CALIBRATING THE INTENSITY AND SHAPE OF SPECTRAL LINES

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Contents

Here we discuss the techniques for recovering the spectral line shape from your data. There are two ways to do this; you can ruin your results by using the wrong one because you introduce too much noise. Accordingly, we provide a brief discussion of uncertainties and how they propagate with arithmetic operations. Moreover, the equipment introduces artifacts in the reduced spectrum which usually consist of slopes and curvature; we tell how to least-squares fit the "baseline" to remove these artifacts.

1. FIGURE 1

Let's take some time to analyze Figure 1.

1.1. The Top Panel

The top panel shows the *actual* system temperature $T_{sys}(\nu)$ over a fairly wide bandwidth for two conditions, one with the noise diode on ("cal on") and one with cal off. The cal adds 20 K to the system temperature.

The top panel shows noise on the spectrum. In fact, of course, the system temperature itself has no noise on it; it's our *measurement* procedure that *introduces* the noise. As we discuss elsewhere, the r.m.s. noise in the system temperature for each channel ΔT_{sys} is approximately

$$\Delta T_{sys} = \frac{T_{sys}}{\sqrt{\Delta\nu\tau}} \tag{1}$$

where $\Delta\nu$ is the frequency width of each channel and τ is the integration time. The product $\Delta\nu\tau$ is known as the time-bandwidth product. Note that the noise decreases as $\frac{1}{\sqrt{\tau}}$. The noise level on the top panel of Figure 1 is what a perfect system would achieve with a time-bandwidth product of about 1000. For the HI line's typical frequency resolution of 5 kHz, that's $\tau = 0.2$ sec.

The *system temperature* $T_{sys}(\nu)$ is a measure of the total power of the system. There are two types of system temperature. One is independent of frequency, and is usually called *continuum*, meaning that there is no structure with frequency. The other is frequency-dependent, and because the spectral line is probably the dominant contributor this is usually called *line*. So we have

1. *Continuum contributions.* For these there is no frequency dependence, so so we drop the parenthetical (ν) and write, for example, T_{rcvr} instead of $T_{rcvr}(\nu)$. Contributors include
   (a) The *receiver temperature* T_{rcvr}. This is the portion contributed by the electronics. In a well-designed system all of this noise comes from the first amplifier in the chain, the one that is connected directly to the antenna. For the case of Figure 1, $T_{rcvr} \sim 70$ K. s
   (b) The *continuum antenna temperature* $T_{ant,cont}$, which comes primarily from synchrotron radiation in the Galaxy. Galactic ionized gas and the Earth's atmosphere contribute to what is usually a much smaller extent. For typical positions in the sky, this amounts to about 10 K.
   (c) For the case of Figure 1, $(T_{rcvr} + T_{ant,cont}) = 80$ K. This is reflected in the top panel.
   (d) The *cal temperature* T_{cal}, which is noise generated by a noise diode. We switch this on and off to calibrate the intensity scale. Because this adds to the system temperature, and thus ΔT_{sys}, we want to obtain our data with the cal turned off. Figure 1, $T_{cal} = 20$ K. This is reflected in the top panel.

