{F(F+1)(2F+1)}$$

$$\Delta M_F = \pm 1: \quad S_{M', M''} = \frac{3(F \mp M_F)(F+1 \pm M_F)}{4F(F+1)(2F+1)}$$

K: atomic angular momentum

J: orbital angular momentum

F: total angular momentum

Magneto optical matrices:

$$A_{\sigma_{\pm}} = \begin{pmatrix} 1 + \cos^2 \theta & \cos(2\eta) \sin^2 \theta & \sin(2\eta) \sin^2 \theta & \mp 2 \cos \theta \\ \cos(2\eta) \sin^2 \theta & 1 + \cos^2 \theta & 0 & 0 \\ \sin(2\eta) \sin^2 \theta & 0 & 1 + \cos^2 \theta & 0 \\ \mp 2 \cos \theta & 0 & 0 & 1 + \cos^2 \theta \end{pmatrix}$$

$$A_{\pi} = \begin{pmatrix} \sin^2 \theta & -\cos(2\eta) \sin^2 \theta & -\sin(2\eta) \sin^2 \theta & 0 \\ -\cos(2\eta) \sin^2 \theta & \sin^2 \theta & 0 & 0 \\ -\sin(2\eta) \sin^2 \theta & 0 & \sin^2 \theta & 0 \\ 0 & 0 & 0 & \sin^2 \theta \end{pmatrix}$$

Correlation between Stokes I and V

From the RT equation directly follows:

$$I = F(\nu_0 + \Delta\nu_z - \nu, a)(1 + \cos^2 \theta) + 2F(\nu_0 - \nu, a) \sin^2 \theta + F(\nu_0 - \Delta\nu_z - \nu, a)(1 + \cos^2 \theta)$$

$$V = [2F(\nu_0 + \Delta\nu_z - \nu, a) - 2F(\nu_0 - \Delta\nu_z - \nu, a)] \cos \theta$$

It can be shown that Stokes V and I are correlated

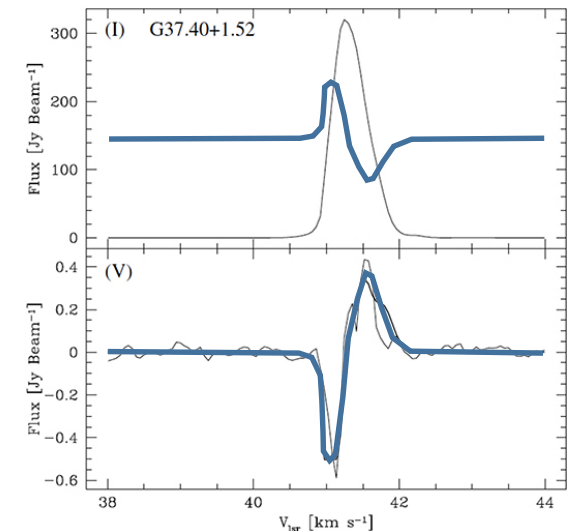
$$V = \left(\frac{dI}{d\nu} \right) \Delta\nu_z \cos \theta$$

Crutcher 1993

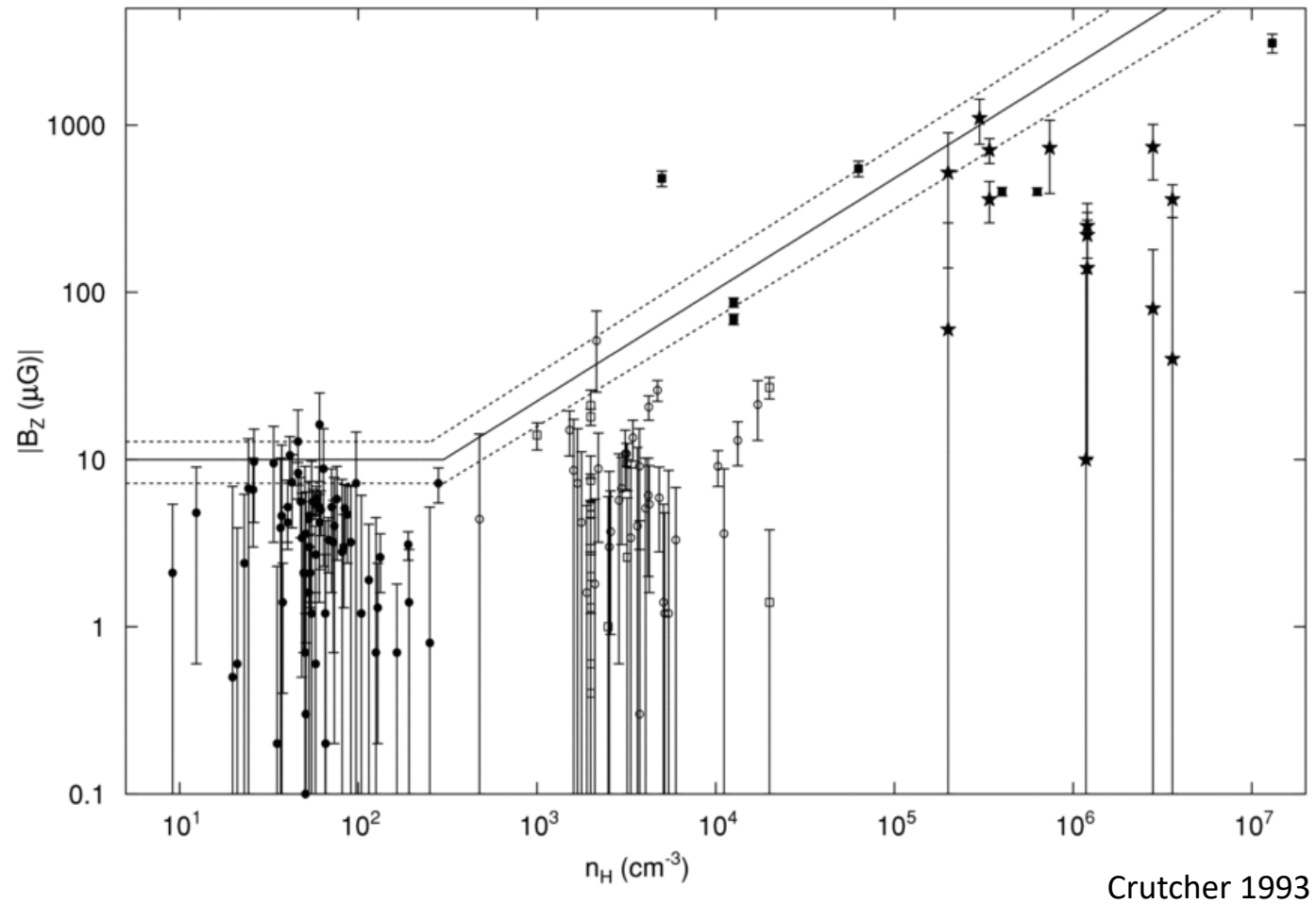
where $\Delta\nu_z$ is the Zeeman shift

$$\Delta\nu_z = \frac{B\mu_b}{h} (g' M' - g'' M'')$$

→ Zeeman observations can trace the LOS magnetic field strength $B_{||} = B_0 \cos \vartheta$

