Chapter 13

Spectral Line Observations

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This chapter is intended as an introduction to spectral line observations at radio wavelengths. While an attempt will be made to put together most of the relevant details, it is not intended to be an exhaustive guide to spectral line observations but instead focuses more on the basics of spectral line observations, keeping in mind synthesis arrays like the Giant Meterwave Radio Telescope (GMRT).

13.1 Spectral Lines

Spectral lines originate under a variety of circumstances in Astronomy. The most ubiquitous element in the Universe, the Hydrogen atom, gives rise to the 21-cm-line ($\nu \sim$ 1420.405 MHz) due to a transition between the hyperfine levels of its ground state. If the Hydrogen atom is ionized, subsequent recombinations of electrons and protons lead to a series of recombination lines of the Hydrogen atom. It is easy to see that such transitions between higher Rydberg levels give rise to spectral lines at radio wavelengths. Transitions around Rydberg levels of 280, for e.g., give rise to recombination lines at $\nu \sim 300$ MHz. In cold (kinetic temperature ~ 100 K), and dense (~ 1000 cm^{-3}) environments Hydrogen atoms form molecules. The CO molecule which has been used as a tracer of molecular Hydrogen has a rotational transition at $\nu \sim 115$ GHz. These are a few illustrative examples.

The widths of spectral lines arise due to different mechanisms. One such is the Doppler effect. The particles in a gas have random motions corresponding to the kinetic temperature of the gas. The observed frequency of the line is thus different from the rest frequency emitted by the particles. In a collision-dominated system, the number density of particles as a function of velocity is expected to be a Maxwellian distribution. The width of this distribution will result in a corresponding broadening of the observed spectral line due to Doppler Effect. This width, arising due to the temperature of the gas, is called thermal broadening. In addition to the thermal motion of the particles, there can also be turbulent velocities associated with macroscopic gas motions. These motions are often accounted for by an effective Doppler width, which includes both thermal and turbulent broadening, assuming a gaussian distribution for the turbulent velocities also. Another mechanism which can contribute to the line width is pressure broadening. This arises due to collisions and is particularly relevant in high density environments and/or for lines arising through transitions between high Rydberg levels. In addition, there is always a natural width to the spectral line imposed by the uncertainty principle, but it is almost always overwhelmed by that due to the mechanisms mentioned earlier.

An observed spectral feature can be much wider than that expected on the basis of the above mentioned mechanisms. This is usually due to systematic motion of the gas responsible for the spectral feature like, for e.g., rotation of a gas cloud, expansion of a gas cloud, differential rotation of a galaxy, etc..

13.2 Rest Frequency and Observing Frequency

The rest frequency of a spectral line of interest can be calculated if it is not already tabulated. The apparent frequency (or, the observing frequency), however, needs to be calculated for each source since it depends on the relative velocity between the source and the observer. The observed frequency (ν_o) of a given transition is related to the rest frequency of the line (ν_l) and the radial velocity of the source w.r.t the observer (v_r) as $(\nu_l - \nu_o)=\nu_o v_r/c$, where, c is the velocity of light. This relation is valid for $v_r \ll c$, and $\theta \ll \pi/2$, where θ is the angle between the velocity vector and the radiation wave vector. The radial velocity is positive if the motion is away from the observer and the observed frequency is smaller than the rest frequency of the line. In this situation, the line is redshifted. If the velocity (v_r) is known, the observing frequency can be calculated. While dealing with extragalactic systems, one quotes the redshift rather than the radial velocity. The redshift (z) is related to the rest and observed frequencies as $z = (\nu_l - \nu_o)/\nu_o$ and approximates to v_r/c for $v_r \ll c$.

It is more useful, and common to define velocities w.r.t. the 'local standard of rest' than w.r.t. an arbitrary frame of reference. This transformation takes into account the radial velocity corrections due to the rotation of the earth about its own axis, the revolution of the earth around the Sun, and the motion of the Sun w.r.t. the local group of stars. The magnitudes of these corrections are within $\sim$ 1 km s^{-1}, 30 km s^{-1}, and 20 km s^{-1} respectively. The actual value of the total correction depends on the equatorial coordinates of the source, the ecliptic coordinates of the source, the longitude of the Sun, the hour angle of the source, and the geocentric latitude of the observer.

