

Spectral Line Interferometry

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Outline

Part 1: Spectral Line Science

- What are spectral lines?
- Key physical processes doppler velocities, proper motions
- Conditions how spectral line emission is detectable
- Chemistry
- Fundamental physics

Part 2: Spectral line data reduction

- Differences between continuum observing and spectral lines
- How to set up spectral line observations

Part I: Spectral line science

Atoms & molecules in space

- There is a lot of 'stuff' between the stars (but we still don't know what dark matter is!)
 - > 200 molecular species have been identified
 - Gas and dust is concentrated in molecular clouds
 - Molecular clouds are where star formation takes place
 - A wide range of densities and temperatures
- Atoms and molecules in space produce spectral lines which act like fingerprints that we can use to identify them
- Chemistry in space
- Spectral lines are powerful diagnostics of the physical and chemical conditions in astronomical objects

Molecular clouds are composed of:

- Mostly hydrogen H₂ (~75%)
- Helium **He** (~25%)
- Dust (1%)
- Carbon Monoxide **CO** (10⁻⁴ by number)
- And >200 other molecules with low abundances (<10⁻⁴)



http://www.cv.nrao.edu/php/splat/http://physics.nist.gov/cgi-bin/micro/table5/start.pl

Spectral lines

- Temperature variations in the ISM lead to transition zones called photodissociation regions or PDRs.
- These exist between the hot (ionised) and cold (neutral) ISM.
- The physical and chemical properties of a PDR change with distance as the photons are absorbed
- When the density of dust and molecules is high enough it shields the interior from UV radiation
- This leads to a rich variety of atoms and molecules



Spectral lines

Orion KL survey at 100 GHz



Orion KL survey at 100 GHz

Tercero et al. (2010)



Spectral lines

Spectral line origins



• Spontaneous emission rate depends on temperature i.e. Boltzmann distribution of molecular energies

- Absorption rate also depends on the energy field (more specifically the energy density, U_v)
- Stimulated emission

All these depend on the Einstein coefficients i.e. A_{UL} , B_{LU} , B_{UL}

Electron transitions

- Transition between energy levels results in emission at discreet wavelengths.
- Discrete energy levels allows us to know which species is present!
- Due to the higher energy, the emission is at much shorter wavelengths / higher frequency
- Ha emission is generated when an electron in hydrogen moves from n=3 to n=2
- This is most likely to happen when a proton captures an electron
- It is a good indicator of ionised gas
- Ionisation on large scales requires the presence of a massive star





n = 1

n = 2

n = 3





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Spectral lines

The 21 cm line



- Observations of the 21 cm line in 1951 marked the birth of spectral line radio astronomy
- Electrons and protons have a quantum property called **spin** which can be in two orientations relative to the proton (parallel & anti-parallel
- Parallel levels have higher energy than anti-parallel
- Flipping between these is the same as the electron being accelerated
- This is a low energy transition leading to 21 cm radio waves
- The probability of this occurring is small
 2.9x10⁻¹⁵ s⁻¹
- 10 million years for a single hydrogen atom
- Despite this we still see 21-cm emission so there must be a lot of hydrogen about!

Spectral lines in molecules

Complex molecules also emit radiation but in different ways to atomic species:

- Electronic, vibrational, rotational transitions
- Collisional or radiative excitation
- Energy levels are quantised (i.e discreet)
- Only certain transitions are allowed between energy states



Molecular energy levels



Spectral lines

Optical depth

Important concept!

 Describes the fraction of radiation that passes through a medium (including absorption & scattering)

$$\tau_{\nu} = \int \kappa_{\nu} ds$$

- Integrated absorptivity times path length at a given frequency through a medium of depth ${\cal S}$
- The observed emission or absorption line is then given by:

$$I_e = B[1 - \exp(-\tau_{\nu})] \sim B\tau \text{ (for } 0 < \tau_{\nu} \ll 1)$$

 $I_a = I_0 \exp(-\tau_{\nu})$



Line profiles

A quantised transition with exact energy would produce a line that is infinitely sharp, however this is not the case:



Every line has **line broadening** due to:

- Natural broadening due to the Uncertainty Principle $\Delta E \Delta t \ge h$
- Thermal Doppler broadening Thermal Boltzmann distribution of atoms / molecules
- Collisional broadening The collision of other particles interrupts the emission process and shortens the time leading to an increase in the uncertainty of the energy emitted
- Zeeman splitting Magnetic fields cause the spectral line emission to split into several features

Kinematics – the Doppler effect

- Movement of an emitting source towards or away from the observer produces a shift in the frequency.
- Analogous to the sound of a passing siren being distorted
- For observations in the Milky Way the differential rotation leads to a shift in the frequency
 - Approaching sources are blueshifted - higher frequency / shorter wavelength
 - Receding sources are redshifted - lower frequency / longer wavelength



The Doppler effect

- The Doppler effect allows us to determine the velocity that an object is moving towards or away from us known as the radial velocity
- If you can measure the shift in the wavelength of a spectral line you can determine the radial velocity via:
 - *v* is the relative radial velocity taken as positive for sources moving away from the observer and negative for sources moving towards the observer
 - Knowing this we can map the distribution of gas in the galaxy





The Doppler effect



Doppler effect in the 21 cm line



HI emission integrated over the velocity range -400 < v < +400 km/s in the LAB dataset, shown in Aitoff projection. The Galactic centre is in the middle. The integrated emission (0 < NH < 2.1022 cm⁽⁻²⁾, logarithmic scale) yields column densities under the assumption of optical transparency; this assumption may be violated at latitudes within about 10° of the Galactic equator. (Kalberla et al. 2005)

Spectral lines

Kinematic distance degeneracy

- The velocity can be used to determine the distance to a source assuming some model of how the Galaxy rotates
- This is called the kinematic distance
- Unfortunately the geometry gives rise to a degeneracy where a source may be located at either a **near** or **far** kinematic distance



Other emission mechanisms

We have only looked at how atoms and molecules emit spectral line radiation and heated objects emit blackbody emission but there exists many other emission mechanisms such as:

Maser emission

- Stimulated emission of an inverted population
- Synchrotron emission
 - Electrons spiralling around magnetic fields (as in most extragalactic GHz radio emission)
- Thermal Bremsstrahlung (free-free) emission
 - Electrostatic interactions in ionised (HII) regions

Other emission mechanisms

Maser emission

A group of molecules are pumped into an excited state. When photons with an energy equal to the energy separation between E1 and E2 pass it stimulates a cascade. Leads to discrete emission.

Synchrotron emission

As a charged particle (normally electrons) spirals around a magnetic field it will release photons. The frequency is directly related to the speed of the particle, very fast (relativistic) electrons are required. The particle loses energy as it emits photons and slows thus releasing energy at longer wavelengths.

Free-free emission

Unlike the previous two, this is a thermal emission mechanism (depends on temperature). In an ionised gas (plasma) charged particles undergo interactions. Electrons can be accelerated by charged particles. A wide range of frequencies are generated based on the speed



HI absorption



FIG. 1.—Global (spatially integrated) H I absorption spectra of Seyfert l nuclei. The spectra are continuum subtracted and corrected back to zero est velocity based on the observed recessional velocities in Table 2. The only nondetection among the Seyfert 1 nuclei was Mrk 668.

Gallimore et al. 1999

Radio continuum grey scale

Absorption measurements

Can be used to resolve the kinematic distance ambiguity (Urquhart et al. 2012)



Figure 3. Source-averaged, high-resolution continuum-included H_I spectra towards the H_I regions observed with ATCA. The source velocity (v_S) , the velocity of the tangent point (v_T) and the position of the first absorption minimum (v_A) are shown by the red, blue and green vertical lines, respectively. The grey vertical band covers the velocity region 10 km s^{-1} either side of the source velocity and is provided to give an indication of the uncertainty associated with it due to streaming motions. The dotted horizontal line shows the $4\sigma_{rms}$ noise level determined from absorption-free parts of the spectra (see Section 2.3 for details). In the top and bottom panels, we provide examples of sources placed at the near and far distances, respectively. The full version of this figure is available in the online version of the journal – see Supporting Information.