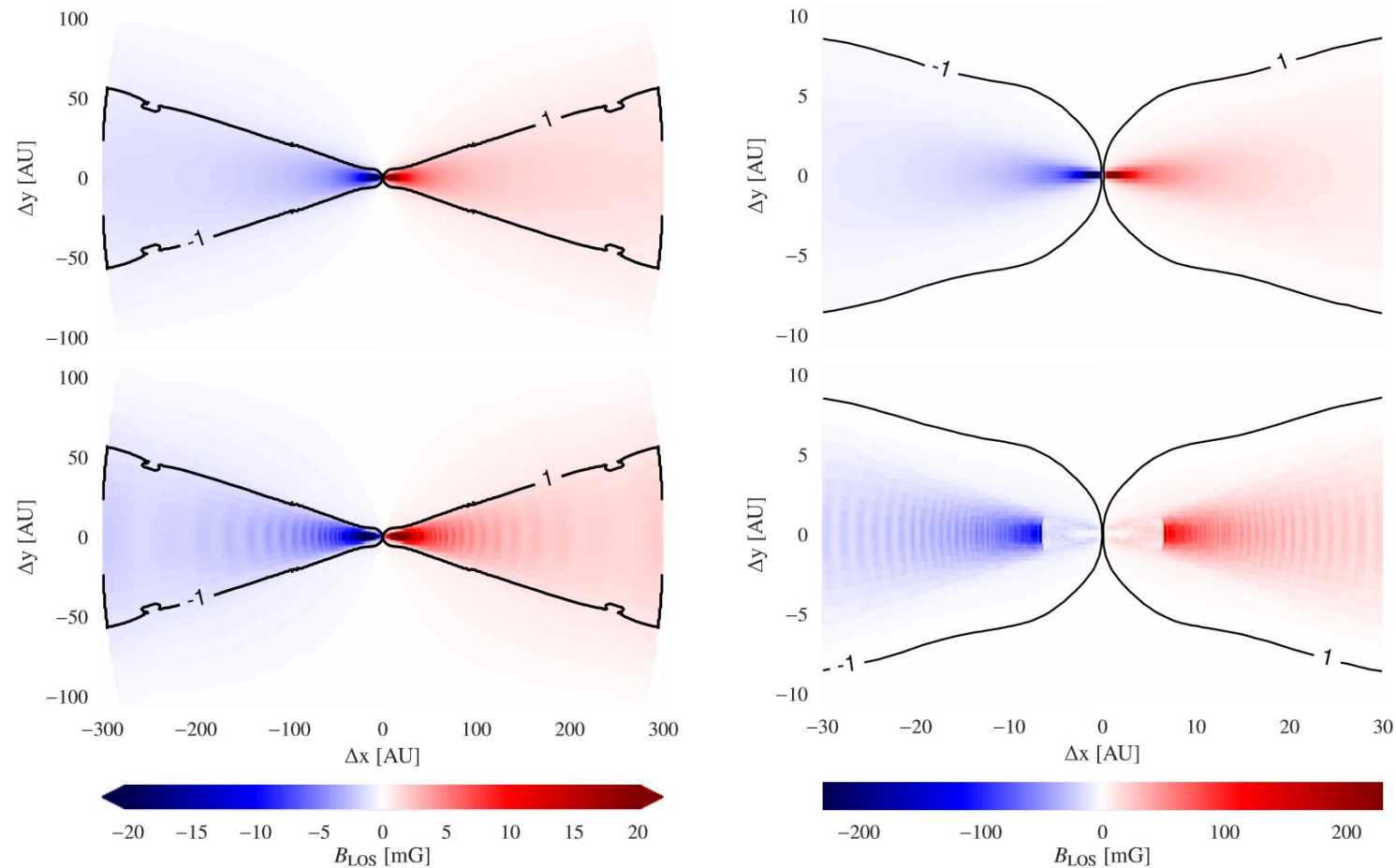


B-field strengths molecular clouds



Zeeman effect in disks

Synthetic 113.170 GHz CN line emission including Zeeman effect

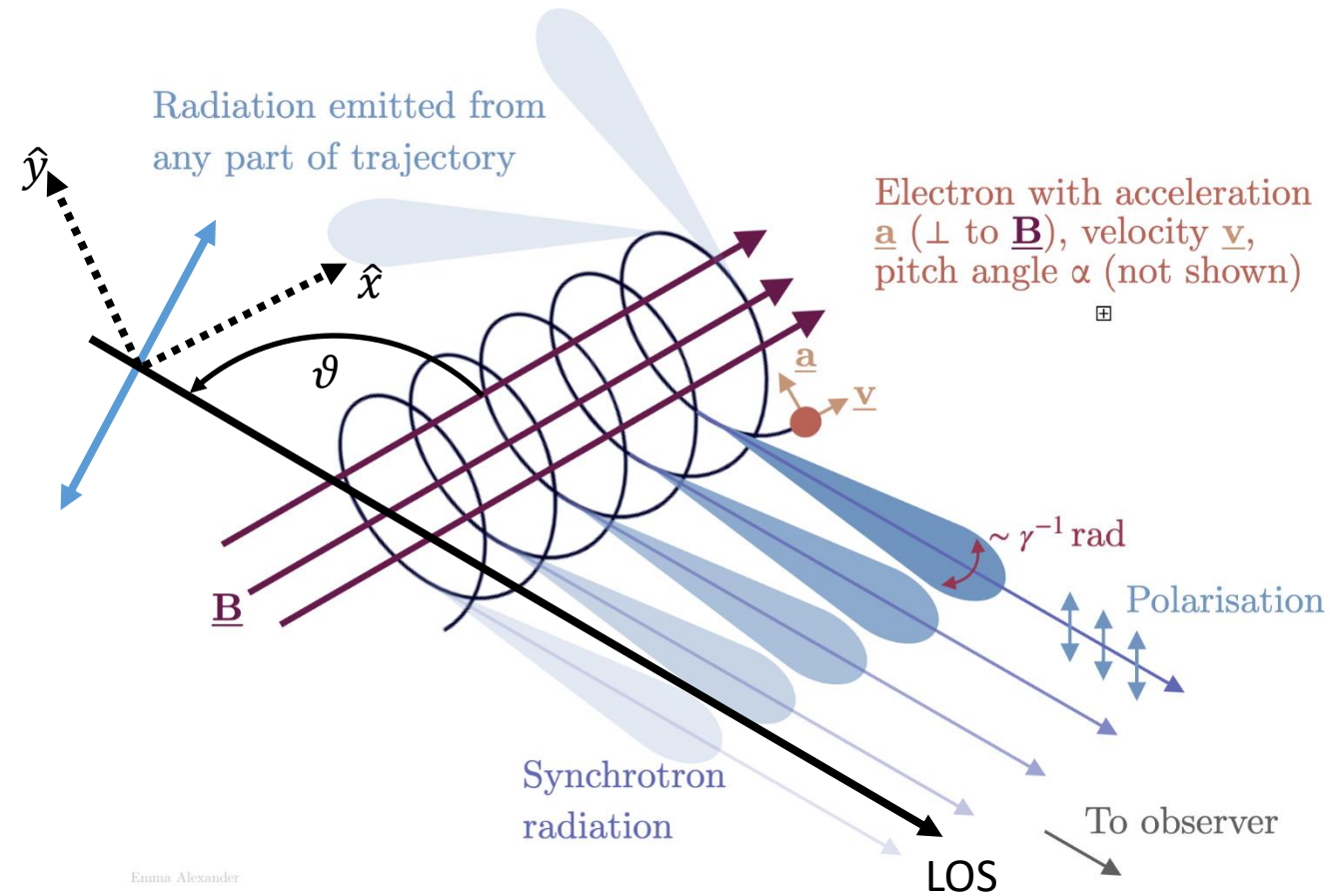


Brauer+ 2017

The Zeeman effect is detectable for inclinations $< 60^\circ$ and fields $< 1\text{mG}$

**Polarized Synchrotron Emission
&
Faraday Rotation**

Synchrotron emission



- Synchrotron emission is produced by highly energetic cosmic rays (CR) spiraling in a magnetic field
- Due to relativistic effects linearly polarized light is emitted in a very narrow beam

- Characteristic cyclotron frequency $\nu_c = \frac{eB}{2\pi m_e c}$

- Spectrum of a single electron

$$P(\nu) = \frac{\sqrt{3}e^3 B \sin \alpha}{m_e c^2} \left(\frac{\nu}{\nu_c}\right) \int_{\nu/\nu_c}^{\infty} K_{5/3}(\eta) d\eta$$