In principle, the apparent frequency of a spectral line from a source is always changing due to the change in the radial velocity between the source and the observer. In a given observing session during a day the source can be observed from rise to set. During this period the radial component of the velocity between the source and the earth due to the rotation of the earth can (in an extreme case) change from -0.465 to +0.465 km s^{-1}. Consider observing a narrow spectral line (width $\sim$ 0.5 km s^{-1}) from this source using a spectral resolution $\sim$ 0.1 km s^{-1}. If no extra precautions are taken, the peak of the spectral line will appear to slowly drift across the channels during the course of the day. This drift, if not accounted for, will decrease the signal-to-noise ratio of the line, and increase its observed width in the time-averaged spectrum. Depending on the circumstances, this can completely wash out the spectral line. In order to overcome this, the continuous change in the apparent frequency is to be corrected for during an observing session so that the spectral line does not drift across frequency but stays in the same channels. This process of correction is known as Doppler Tracking. I would like to emphasize that this is important if one is observing narrow lines with high spectral resolution and that there is a significant change in the sight-line component of the earth's rotation during the observing session.

13.3 Setting the Observing Frequency and the Bandwidth

Once the apparent frequency ν_o of the transition of interest is known, the Local Oscillator (LO) frequencies can be tuned to select this frequency for observations. In general, there can be more than one LO that need to be tuned. Consider the situation at the GMRT. The First LO (ν_{ILO}) can be chosen such that $\nu_{ILO} = \nu_o \pm \nu_{IF}$, where, ν_{IF} is the Intermediate Frequency (IF). The First LO can be tuned in steps of 5 MHz. The IF is 70 MHz. The IF bandwidth ($\delta\nu_{IF}$) can be chosen from one of 6, 16, and 32 MHz. Thus, the output of the first mixer will be over a frequency range of $\nu_{IF} \pm \delta\nu_{IF}/2$. The baseband LO ($\nu_{BBLO}$) can be tuned in the range of 50 to 90 MHz in steps of 100 Hz to bring the IF down to the baseband. The bandwidth of the baseband filter ($\delta\nu_{BB}$) can be chosen from 62.5 KHz to 16 MHz in steps of 2. The bands from $-\delta\nu_{BB}/2$ to 0, and from 0 to $\delta\nu_{BB}/2$, which are the lower, and the upper side bands respectively, will be processed separately. The FX Correlator at the GMRT will produce 128 spectral channels (0 – 127) covering each of these bands. The 0th channel corresponds to a frequency of $\nu_o + \nu_{BBLO} - \nu_{IF}$ and the frequency increases with channel number in the USB spectrum and decreases with channel number in the LSB spectrum.

While setting the LO frequencies one needs to make sure that (a) the desired LO frequency is in the allowed range and that the oscillator is 'locked' to a stable reference, and, (b) that the required power output is available from the oscillator. The choice of the baseband filter bandwidth depends on the velocity resolution and the velocity coverage required for a given observation. In addition, it is preferable to have as many line-free channels in the band as there are channels with the line in order to be able to obtain a good estimate of the observed baseline (or reference spectrum). One would also like to center the spectral feature within the observed band so that line-free channels on either side can be used to estimate the baseline. The velocity resolution should be at least a factor of two better than the full width at half maximum of the narrowest feature one is expecting to detect.

At present, the FX Correlator at the GMRT produces 128 channels per side band for each of the two polarizations. The two polarizations are identified as the 130 MHz and the 175 MHz channels. In principle it should be possible to drop one of the polarizations to obtain 256 channels for one polarization. This will improve the spectral resolution by a factor of 2 keeping the velocity coverage (the bandwidth) the same. This can be very useful in observing narrow lines over a wider range of velocities.

13.4 Calibration

The observed spectrum has to be corrected for the telescope response as a function of frequency across the band to obtain an estimate of the true spectrum. The telescope response is in general complex with both amplitude and phase variations across the observing band. This overall response across the band can be split into two components : (1) an overall gain (amplitude and phase) of the telescope for a reference radio frequency (RF) within the observing band, and (2) a variation of this gain across channels (the bandshape). The telescope response is thus a combination of RF gain calibration and IF bandshape calibration. This way of looking at the telescope calibration is useful since the requirements for determining these two parts of the telescope response can be different. For e.g., the IF bandshape variation is expected to be slower in time than the RF gain variation and hence need to be estimated less often. The spectral scale for the IF bandshape is however narrower compared to that of the RF gain.