Summary of part I

- We have looked at where spectral lines come from and some of the science
- A wide range of spectral lines probe varied environments
- Determine gas abundances, chemistry, kinematics, densities, temperatures
- Continuum and spectral line observations give complimentary information

Thanks to Jack Radcliffe, Luke Hindson, Joe Callingham and Sharmila Goedhart for the content of these slides

Part II – Spectral line data reduction

- We have discussed some of the science you can do with spectral lines
- In this part we will explore the important differences between spectral line and continuum data reduction
 - Setting up your observations
 - Data reduction
 - Image and spectral analysis

What is spectral line interferometry?

- Observing many adjacent frequency channels with an interferometer for an object whose flux changes rapidly with frequency
- Results in a third axis: frequency or velocity



CO (6-5) emission from a high redshift quasar observed with the Plateau de Bure interferometer (Wang et al. 2010)

What is spectral line interferometry?

- However, today even continuum observations are carried out with many channels (called pseudo continuum)
- Therefore, you need to understand spectral line interferometry to do (almost all) interferometry

Plot of response across a band for one EVN antenna as a function of channel during the reduction of continuum data



Setting up your observations

- 1. Choose your science case and lines(s)
- 2. Choose your source(s) and research its properties
- 3. Choose your interferometer and configuration
- 4. Check source velocity reference frame, on-line Doppler tracking
- 5. Choose the channel width, total bandwidth, and number of channels
- 6. Determine your required sensitivity and time on source
- 7. Choose your calibrators
- 8. Data rate and size considerations

I. Choose your science case(s) and line(s)

- 1. Choose spectral line(s) for science case
- 2. Find which telescopes have bands that can observe the line(s)

Doppler shifts \rightarrow Velocity fields



Velocity field of galaxy M33 in HI. Colours show Doppler shift of line and brightness is proportional to HI column density (NRAO, Thilker et al.) Physical properties from lines for science case

Column density Chemistry

Excitation Temperature

Dynamics

Magnetic field strength

Density

Optical depth

Turbulent motions

Commonly observed lines:

HI – the hydrogen spin-flip transition



Can determine:

- Morphology of atomic gas
- Dynamics
 - Gives enclosed mass (inc. dark matter)
- Column density and mass of optically thin gas
- Temperature of optically thick gas
- Distance via Hubble law

Commonly observed lines

RRLs – Radio Recombination Lines



Can determine:

- Ionised gas dynamics
- Optical depth and electron temperature (in Local Thermodynamic Equilibrium, LTE)
- Gas density from collisional broadening of the lines
- Speed of turbulent motions from linewidths (for low n)
- Abundance ratio of H/He/C
- Magnetic field strengths from Zeeman splitting

Commonly observed lines

Molecular lines



Common molecular lines:

- CO, OH, H₂O, SiO, HCN, NH₃
- Can also observe absorption lines and masers.

Can determine:

- Morphology of molecular gas
- Dynamics
- Gas column and volume density
- Optical depth
- Temperature
- Abundances
- Magnetic field strength
- Chemistry
- Presence of shocks (SiO)

2. Choose source and research properties

Learn about the object you wish to study e.g:

- Position (and equinox)
- Size
- Velocity (and reference frame)
- Estimated brightness

Search for literature on your source using resources like:

- ADS (<u>http://www.adsabs.harvard.edu/</u>)
- NED (<u>https://ned.ipac.caltech.edu/</u>)
- CDS (<u>http://cds.u-strasbg.fr/</u>)

3. Choose interferometer and configuration

- Large number of possible instruments to name just a few:
 - (J)VLA, ALMA, MWA, LOFAR, PdB, ATCA, EVN, AVN
- Read about the telescope online e.g for the VLA



3. Choose interferometer and configurations

(J)VLA



Larger arrays: better resolution! Good for absorption studies as want to detect a small, bright background source

Part of the ALMA Compact Array



Smaller arrays: have better surface brightness sensitivity so easier to detect extended or faint emission

4. Check source velocity reference frame

• Need to always specify the velocity reference frame.