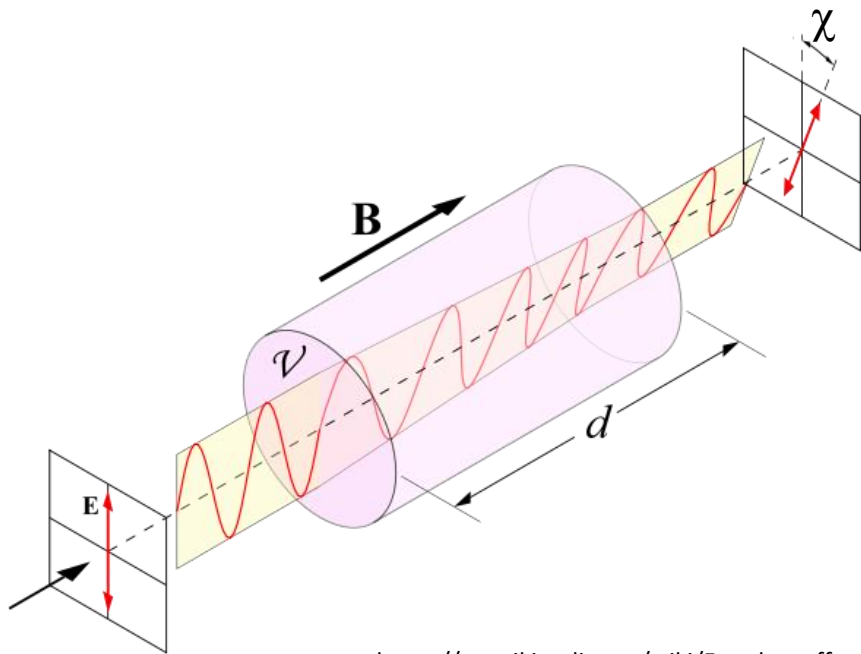
where $K_{5/3}$ is a modified Bessel function

- The energy distribution of cosmic-ray electrons is roughly a power law

$$n_{CR}(\gamma) = \begin{cases} \gamma^{-p} & \text{for } \gamma_{min} < \gamma < \gamma_{max} \\ 0 & \text{else} \end{cases}$$

with power-law index p and Lorentz factor γ

Thermal electrons



https://en.wikipedia.org/wiki/Faraday_effect

- In hot, diffuse regions of the ISM, the gas can be highly ionized leading to thermal (free) electrons
- Thermal electrons with a dimensionless electron temperature: $\Theta = \frac{k_B T_e}{m_e c^2}$
- These electron may be relativistic but not energetic enough for synchrotron radiation
- For temperatures $\Theta > 1$ the thermal electrons follow a velocity distribution

$$N_{\text{th}}(\gamma) = \frac{n_{\text{th}} \gamma^2 \beta \exp(-\gamma/\Theta)}{\Theta K_2(\Theta^{-1})}$$

- Light traversing a magnetized relativistic plasma undergoes both Faraday conversion (FC) ($U \leftrightarrow V$, s. dust polarization) and Faraday rotation (FR) ($Q \leftrightarrow U$)

⇒ Faraday rotation traces the LOS magnetic field strength B_{\parallel}

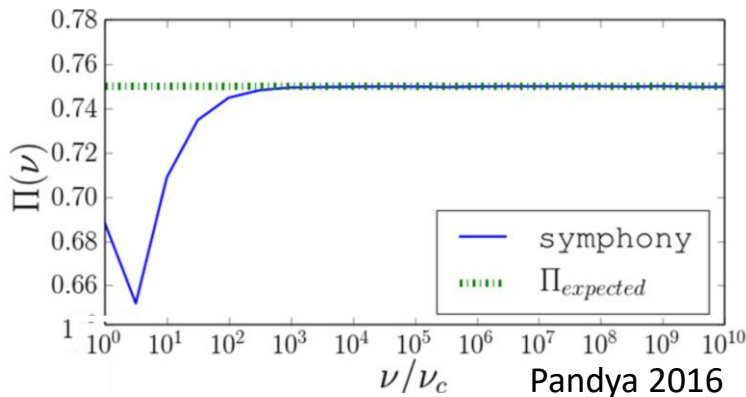
Transfer coefficients

Since the total power

$$P = \int_{\gamma_{min}}^{\gamma_{max}} P(\gamma) n_{CR}(\gamma) d\gamma$$

may be evaluated by a double integral over a Bessel function, the calculation of each matrix element is very time consuming

⇒ Use approximate solutions for $\nu > \nu_c$



The synchrotron emissivity e.g. is then

$$j_I \approx n_{CR} \left(\frac{e^2 \nu_c}{c} \right) \frac{3^{p/2} (p-1) \sin \theta}{2(p+1) (\gamma_{min}^{1-p} - \gamma_{max}^{1-p})} \Gamma\left(\frac{3p-1}{12}\right) \Gamma\left(\frac{3p+19}{12}\right) \left(\frac{\nu}{\nu_c \sin \theta} \right)^{-(p-1)/2}$$

Note that $P_l = \frac{j_I}{j_Q} = \frac{p+1}{p+7/3}$ i.e. the maximal linear polarization is completely determined by the power-law index p .

Similar approximations exist for the emissivities j_Q and j_V and the absorption coefficients α_I , α_Q , and α_V .

FR and FC can be exactly calculated:

FC coefficient $\kappa_Q(\lambda, \vartheta) = \frac{1}{4\pi^2} \frac{n_{th} e^4 B^2}{m_e^3 c^6} \lambda^3 \sin^2(\vartheta)$

FR coefficient $\kappa_V(\lambda, \vartheta) = \frac{1}{2\pi} \frac{n_{th} e^2 B}{m_e^2 c^4} \lambda^2 \cos(\vartheta)$

The RT equation

First, rotate Stokes vector in the reference frame of the magnetic field

Synchrotron RT equation including FC and FR:

synchrotron emission

$$\frac{d}{dr} \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} = - \begin{pmatrix} \alpha_I & \alpha_Q & 0 & \alpha_V \\ \alpha_Q & \alpha_I & \kappa_V & 0 \\ 0 & \kappa_V & \alpha_I & \kappa_Q \\ \alpha_V & 0 & -\kappa_Q & \alpha_I \end{pmatrix} \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} + \begin{pmatrix} j_I \\ j_Q \\ 0 \\ j_V \end{pmatrix}$$

Stokes I \leftrightarrow Q

Stokes I \leftrightarrow V

Stokes U \leftrightarrow V

Stokes Q \leftrightarrow U
Faraday rotation

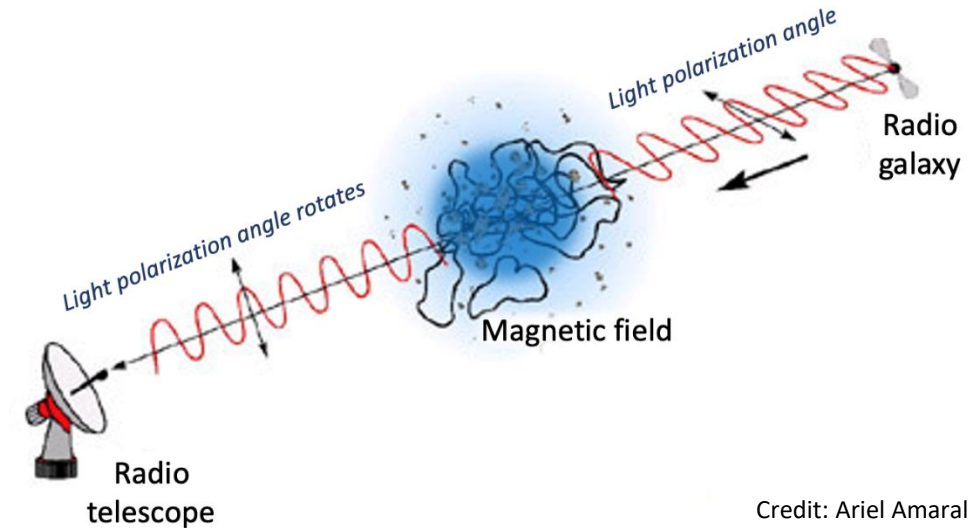
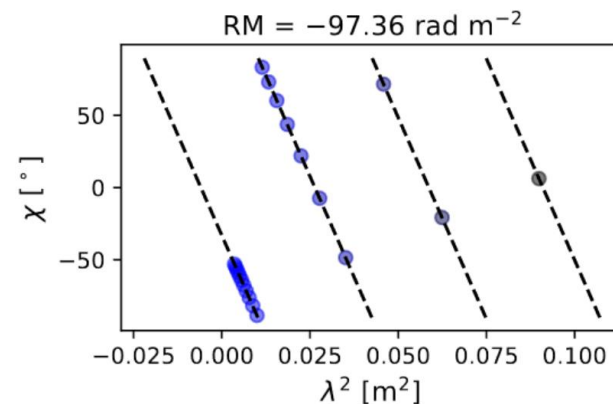
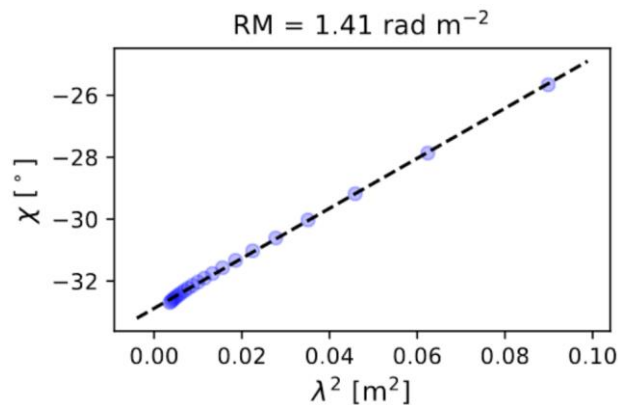
Faraday depth vs. rotation measure