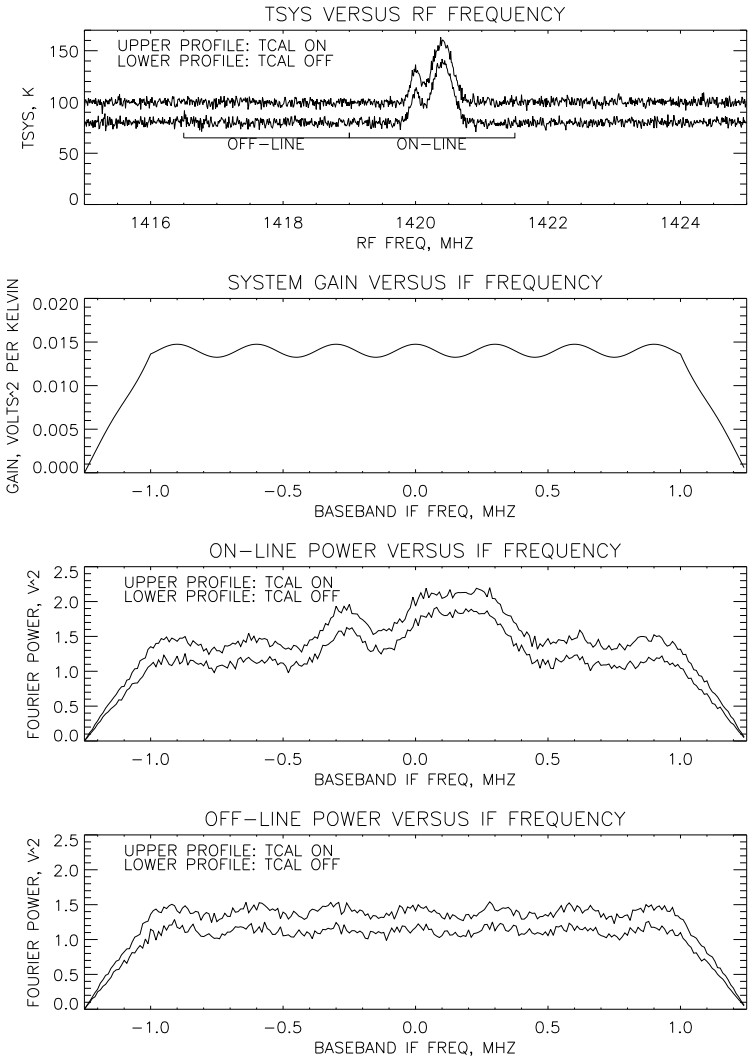

Fig. 1.— An HI line profile and its system contaminates, which must be removed by calibration.

2. *Spectral line contributions.* For our work, this is the HI line, so we have as the sole contributor

   (a) The *spectral antenna temperature* $T_{ant,HI}(\nu)$, which maxes out at perhaps 30 K for the 21-cm line as seen with our broad-beam horn.

The total system temperature is the sum. Thus, when the cal is off, we have

$$T_{sys}(\nu) = T_{rcvr} + T_{ant,cont} + T_{ant,HI}(\nu) = T_{sys} + T_{ant,HI}(\nu) \tag{2a}$$

The totality of the frequency independent portion, $T_{rcvr} + T_{ant,cont}$ is usually referred to as the *system temperature* T_{sys}[1]. When the cal is on we have

$$T_{sys}(\nu) = T_{rcvr} + T_{ant,cont} + T_{cal} + T_{ant,HI}(\nu) = T_{sys} + T_{cal} + T_{ant,HI}(\nu) \tag{2b}$$

The top panel shows these two conditions, cal on and cal off. It also shows the nonzero system temperature off of the line; the line adds to what's already there in the continuum. The only way to know how much the line contributes to $T_{sys}(\nu)$ is to observe a large enough bandwidth so that you are sure that the line has dropped to zero. Sometimes "being sure" is not so easy (see §4).

1.2. The Second Panel

The total system power, which consists not only of T_{ant} but also T_{rcvr}, goes through our receiver system, which consists of amplifiers, mixers, filters, and cables connecting them all. The system spoils the signal because the system has a frequency dependent gain. This gain multiplies the system temperature. The second panel shows this gain versus IF frequency.

1.2.1. The frequency dependence of gain occurs at IF

The second panel exhibits a typical frequency-dependent gain $G(\nu)$. This requires a bit of explanation. We make the assumption that we can split the gain into two components, one being before the first mixer [and thus at RF: $G_{RF}(\nu)$] and one after [and thus at IF: $G_{IF}(\nu)$]. We assume that the gain *before* the first mixer has *no* frequency dependence, so that $G_{RF}(\nu) = G_{RF}$. We assume that *only* the components *after* the first mixer exhibit frequency dependence. This assumption allows us to write

[1]Strictly speaking, the system is the sum of *all* contributions, even including $T_{ant,HI}$, and is thus frequency dependent.

$$G(\nu) = G_{RF} \cdot G_{IF}(\nu) \tag{3}$$

Again, we emphasize the fact that we assume $G(\nu)$ depends *only on the IF frequency* and is is *independent of RF frequency*. This means that, in the power spectrum we derive using the FFT, $G(\nu)$ is a function of the frequency index j; and, additionally, $G(\nu)$ does *not* depend on the LO frequency. In radio astronomy jargon, j is called the *channel number*.

Our assumption means that we can write G_j in place of $G(\nu)$, and G_j completely specifies the gain no matter what the LO frequency is. The channel number refers explicitly to the IF frequency, not the RF frequency, because it is computed from the baseband signal. In the example of Figure 1, the IF frequency runs from –1.25 to +1.25 MHz and j runs from, we shall say, 0 to $2J - 1$; the total number of channels is $2J$.