13.4.1 Gain Calibration

This is usually achieved by observing a bright, unresolved source which is called a calibrator. In the case of a synthesis array like, for e.g., the GMRT, the gain calibration amounts to estimating the gains of the individual antennas in the array. The gains of any given pair of antennas reflect in the visibility (or the cross correlation) of the calibrator measured by them. In an array with N antennas, there are N(N-1)/2 independent estimates of the calibrator (an unresolved bright source) visibility at any give instant of time. However, there are only 2N unknowns, viz., N amplitudes and N phases of the N antennas. Hence, the measured visibilities can be used in a set of simultaneous equations to solve for these 2N unknowns. In practice, a calibrator close (in direction) to the source is observed for a suitable length of time using the same setup as that for the spectral line observations towards the source. A suitable number of spectral channels are averaged to improve the signal-to-noise ratio on the calibrator which is then used to estimate the gains of the antennas. Apart from the instrumental part, the gains include atmospheric offsets/contributions also. The proximity of the calibrator to the source ensures that the atmospheric offsets/contributions are similar in both observations and hence get corrected for through the 'calibration' process.

How often does one do the calibration depends on various factors, like for e.g., the observing frequency, the length of the baseline involved, the telescope characteristics, the time scale for variations in the atmospheric offsets/contributions, etc.. The frequency of calibration can vary from once in $\sim$ 10 minutes to once in an hour depending on these factors.

13.4.2 Bandshape Calibration

In this case too, a bright, unresolved source is used as a calibrator but the nearness requirement (as in the gain calibration) is not essential. On the other hand, the calibrator should not have any spectral features in the band of interest. The measured visibilities from the calibrator across the band of interest can once again (like in the earlier gain calibration) be used to estimate the antenna bandshapes. The observed spectrum from the source is divided by the bandshapes to obtain the true spectrum. The bandshape should have a signal-to-noise ratio (snr) significantly greater than that of the observed spectrum so that the snr in the corrected spectrum is not degraded. For e.g., if the bandshape and the observed spectrum have equal snr, then the corrected spectrum will have an snr which is square root of 2 worse (assuming gaussian statistics of noise). Ideally, one wouldn't want the corrected spectrum to degrade in its snr by more than $\sim$ 10%. This can be used as a criterion to judge if a given calibrator is bright enough and to decide the amount of integration time required for the source and for the calibrator.

There are two methods of bandshape calibration.

(1) Position Switching : In this method, the telescope cycles through the source and a bandshape calibrator but observing both at the same frequency and bandwidth. Depending on the accuracy to which the corrected bandshape is required, and the stability of the receiver, the frequency of bandshape calibration can vary from once in $\sim$20 minutes to once in a few hours.

(2) Frequency Switching : There are situations when position switching is not a suitable scheme to do the bandshape calibration. This can happen due to (at least) two reasons : (a) the band of interest covers the Galactic HI. In this situation, all calibrators will also have some spectral feature within this band due to the ubiquitous presence of Galactic HI. No calibrator is suitable for bandshape calibration. (b) The band is outside the Galactic HI but the source of interest is a bright unresolved source. In this case one

might end up observing any other calibrator much longer ($\sim$ 10 times) than the source in order to achieve the desired signal-to-noise ratio on the bandshape. In either of these situations position switching is not desirable. An alternative scheme is employed.