- Faraday depth: $\phi = \frac{1}{2\pi} \frac{e^2}{m_e^2 c^2} \int_{\text{source}}^{\text{observer}} n_{th} B_{\parallel} dr$, $\phi = 0.811 \text{ rad m}^{-2} \int_{\text{source}}^{\text{observer}} \left(\frac{n_{th}}{\text{cm}^{-3}} \right) \left(\frac{B_{\parallel}}{\mu\text{G}} \right) \left(\frac{dr}{\text{pc}} \right)$

- Rotation measure (RM): $RM = \frac{d\chi}{d\lambda^2}$ where χ is the polarization angle

- In general both are not the same $\phi \neq RM!$

\Rightarrow Observed polarization angle $\chi = \chi_{\text{source}} + \phi \lambda^2$



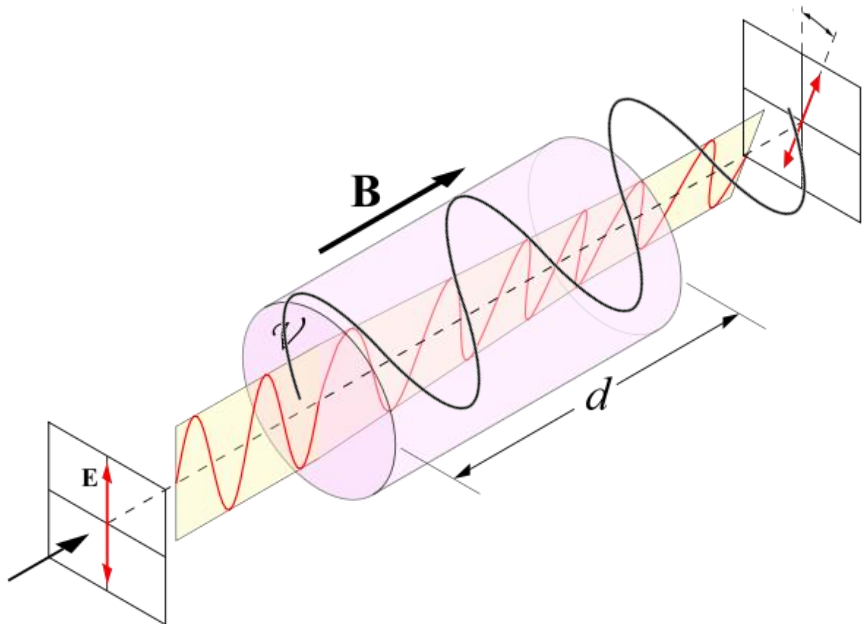
Credit: Ariel Amaral

Here, $\phi \equiv RM$ but note that the polarization angle χ may be ambiguous by $\chi \rightarrow \chi + n\pi$!

Faraday rotation measure synthesis

Observational ambiguities:

- The medium is synchrotron active i.e. emits polarized radiation
- The polarization angle of the source is not constant over λ



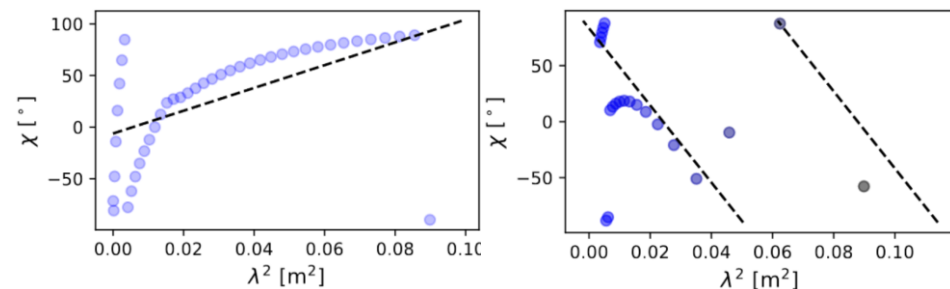
Idea: Define complex polarization $\mathcal{P}(\lambda^2) = Q + iU$ and calculate the Faraday dispersion function: $F(\phi) = \int_{-\infty}^{\infty} \mathcal{P}(\lambda^2) \exp(-2\pi i \phi \lambda^2) d\lambda^2$

Problem: Observational range is not infinite but limited within $\{\lambda_{min}, \lambda_{max}\}$ defining a window function

$$\mathcal{W}(\lambda^2) = \begin{cases} 1 & \text{if } \lambda_{min}^2 \leq \lambda^2 \leq \lambda_{max}^2 \\ 0 & \text{otherwise} \end{cases}$$

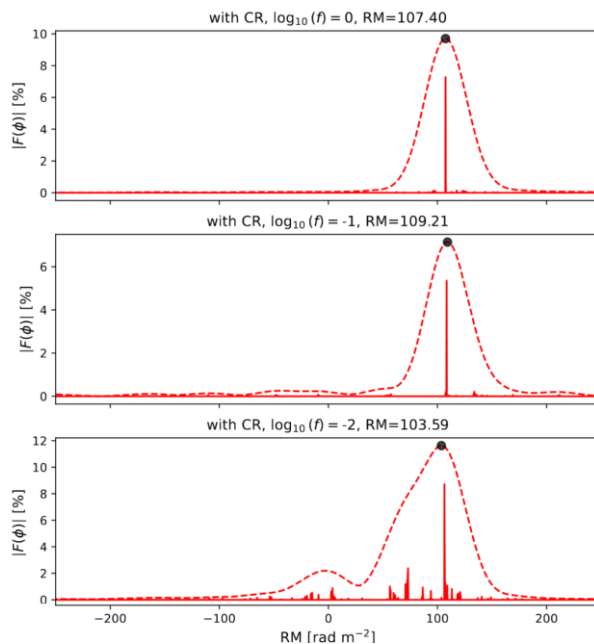
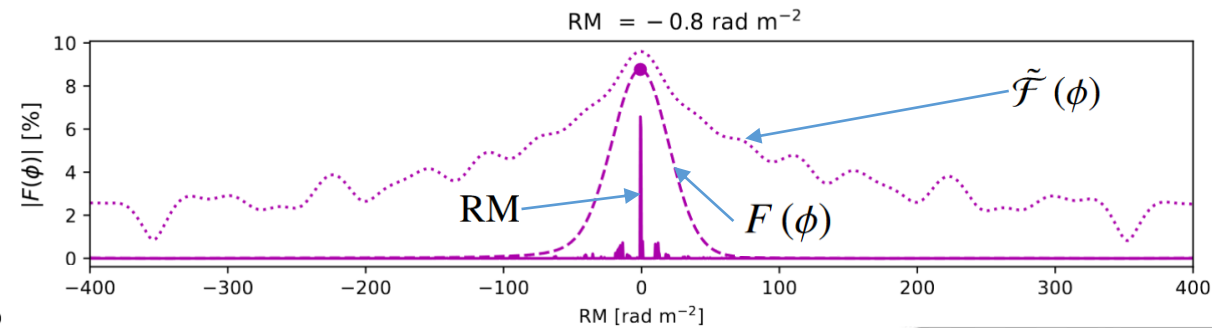
What we get is the convolution

$$\tilde{\mathcal{F}}(\phi) = \int_{-\infty}^{\infty} \mathcal{P}(\lambda^2) \mathcal{W}(\lambda^2) \exp(-2\pi i \phi \lambda^2) d\lambda^2 = \mathcal{P}(\lambda^2) * \mathcal{W}(\lambda^2)$$