Rest Frame	Corrected for	Amplitude of Correction (km/s)
Topocentric	Nothing	0
Geocentric	Earth rotation	0.5
Earth-Moon Barycentric	Effect of Moon on Earth	0.013
Heliocentric	Earth's orbital motion	30
Solar System Barycentric	Effect of planets on Sun	0.012
Local Standard of Rest (LSRK/D)	Solar motion	20
Galactocentric	Milky Way Rotation	230
Local Group Barycentric	Milky Way Motion	~100
Virgocentric	Local Group Motion	~300
Microwave background	Local Supercluster motion	~600

4. Check source velocity reference frame

- Optical Barycentric or Heliocentric system often used for extragalactic observations
- Radio Local Standard of Rest (LSR) used for Milky Way observations

$$\frac{\nu_{\rm radio}}{c} = \frac{\nu_0 - \nu}{\nu_0}$$

Doppler shift and Doppler tracking

- **On-line Doppler** tracking automatically corrects to a given reference frame during the observation in real time
- The tracked or observed frequency is usually called the sky frequency
- However, for wide frequency bands, on-line Doppler tracking is not done as correction is only strictly correct at one frequency.
- Instead **Doppler setting** is used i.e. the sky frequency is calculated once at the start of the observation
- Further corrections can be made during the data reduction and imaging stages (need > 4 channels across the line to go a good correction

5. Choose channel width, bandwidth and number of channels

- Channel width determined by required spectral resolution and sensitivity
- Total bandwidth should leave good line free channels at the ends of the band for continuum subtraction (end channels often bad)
- In a "lag" correlation, total number of channels is conserved, so total bandwidth is directly related to channel width

Velocity coverage

• For radio/millimetre frequency observations:

$$\frac{\Delta f}{f} \simeq \frac{\Delta v}{c}$$

Where Δf is the bandwidth (Hz), f the rest frequency (Hz), Δv is the velocity span (km s⁻¹) and $c = 3 \times 10^5$ km s⁻¹, the speed of light

So if you want a velocity coverage of 100 km s⁻¹ at a frequency of 22.2 GHz then:

$$\Delta f = \frac{100}{3 \times 10^5} \times 2.22 \times 10^{10} = 7.4 \,\mathrm{MHz}$$

• Need to allow some leeway for filter edge effects.

Velocity resolution

- It is good practice to have a velocity resolution with at least 3 channels between the half power points of a typical spectral line
- So if you have lines with typical FWHM of 1 km s⁻¹ at 22.2 GHz then you want a spectral resolution of:

$$\Delta f = \frac{0.33}{3 \times 10^5} \times 2.22 \times 10^{10} = 25 \,\mathrm{kHz}$$

• Many correlators have a maximum channel bandwidth product. Often you want to select the configuration with maximum bandwidth for the required velocity resolution

Gibbs ringing and Hanning smoothing



- Seen at channel edges
- Also see for bright lines e.g masers, RFI

Con – reduces spectral resolution by 2

6. Determine your required channel sensitivity and time on source

- Determine how many channels needed to adequately resolve your line (e.g. >5)
- If detection is important, need to detect line peak channel with >3-5 sigma
- If need to resolve emission in different channels for e.g. dynamics, need to detect line in faintest of these channels with >3-5 sigma
- You should determine the estimated flux of the source (May need to convert from brightness temperature T_b or expected column density)
- Use sensitivity calculator to determine required time on-source (e.g. VLA, ALMA, SMA, ATCA)

7. Choose your calibrators

Bandpass calibration

The bandpass is the spectral frequency response of an antenna to spectrally flat source of unit amplitude



The observed phase and amplitude is not ideal because of delay error and limitation of the antenna transmission and electronics

Why bandpass calibration is important

The quality of the bandpass calibration is a key limiting factor in the ability to detect and analyze spectral features

v-dependent amplitude errors:

- Limits ability to detect/measure weak emission/absorption lines
 superposed on the continuum
- May mimic changes in structure

v-dependent phase errors:

- May lead to spurious positional offsets between spectral features as a function of frequency, imitating Doppler motions
 - Relative positional accuracy in channel images $\Delta \theta / \theta_B = \Delta \phi / 360^\circ$ where θ_B is the synthesized beam and $\Delta \phi$ is the scatter in the phase

For pseudo-continuum experiments conducted in spectral line mode, dynamic range of final images is limited by bandpass quality

Spectral lines

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What makes a good bandpass calibrator?