If a spectral feature covers a bandwidth of $\delta\nu$ centered at ν, quite often it is possible to find line-free regions in the bands centered at $\nu \pm \delta\nu$. The bandshapes at these adjacent frequencies can be used to calibrate the observed spectrum. This works well because the bandshape is largely decided by the narrowest band in the signal path through the telescope. This is usually decided by the baseband filter. The bandwidth of this filter is selected to be the same while observing at frequencies $\nu - \delta\nu$, ν, and $\nu + \delta\nu$. It is important to keep in mind that frequency switching works as long as $\delta\nu$ is small compared with the bandwidth of the front-end devices, and feeds. This is usually the case. For e.g., at the GMRT, the 21-cm feeds have a wide-band response, over 500 MHz. This is divided into 4 sub-bands each of 120 MHz width. If the amount by which the frequency is switched is small compared to 120 MHz this technique should work quite satisfactorily. A typical frequency switching observation would thus have an "off1", "on", and an "off2" setting. The "on" setting centers the band at the spectral feature of interest (at ν) with a bandwidth of $\delta\nu$ while the "off1" and "off2" settings will be centered at $\nu - \delta\nu$ and $\nu + \delta\nu$ respectively. The three settings will be cycled through with appropriate integration times. The average of the "off1" and "off2" bandshapes can be the effective bandshape to calibrate the "on" spectrum. In this situation, equal amounts of time are spent "off" the line and "on" the line to achieve the optimum signal-to-noise ratio in the final spectrum. However, the switching frequency itself will depend on the receiver stability, and the flatness of the corrected bandshape required. This could vary from once in $\sim$20 minutes to once in a few hours.

There are situations when one might to do both frequency and position switching. If one is observing Galactic HI absorption towards a weak continuum source, it is advantageous to obtain bandshape calibration by observing a brighter continuum source with frequency switching.

13.5 Smoothing

The cross power spectrum is obtained by measuring the correlation of signals from different antennas as a function of time offset between them. A spectrum with a bandwidth $\delta\nu$ and N channels is produced by cross correlating signals sampled at interval of τ with relative time offset in the range –Nτ to (N-1)τ, where τ = 1/(2$\delta\nu$). Because of this truncation in the offset time range amounting to a rectangular window, the resulting spectrum is equivalent to convolving the true spectrum by a Sinc function. Thus, a delta function in frequency (a narrow spectral line, for e.g.) will result in an appropriately shifted sin($N\pi\nu/\delta\nu)/(N\pi\nu/\delta\nu$) pattern, where $\delta\nu$/N is the channel separation. The full width at half maximum of the Sinc function is 1.2$\delta\nu$/N. This is the effective resolution. Any sharp edge in the spectrum will result in an oscillating function of this form. This is called the Gibbs' phenomenon. There are different smoothing functions that bring down this unwanted ringing, but at the cost of spectral resolution. One of the commonly used smoothing functions in radio astronomy is that due to Hanning weighting of the correlation function. This smoothing reduces the first sidelobe from 22% (for the Sinc function) to 2.7%. The effective resolution will be 2$\delta\nu$/N. After such a smoothing, one retains only the alternate channels. For Nyquist sampled data, the Hanning smoothing is achieved by replacing every sample by the sum of one half of its original value and one quarter the original values at the two adjacent positions.

Apart from Hanning smoothing which is required to reduce the ringing, additional smoothing of the spectra might be desirable. The basic point being that a spectral line of given width will have the best signal-to-noise ratio when observed with a spectral resolution that matches its width. This is the concept of 'matched-filtering' and is particularly important in detection experiments.

13.6 Continuum Subtraction

Quite often spectral line observations include continuum flux density present in the band. The continuum in the band can arise due to a variety of reasons. Ionized Hydrogen regions, for e.g., give rise to the radio recombination lines of Hydrogen due to bound-bound transitions and the radio continuum due to thermal bremsstrahlung. Galaxies can have strong non-thermal radio continuum as well as 21-cm-line emission and/or absorption. In addition, any absorption spectral line experiment involves a bright continuum background source. In these and similar situations, detecting a weak spectral line in the presence of strong continuum contribution can be very difficult. Depending on the complexity of the angular distribution of the continuum flux density and that of the spectral feature this task might almost become impossible.

The basic problem here is one of spectral dynamic range (SDR). The spectral dynamic range is the ratio of the weakest spectral feature that can be detected to the continuum flux density in the band. This is limited by the residual errors which arise due to a variety of reasons like, for e.g., the instrumental variations, the atmospheric gain changes, the deconvolution errors, etc.. Of these, the multiplicative errors limit the SDR depending on the continuum flux density in the band. Thus, if the multiplicative errors are at 1% level, and , if the continuum flux density in the band is 10 Jy, no spectral line detection is possible below 100 mJy. On the other hand, a continuum subtraction (if successful) will lead to a situation where the SDR is decided by the peak spectral line flux density rather than the continuum flux density. Apart from the continuum flux density any other systematics which have a constant value or a linear variation across frequency will be subtracted out in the continuum subtraction procedure. This can lead to improvements in the SDR by several orders of magnitude.