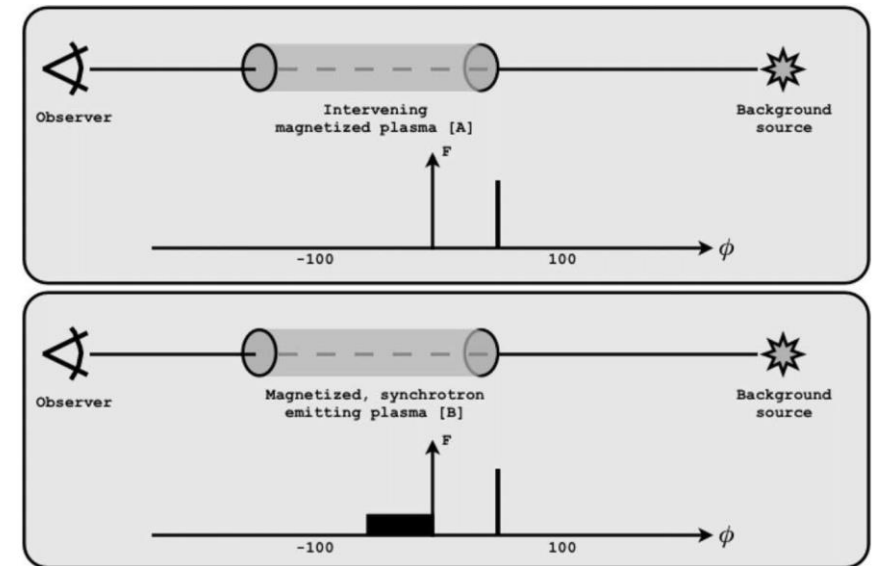


Faraday rotation measure synthesis

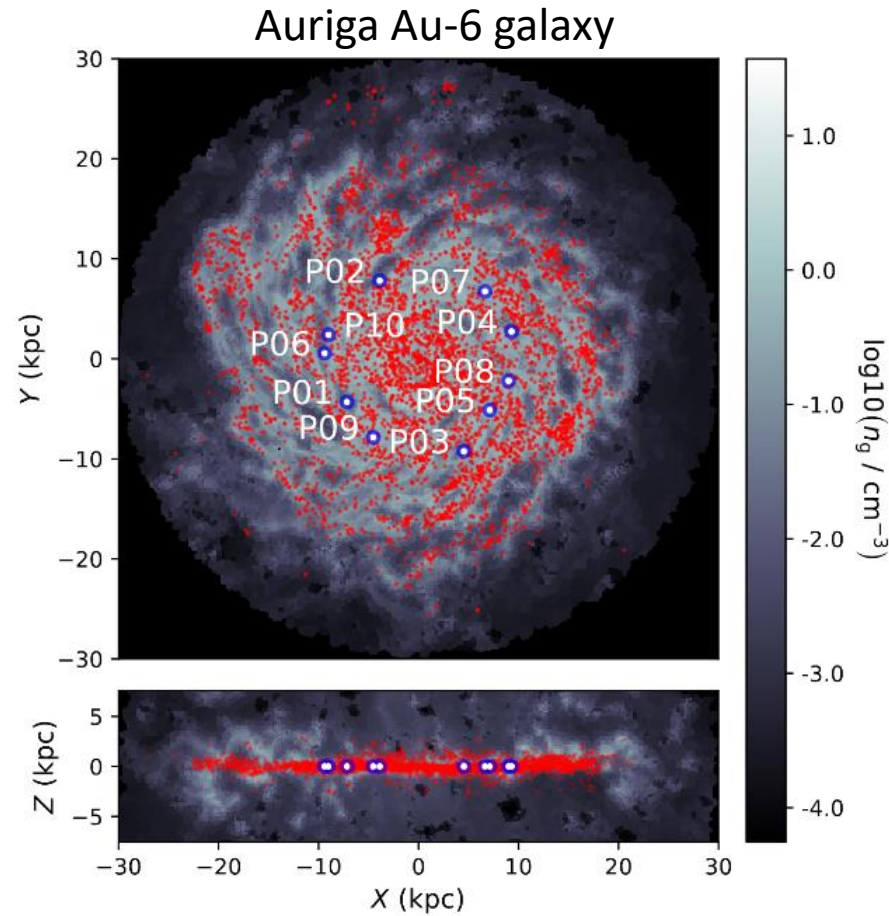
The Faraday rotation measure synthesis is a mathematical technique of deconvolution to recover the dispersion function $F(\phi)$ and even individual RM components. <https://github.com/crpurcell/RM-tools>



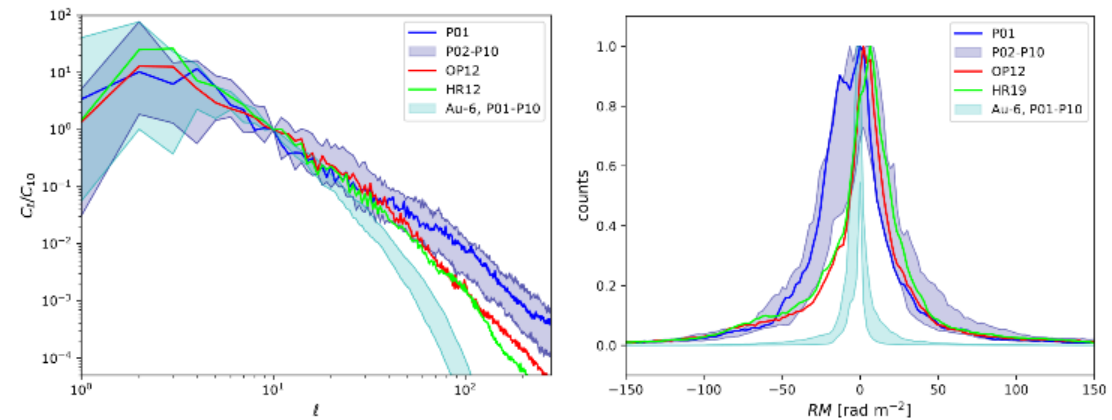
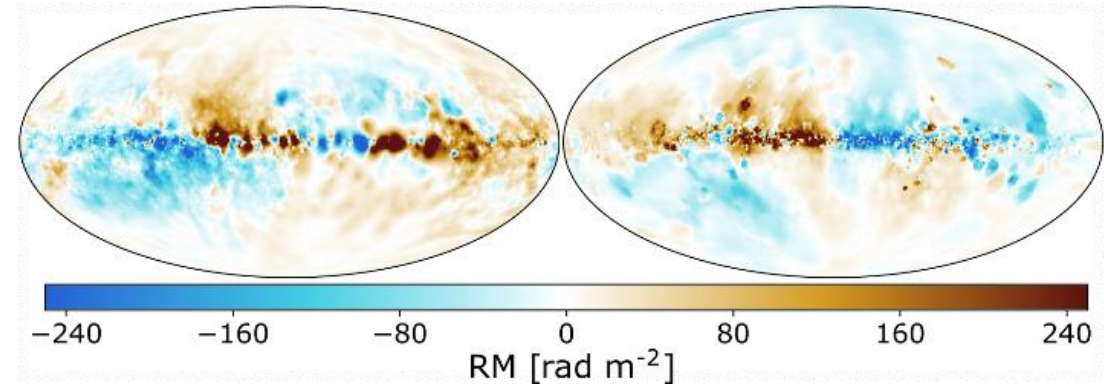
“Numerical experiment”: By reducing the intensity of the background source, the synchrotron active medium becomes apparent. The dominant RM can still be recovered in the spectrum.