Select a bright continuum source with:

- High SNR in each channel
- Intrinsically flat spectrum
- No spectral lines/features
- No changes in structure across band (e.g. point source at all frequencies)

Calibration should not contribute to noise in target spectrum, i.e. in one channel:

bandpass SNR > target SNR

Can smooth the bandpass or fit polynomial to increase the SNR

May need a higher SNR for bandpass calibrator if looking for faint lines on strong continuum



7. Choose your calibrators

Flux calibration

- In mm/sub-mm observing, if using solar system object with an atmosphere for calibration (Jovian or Saturnian moons, for example), be aware that these objects often have absorption lines
- Check your calibrator spectrum carefully, particularly if that source is not red-shifted
- You should exclude affected channels (or even baseboards if the absorption is broad)



Titan clearly shows multiple emission features Finally, many observatories impose a maximum data rate for a given observation

For instance, for the VLA the data rate depends on:

- Number of channels
- Number of spectral windows
- Number of polarisations observed
- Length of one integration in seconds
- Number of antennas

It is not uncommon for datasets to be in the many 100s of GBs. Large datasets are difficult to transfer and reduce.... only use high spectral and time resolution if you really need it.

Data reduction

- Flagging methods
- Bandpass calibration
- Doppler correction
- Continuum subtraction
- Self-calibration
- Imaging of cubes

Flagging methods - in frequency

- For large data sets, checking the data channel-by channel is not practical
- This task can be simplified using approaches such as:
 - Examination of scalar-averaged cross-power spectra: check for dips or spikes
 - Use of automated flagging routines: these can flag based on deviation from expected spectral behaviour (e.g. SERPent, AOFlagger, pieflag)

But... if you are planning to make image cubes then avoid excessive frequency dependant flagging which changes the *uv*-coverage across the band

Bandpass calibration

Has it gone well??



Examples of good-quality bandpass solutions for 2 antennas

- Solutions should look comparable for all antennas
- Mean amplitude ~1 across useable portion of the band
- No sharp variations in the amplitude and phase
- Variations are not dominated by noise

Bandpass calibration

Another good way to check - examine cross-power spectra of a continuum (flat spectrum) source with BP corrections

Checklist:

- \checkmark Phases are flat across the band
- ✓ Amplitude is constant across the band
- ✓ Corrected data do not have significantly increased noise
- Absolute flux level is not biased high or low



Bandpass calibration

When has your bandpass calibration gone bad?



The solutions shown are clearly bad

Problems:

- Amplitude different normalization for different antennas
- Noise levels are high, and are different for different antennas

Doppler correction

- Often now done using **Doppler Setting** and further finer corrections during post-processing and imaging
- Within one observation, Doppler Setting can correct for the Heliocentric velocity (~30 km/s), but cannot exactly correct for the ~0.5 km/s for the Earth's rotation on its axis
- Remaining corrections done in e.g. tasks clean or cover in CASA and task CVEL in AIPS (after bandpass calibration). CASA task plots can correct on-the-flv (less accuratelv).



Continuum subtraction

As well as lines, spectral-line data often contains continuum sources (either from the target or from nearby sources in the field)

- This emission complicates the detection and analysis of line data
- Continuum emission limits the achievable spectral dynamic range



Spectral line cube with two continuum sources (structure independent of frequency) and one spectral line source near the field centre Roelfsma(1989)



Continuum subtraction

Method:

- 1. Examine the data
- 2. Assess which channels appear to be line-free
- 3. Use line-free channels to estimate the continuum level
- 4. Subtract the continuum
- 5. Evaluate the results



Continuum subtraction

Two methods

1. In the *uv*-plane - subtract continuum then clean line & continuum separately

- Use AIPS tasks such as UVLIN, UVLSF, UVSUB
- Use CASA tasks such as uvcontsub
- 2. In the image-plane FT data, subtract continuum from the "dirty" cube then clean both continuum & line

Use AIPS task such as IMLIN

Use CASA tasks such as imcontsub

No one single subtraction method is appropriate for all experiments!