There are several methods for subtracting the continuum flux density from a spectral line data. It is beyond the scope of this lecture to discuss all of these. A brief mention will be made of one of these simpler methods to illustrate some of the principles involved. In this method, which has been called 'visibility-based subtraction', a linear fit to the visibilities as a function of frequency is performed for every sample in time. This best-fit continuum can then be subtracted from the original visibilities. The resulting data can be Fourier transformed to produce continuum-free images. This method works quite well if the continuum emission is spread over a sufficiently small field of view. This limitation can be understood in the following way. Consider a two-element interferometer separated by d. Let each of the elements of the interferometer be pointing towards θ_0 which is also the fringe tracking (phase tracking) center. The phase difference between θ_0, and an angle θ close to this, is $\phi = 2\pi\nu d(sin(\theta) - sin(\theta_0))/c$, where, ν is the observing frequency, and c is the velocity of light. For the present purpose of illustration, assume that θ is in the plane containing the pointing direction (θ_0) and d. The visibilities from a source at θ will have the form $A_\nu\cos(\phi)$ and $A_\nu\sin(\phi)$, where, A_ν is the amplitude of the source at ν. Writing $\nu = \nu_0 + \delta\nu$, and $\theta = \theta_0 + \delta\theta$, where, ν_0 is the frequency of the center of the band, it can be shown that the frequency-dependent part of the phase is $\phi_\nu = 2\pi\delta\nu d cos(\theta_0)\delta\theta/\nu_0\lambda_0$, where, $c = \nu_0\lambda_0$. It is easy to see that the variation of visibilities as a function of frequency is linear if $\phi \ll 2\pi$. This implies that $\delta\nu\delta\theta/(\nu_0\theta_{syn}) \ll 1$, where, $\theta_{syn} = \lambda_0/d$. Thus, this method of continuum subtraction works if most of the continuum is within $\nu_0/\delta\nu$ synthesized beams from the phase tracking center.

13.7 Line Profiles

If the line width is greater than the spectral resolution one can discuss the variation of the intensity of the line as a function of frequency. This description, called the line profile, can be denoted by $\phi(\nu)$. If the reason for the line width is thermal broadening or turbulent broadening, the line profile will have a gaussian profile such that $\phi(\nu) \propto e^{-(\nu-\nu_l)^2/(\delta\nu)^2}$, where ν_l is the frequency at the line center and $\delta\nu$ is the rms value of the gaussian. The width of the line refers to the full-width at half-maximum and is equal to ~ 2.35 $\delta\nu$. The observed width of the line ($\delta\nu_o$) and the true width of the line ($\delta\nu_l$) are related by $\delta\nu_o^2 = \delta\nu_l^2 + \delta\nu_r^2$, where, $\delta\nu_r$ is the width of each channel (spectral resolution). This simple relation is strictly true only when the spectral channels have a gaussian response. In addition, this is relevant if the widths of the spectral line and the spectral channel are comparable.

Pressure broadened lines show Voigt profiles. This will have a Doppler (gaussian) profile in the center of the line whereas the wings are dominated by the Lorentz profile. Obviously an analysis of the line profile is crucial in understanding the physical conditions of the system producing the spectral line.

Acknowledgments: I would like to thank A.A. Deshpande for a critical reading of the manuscript and for useful comments to improve its clarity.

13.8 Further Reading

1. Cornwell, T. C. et al., 1992, A&A, 258, 583.

2. Harris, 1978, Proc. IEEE, 66, 51.

3. Lang, K. R. “Astrophysical formulae : a compendium for the physicist and astrophysicist”, Springer-Verlag, Berlin.

4. R. A. Perley, F. R. Schwab, & A. H. Bridle, eds., ‘Synthesis Imaging in Radio Astronomy’, ASP Conf. Series, vol. 6.

5. Rybicki, G. B. & Lightman, A. P., “Radiative Process in Astrophysics”, John Wiley, New York.

6. Thompson, R. A., Moran, J. M. & Swenson, G. W. Jr., ‘Interferometry & Synthesis in Radio Astronomy’, Wiley Interscience, 1986.