RM in the MW

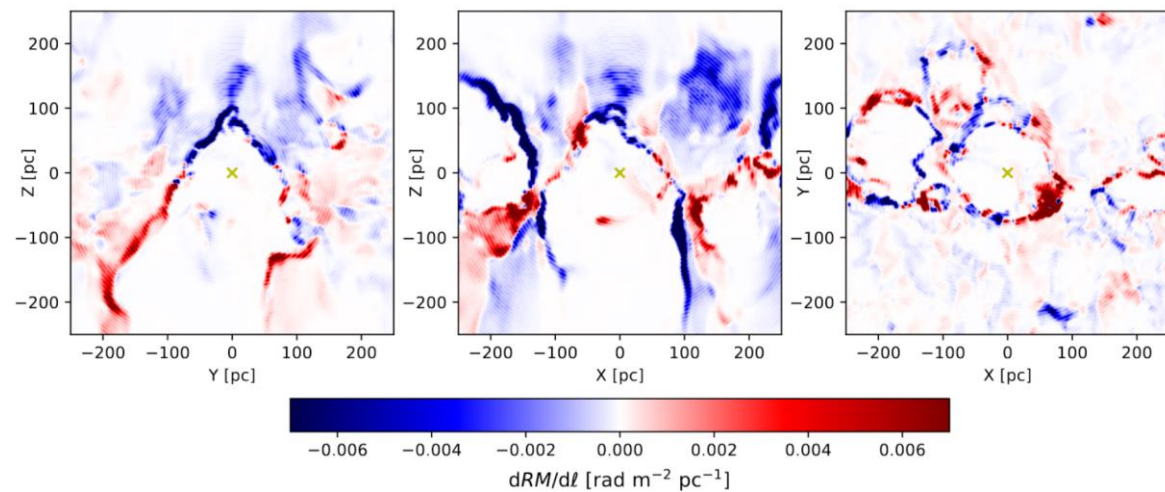
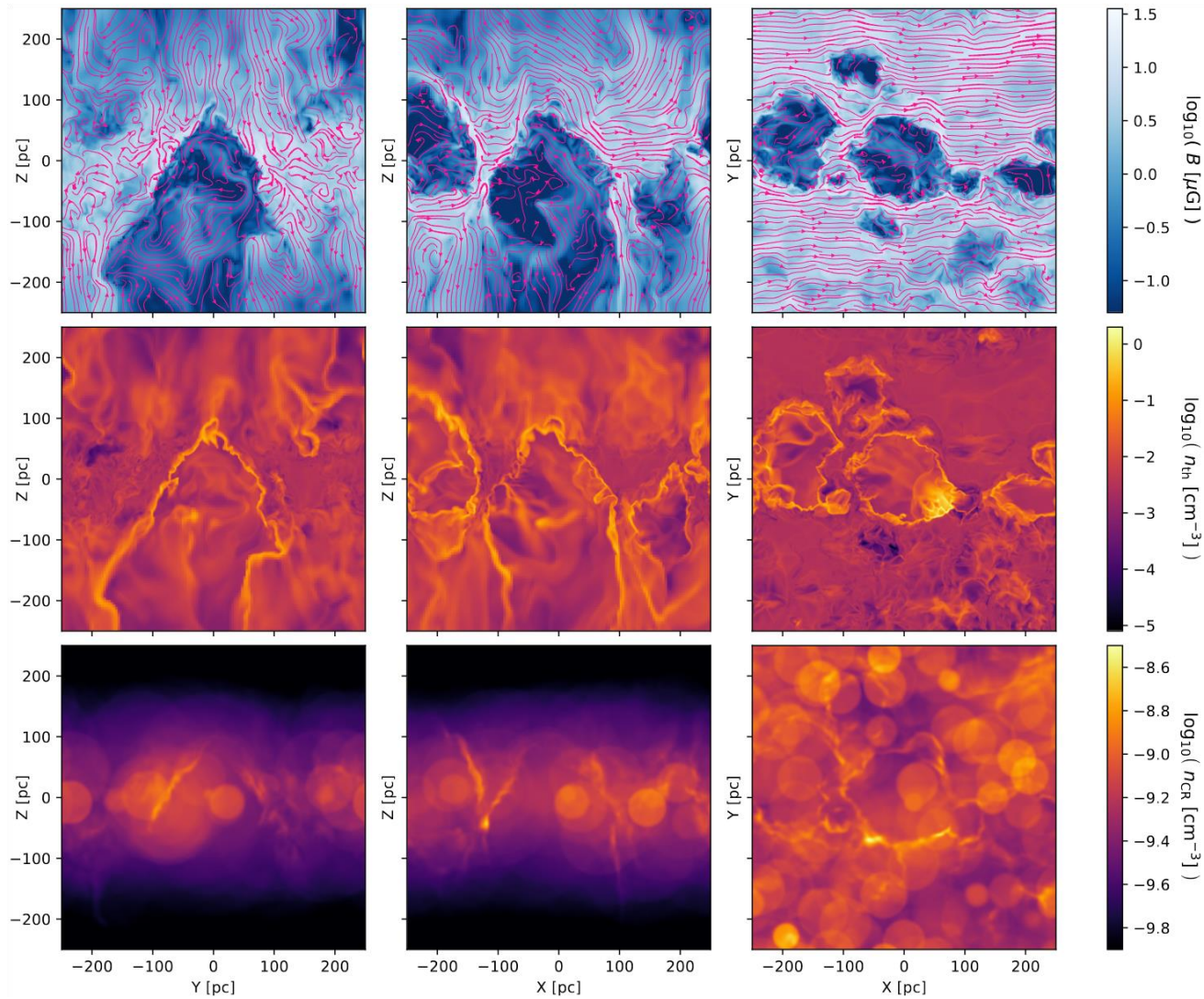


Grand+ 2017, Pellegrini+ 2018



Reissl, Klessen, Pellegrini, Rahner, Pakmor, Grand, Gómez,
Marinacci & Springel Nat Astron 2023

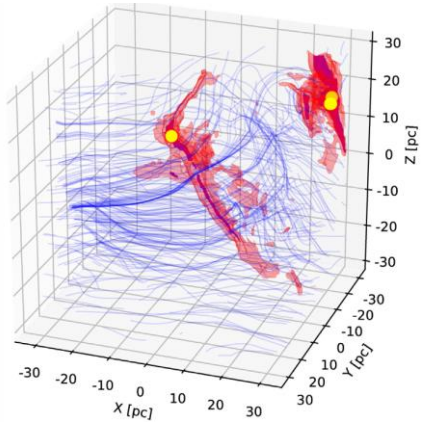
The local bubble in RM



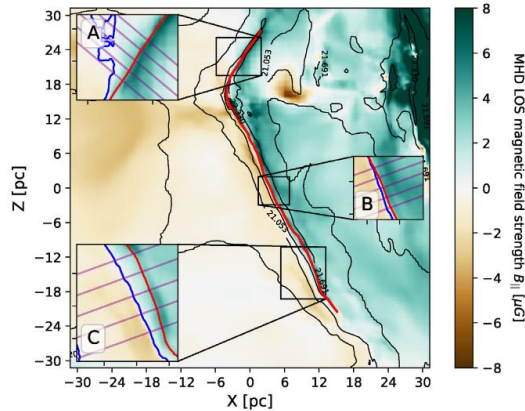
Maconi, Reissl, Soler, Girichidis, & Klessen in prep.