Self-calibration

Can apply self-calibration solutions to improve quality of line data

Two cases:

- 1. Strong line emission (i.e. maser)
 - Choose a strong channel with "simple" structure
 - Self-cal that channel & apply solutions to all other channels
 - Allows imaging of weak continuum (& channels) with improved SNR
- 2. Weak line and strong continuum emission
 - Apply solutions from the continuum to individual channels
 - Allows imaging of weak lines with improved SNR

Get good positions of line features relative to continuum, but lose absolute positional information

Imaging of cubes

- Principles for continuum imaging mostly apply to line data as well (cleaning, weighting, etc.)
- But keep in mind that deconvolution of spectral line data often poses special challenges:
 - Cleaning many channels is computationally expensive (do you need the full spectral resolution or can you average?)
 - Emission *structure* changes from channel to channel (may have to change cleaning boxes for each channel)
 - If you are interested in *both* high sensitivity (to detect faint emission) and high spatial/spectral resolution (to study kinematics):
 - Robust weighting with -1<R<1 good compromise

After mapping all channels in the data set, we have a **spectral line 3D data** *cube* (RA, Dec, Vel or Freq)

To visualise the information we usually make 1-D or 2-D projections providing differing analysis methods:

- Line profiles (1-D slices along velocity axis)
- Channel maps (2-D slices along velocity axis)
- Moment maps (integration along the velocity axis)
- Position-velocity (PV) plots (slices along spatial dimension)
- Movies (2-D slices along velocity axis)

Line profiles



Channel maps

- Channel maps of ¹²CO (J=1-0) towards G305
- Steps through channels from -57 km/s to -1 km/s
- Integrates emission over 4 km/s



FIGURE 4.13: Channel map of the ¹²CO data cube beginning at -57.1 km s⁻¹ in the bottom left and proceeding to the right and returning to the left at the end of each row. The emission is integrated over 3.7 km s⁻¹ channels per image up to -1.2 km s⁻¹ in the top right.

Moment maps

$$\begin{split} I_{\text{tot}}(\alpha, \delta) &= \Delta v \sum_{i=1}^{N_{\text{chan}}} S_{\nu}(\alpha, \delta, \nu_{i}) & \text{Total intensity (moment 0)} \\ \overline{v}(\alpha, \delta) &= \frac{\sum_{i=1}^{N_{\text{chan}}} v_{i} S_{\nu}(\alpha, \delta, \nu_{i})}{\sum_{i=1}^{N_{\text{chan}}} S_{\nu}(\alpha, \delta, \nu_{i})} & \text{Intensity-weighted velocity (moment 1)} \\ \sigma_{v}(\alpha, \delta) &\equiv \sqrt{\left\langle \left(v_{i} - \overline{v}(\alpha, \delta)\right)^{2} \right\rangle} & \text{Intensity-weighted velocity dispersion} \\ &= \sqrt{\frac{\sum_{i=1}^{N_{\text{chan}}} (v_{i} - \overline{v}(\alpha, \delta))^{2} S_{\nu}(\alpha, \delta, \nu_{i})}{\sum_{i=1}^{N_{\text{chan}}} S_{\nu}(\alpha, \delta, \nu_{i})}} \end{split}$$

These maps can be made with AIPS tasks like **MOMNT**, CASA's **immoments** or Miriads **moment**

Moment maps



- Moment maps are sensitive to noise so clipping is required
- Sum only over the planes of the data cube that contain emission
- Since higher order moments depend on lower ones (so progressively noise), set a conservative intensity threshold for the 1st and 2nd moments



Position-Velocity (PV) diagrams

- PV diagrams take a slice out of a cube along a "PV cut"
- You can produce PV diagrams in CASA using task impv, or IMMOMENTS
- This PV diagram was created in kpvslice
- Try exploring the CO cubes to see if you can spot any interesting velocity structures
 - Edges of molecular clouds?



(d) South West

Star forming regions?