Realizing that j refers to IF frequency, and that the gain $G(\nu)$ depends only on IF and not on RF frequency, we can define for the gain

$$G_j \equiv G(\nu) \tag{4}$$

1.2.2. The contributors to G_j

There are two primary contributors to the gain G_j. The most important is the overall shape, which is determined by the base-band filter; in our case this is a smooth low-pass filter having a gradual falloff at the upper edge; filters in many radioastronomical systems are *much* less benign (with shapes that are anything but smooth).

Less prominent, but nevertheless important, is wiggles caused by other effects. Here we show sinusoidal wiggles, which are produced by imperfect VSWR's produced by impedance mismatch of the various system components. Sometimes there are additional artifacts produced by God-knows-what.

1.3. The third and fourth panels

We can also use the subscript j for the measured power $P(\nu)$, but here we must realize that the ν in $P(\nu)$ refers to RF frequency. The RF frequency, in turn, depends on the LO frequency, so we need an additional specification for the central RF frequency. Here we use the superscripts $OFFLINE$ and $ONLINE$, so we write

$$P_j^{OFFLINE} \equiv P(\nu)\ for\ offline\ spectrum \tag{5}$$

$$P_j^{ONLINE} \equiv P(\nu)\ for\ online\ spectrum \tag{6}$$

See Figure 1 for the offline and online spectra.

The system gain G_j multiplies the system temperature, so the measured output spectrum P_j is just

$$P_j = G_j T_{sys}(\nu) \tag{7}$$

Panels three and four show P_j for the 2.5 MHz bandwidth segments centered on the line (the $ONLINE$ spectrum) and off the line. If there were no noise, the $OFFLINE$ spectrum would have exactly the same shape as the second panel because it multiplies the frequency-independent system temperature T_{sys}:

$$P_j^{OFFLINE} = G_j T_{sys} \tag{8}$$

2. FIGURE 2: OBTAINING THE CALIBRATED SPECTRUM $T_{sys}(\nu)$ FROM THE MEASUREMENTS

Our goal is to obtain $T_{ant,HI}(\nu)$. To this end we obtain three measurements:

1. The ONLINE, CALOFF measurement, which gives the instrumental response times the HI line

$$P_j^{ONLINE,CALOFF} = G_j(T_{sys} + T_{ant,HI}(\nu)) \ ; \tag{9a}$$

2. The OFFLINE, CALOFF measurement, which gives the instrumental response by itself

$$P_j^{OFFLINE,CALOFF} = G_j(T_{sys}) \ ; \tag{9b}$$

3. The OFFLINE, CALON measurement, which gives us our intensity calibration. T_{cal} is our ultimate intensity calibration: it is the only known temperature in this set of measurements.

$$P_j^{OFFLINE,CALON} = G_j(T_{sys} + T_{cal}) \ . \tag{9c}$$

We need to manipulate these measurements to calculate the best estimate of our desired quantity $T_{ant,HI}(\nu)$. There are two ways to obtain this calibrated spectrum. One is straightforward and not so good; the other is less straightforward and much better.