Zeeman vs. RM

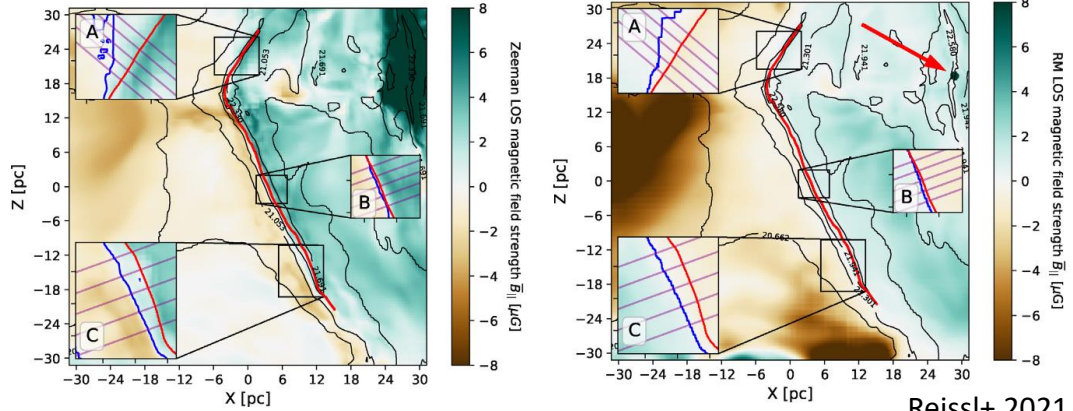
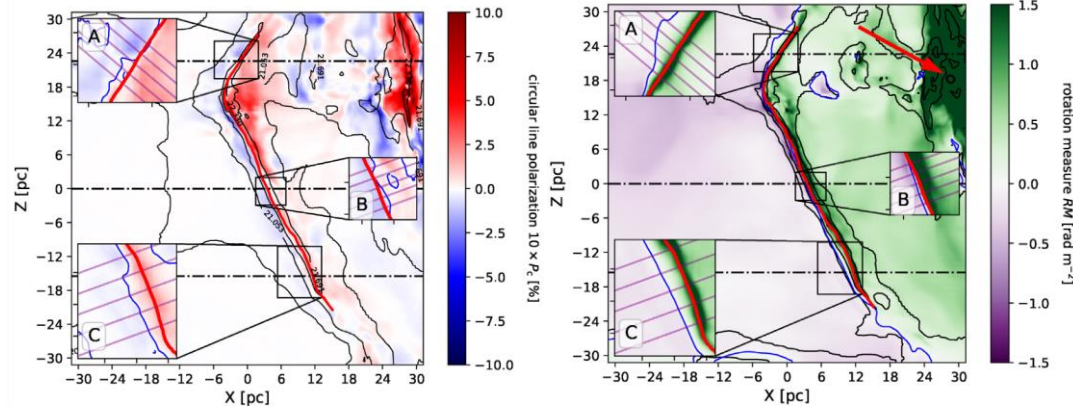
SILLC MHD simulation



Haid+ 2019



Synthetic Zeeman HI and RM observations



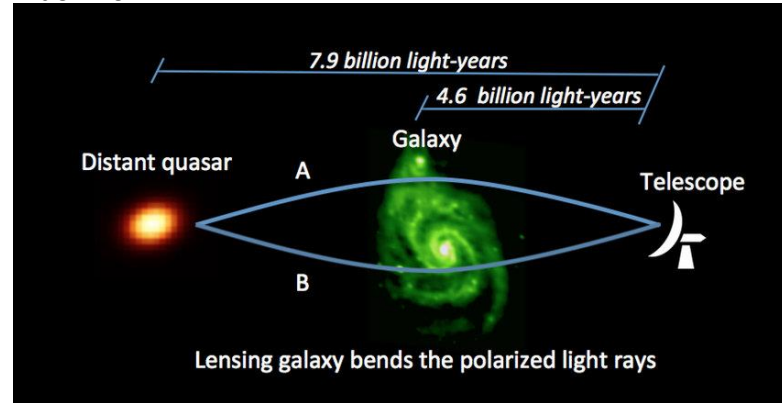
Reissl+ 2021

Thermal electrons may be constrained by relating the $H\alpha$ luminosity to the electron density

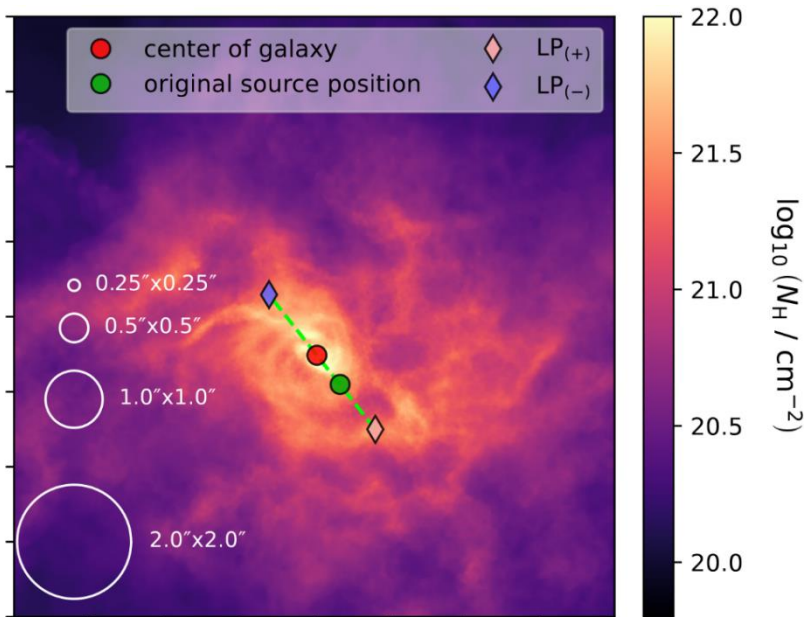
$$RM \sim \int n_{th} B_{||} dr \sim N_{th} \int B_{||} dr$$

B-fields in the early universe

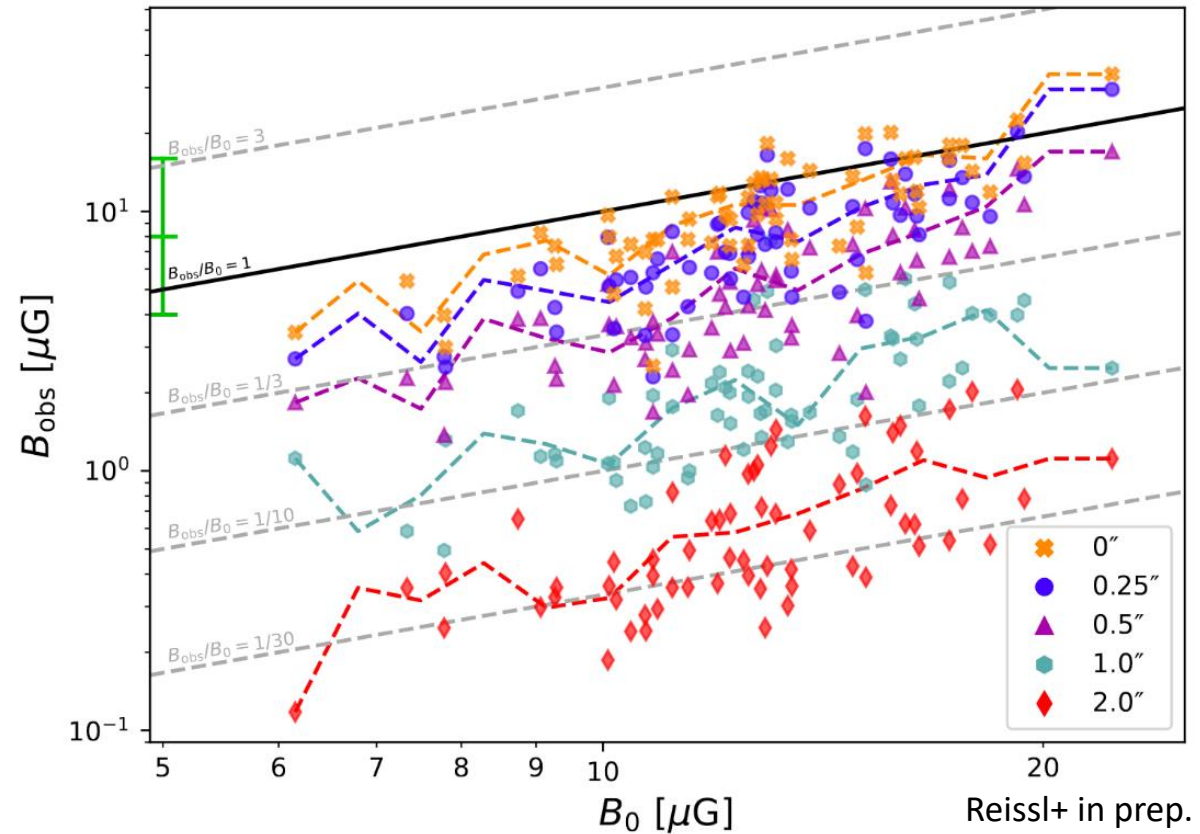
Mao +2017



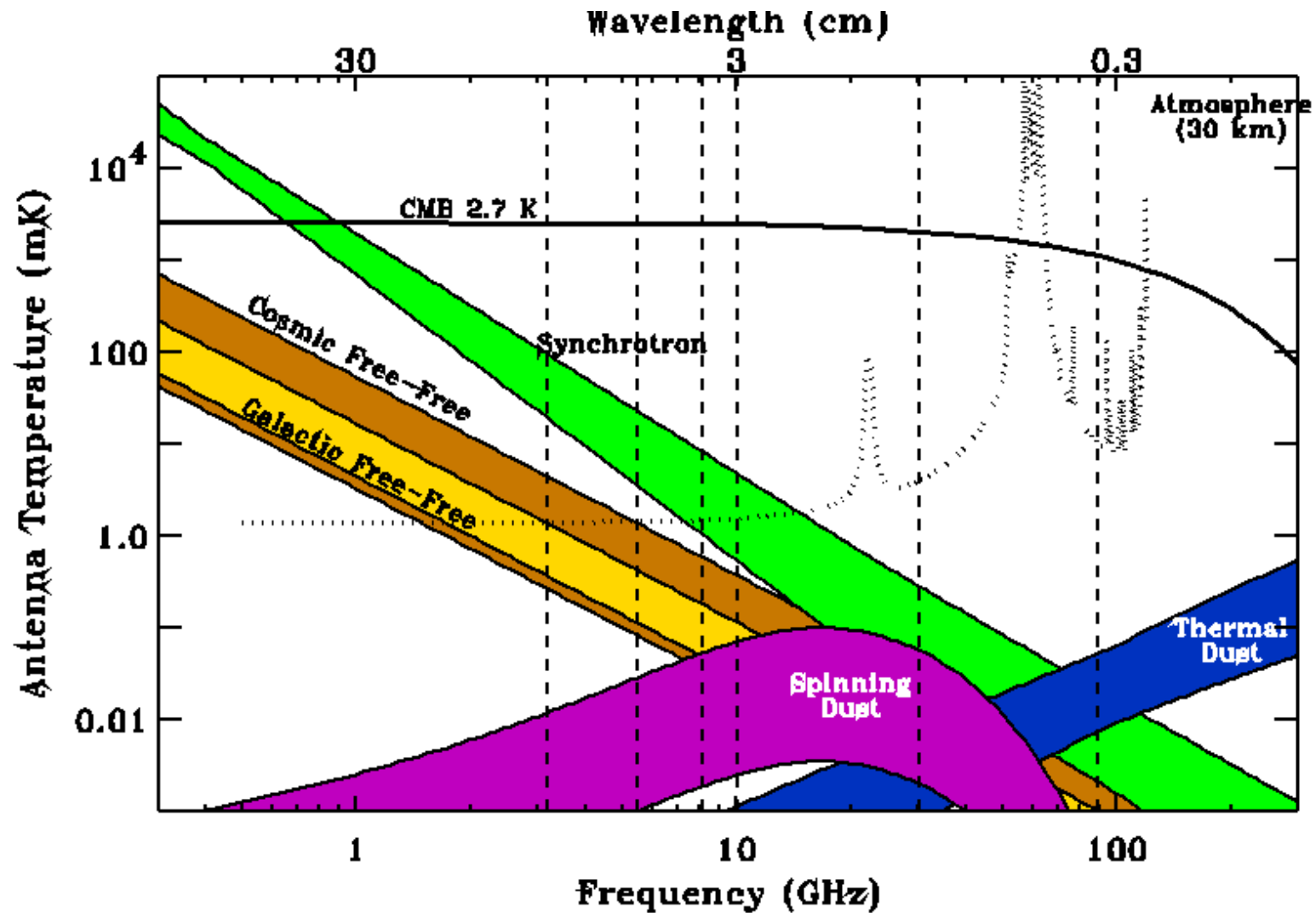
IllustrisTNG galaxy @ $z=0.5$ Nelson+ 2019



Reissl, Klessen, Pillepich, Mao, Pakmor & Nelson in prep.



What tracer is dominant?



Dust scattering needs to be taken into consideration for wavelengths $\lambda < 10 \mu\text{m}$

RT codes

Name	Type	Reference	Main application
SKIRT	MC, RayT	Baes et al. (2003, 2011)	Galaxies, AGN, lines, dust
TRADING	MC	Bianchi, Ferrara & Giovanardi (1996), Bianchi (2008)	Galaxies
RADISHE	MC	Chakrabarti et al. (2007), Chakrabarti & Whitney (2009)	Galaxies
RADMC-3D	MC, RayT	Dullemond in prep.	SF disks, dust & line RT
MOCASSIN	MC	Ercolano, Barlow & Storey (2005)	Photoionized regions
POLARIS	MC, RayT	Reissl+ (2016, 2018)	magnetic field detection, dust & lines
STOKES	MC	Goosmann & Gaskell (2007)	AGN
DIRTY	MC	Gordon et al. (2001), Misselt et al. (2001)	Galaxies, nebulae
TORUS	MC	Harries (2000), Harries et al. (2004)	SF disks
SUNRISE	MC	Jonsson (2006), Jonsson, Groves & Cox (2010)	Galaxies
CRT	MC	Juvela & Padoan (2003), Juvela (2005)	SF clouds
MCMMax	MC	Min et al. (2009, 2011)	SF disks
STSH	MC	Murakawa et al. (2008)	SF disks
MCTRANSF	MC	Niccolini, Woitke & Lopez (2003), Niccolini & Alcolea (2006)	SF disks
mcsim mpi	MC	Ohnaka et al. (2006)	Carbon stars
MCFOST	MC	Pinte et al. (2006)	SF disks
HYPERION	MC	Robitaille (2011)	SF clouds
PHAETHON	MC	Stamatellos et al. (2004, 2005)	SF cores
STEINRAY	FD	Steinacker et al. (2003)	SF disks
(no name)	RayT	Steinacker, Bacmann & Henning (2006)	SF cores
HO-CHUNK	FD	Stenholm, Stoerzer & Wehrse (1991)	SF disks, AGNs
MC3D	MC, RayT	Wolf & Henning (2000), Wolf (2003b)	SF disks, dust

POLARIS

- **MC dust heating:** Continuous absorption and temperature correction, **stochastic heating of small dust grains (PAH)**
- **Dust model:** Independent composition of dust grain materials and size distributions
- **Grain alignment:** Internal alignment, Davis-Greenstein (IDG), radiative torques (RAT, **wrong alignment, MRAT**), **mechanical alignment of dust (MAD), rotational disruption (RATD)**
- **Sources:** Stars, star fields, background radiation, ISRF, thermal dust re-emission, **AGN**, laser
- **Dust polarization:** (Self)scattering, **scattering on non-spherical grains**, dichroic extinction, thermal re-emission, **spinning dust microwave emission**
- **Free-free emission**
- **Line polarization:** Zeeman effect, **atomic alignment**, level population methods of local thermodynamic equilibrium (LTE), free-escape probability (FEP), large velocity gradient (LVG)
- **Synchrotron polarization:** Emission and Faraday rotation by thermal and cosmic-ray electrons
- **Optimization:** Forced first scattering, Wavelength range selection, Peeling-off, sub-pixeling, OpenMP parallelization
- **Native AMR grids:** Spherical, cylindrical, Voronoi, Octree