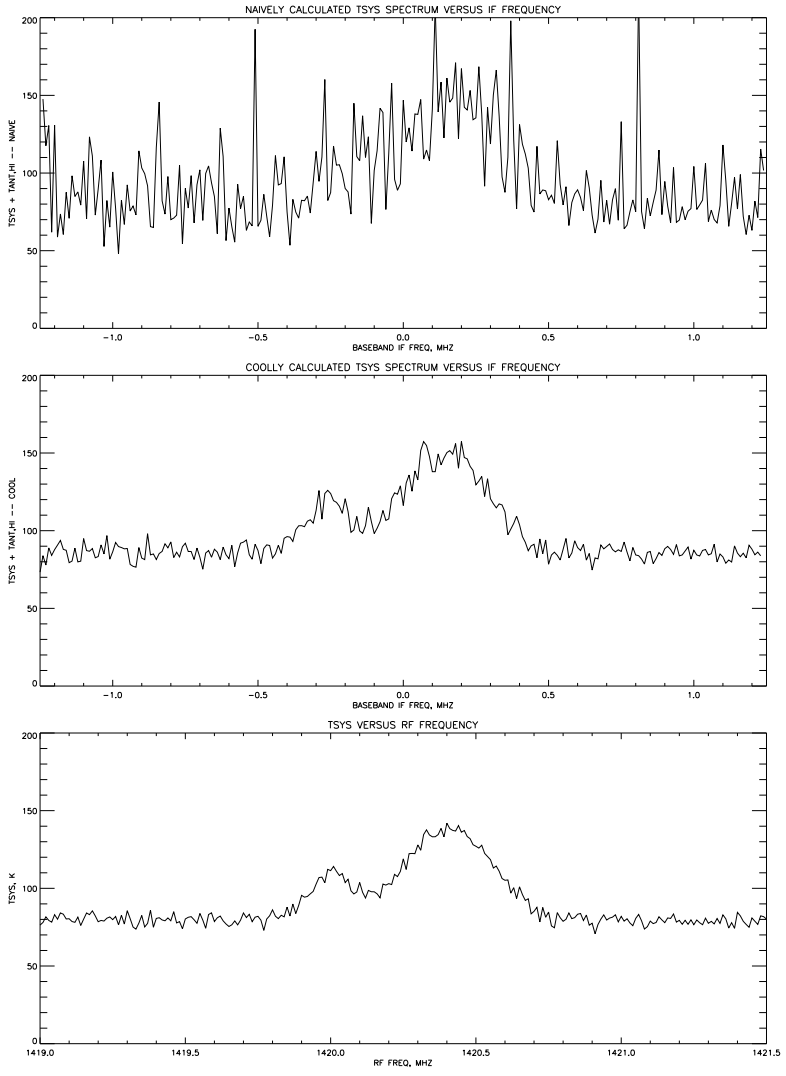

Fig. 2.— Top two panels: two different reduction techniques: naïve and cool. Bottom panel: the ON-LINE spectrum from the top panel of figure 1

2.1. The näive method

With this method, we use the cal in a very straightforward way. First, we use equations 9b and 9c, with $CALON$ and $CALOFF$, and take the difference to give

$$P_j^{OFFLINE,CALON} - P_j^{OFFLINE,CALOFF} = G_j T_{cal} \tag{10a}$$

(Actually, the $CALON - CALOFF$ spectra can be done either $ONLINE$ or $OFFLINE$; all temperatures but T_{cal} drop out in the difference). This equation provides G_j on a channel-by-channel basis:

$$G_j = \frac{P_j^{OFFLINE,CALON} - P_j^{OFFLINE,CALOFF}}{T_{cal}} \tag{10b}$$

Knowing G_j, we can apply it to the $ONLINE, CALOFF$ spectrum in equation 9a. Making this substitution, we obtain

$$T_{sys} + T_{ant,HI}(\nu) = \left[\frac{P_j^{ONLINE,CALOFF}}{P_j^{OFFLINE,CALON} - P_j^{OFFLINE,CALOFF}}\right][T_{cal}] \tag{11}$$

We show this result in the upper panel of Figure 2. We see the line, but it's very *noisy*. That is, there is a lot of channel-to-channel noise. This occurs because the gain of each channel is determined individually and independently.

2.2. The cool method

The cool method very much reduces the channel-to-channel noise by being clever in the determination of the channel gains. Let's begin by doing some elementary rewriting of equations 9. First rewrite equation 9a to explicitly provide our desired quantity $T_{sys} + T_{ant,HI}(\nu)$,

$$T_{sys} + T_{ant,HI}(\nu) = \frac{P_j^{ONLINE,CALOFF}}{G_j} \ . \tag{12a}$$

From this equation it is clear that if we know G_j we know $T_{sys} + T_{ant,HI}(\nu)$. Now rewrite equation 9b to explicitly give G_j

$$G_j = \frac{P_j^{OFF-LINE}}{T_{sys}} \tag{12b}$$

From these two equations it is clear that if we know the constant T_{sys}, we know G_j. This might seem like a tautology, but it's not. Even if we don't know T_{sys}, $P_j^{OFF-LINE}$ tells us the *shape* of G_j—and $P_j^{OFF-LINE}$ has little noise. All we lack is the multiplicative constant T_{sys}, which is a constant, independent of frequency. To be explicit, combine equations 12a and 12b and eliminate G_j, which gives

$$T_{sys} + T_{ant,HI}(\nu) = \underbrace{\left[\frac{P_j^{ONLINE,CALOFF}}{P_j^{OFFLINE,CALOFF}}\right]}_{the shape} \cdot \underbrace{T_{sys}}_{scaling factor} \tag{13}$$

It remains to determine T_{sys} so we can get not only the shape, but the proper "vertical scale".

We get T_{sys} from the cal as follows. First, on a channel-by-channel basis we would have (by combining equations 9b and 9c)

$$T_{sys,j} = \frac{P_j^{OFFLINE,CALOFF}}{P_j^{OFFLINE,CALON} - P_j^{OFFLINE,CALOFF}} T_{cal} \tag{14}$$

This gives us $2J$ different values for T_{sys}. Now realize that T_{sys} is independent of frequency (by assumption; in practice, this assumption is usually very good). With this, we can use the full bandwidth in both the numerator and denominator,

$$T_{sys} = \frac{\sum_{j=0}^{j=2J-1} P_j^{OFFLINE,CALOFF}}{\sum_{j=0}^{j=2J-1} \left(P_j^{OFFLINE,CALON} - P_j^{OFFLINE,CALOFF}\right)} T_{cal} \ , \tag{15}$$

and we insert this *single* number into equation 13. That is, we can write (in direct comparison to equation 11)

$$T_{sys} + T_{ant,HI}(\nu) = \underbrace{\left[\frac{P_j^{ONLINE,CALOFF}}{P_j^{OFFLINE,CALOFF}}\right]}_{the shape} \underbrace{\left[\frac{\sum_{j=0}^{j=2J-1} P_j^{OFFLINE,CALOFF}}{\sum_{j=0}^{j=2J-1} \left(P_j^{OFFLINE,CALON} - P_j^{OFFLINE,CALOFF}\right)}\right] T_{cal}}_{T_{sys}: a\ constant,\ inpdendent\ of\ j} \tag{16}$$

We show this result in the middle panel of Figure 2. Note the much smaller noise!

2.3. Why so cool?

Why is the cool method so cool? Because there's less noise! The reason is clear when we compare the ratios of the various P_j combinations between equations 11 and 16: everything is the same in these equations except that, in the cool method, we average $\frac{P_j^{OFFLINE,CALOFF}}{P_j^{OFFLINE,CALON}-P_j^{OFFLINE,CALOFF}}$ over channels (j). This quantity has lots of channel-to-channel noise because the denominator contains a difference between two measured spectra; by replacing its channel-by-channel noise fluctuations with the channel-independent average, we get rid of this channel-to-channel noise component.

You can look at it another way: the *shape* is given by the lower-noise ratio $\left[\frac{P_j^{ONLINE,CALOFF}}{P_j^{OFFLINE,CALOFF}}\right]$; the *scaling* is given by T_{sys}, which in turn depends on T_{cal}. In contrast, for the näive method, both the shape and the scaling are given by $T_{sys,j}$.

There is more, though. We have implicitly assumed that the integration times for $CALOFF$ and $CALON$ spectra are identical. But we don't want to spend ("waste") any more time than needed on calibrating the intensity scale. This means we'd like to spend only a short time on the $CALON$ spectrum, meaning that it will have increased noise. This, in turn, will increase the noise in $P_j^{CALON} - P_j^{CALOFF}$ compared to what it would be if we had equal time. This would make the näive method *even worse* than the top panel of Figure 2.

2.4. If it's so cool, why...

Look at the bottom panel of Figure 2. This is the original spectrum from the top panel of Figure 1. And it has less noise than the cool method! If the cool method is so cool, why can't it recover the original smaller noise level?

The answer lies in the necessity to remove the effects of G_j. This, in turn, requires combining $P_j^{ONLINE,CALOFF}$, which is the ON-LINE spectrum from the top panel of Figure 1, with the OFF-LINE spectrum from that same panel. Each has noise, and both noises contribute to the final result.

3. ERROR PROPAGATION

This leads us to consider the way in uncertainty (or error, or noise), propagates when we arithmetically combine quanties. This is treated in books on statistics. Probably the best introductory text is Taylor's *An Introduction to Error Analysis*. In chapter three he discusses this propagation.

The basic rule is expressed in his equation 3.47. Suppose the quantity q is a function of x and y, and the errors in x and y are δx and δy. Then the error in q is just

$$\delta q^2 = \left(\frac{\partial q}{\partial x}\delta x\right)^2 + \left(\frac{\partial q}{\partial y}\delta y\right)^2 \tag{17}$$

One important thing to notice is that the errors add *quadratically*. Another important thing to notice is the two most common special cases:

1. For sums and differences, we have

$$q = (x + y) \quad \text{OR} \quad q = (x - y) \tag{18a}$$

$$\delta q^2 = \delta x^2 + \delta y^2 \tag{18b}$$

   So the errors add quadratically, which makes sense.

2. For products and ratios, we have

$$q = xy \quad \text{OR} \quad q = \frac{x}{y} \tag{19a}$$

$$\left(\frac{\delta q}{q}\right)^2 = \left(\frac{\delta x}{x}\right)^2 + \left(\frac{\delta y}{y}\right)^2 \tag{19b}$$

The generatlization to more variables than just x and y should be obvious. Let's apply these rules to our situation:

3.1. Application of equation 18b for *averages*

When we take a long integration and combine many spectra, we are taking the sum of N spectra, each with its independent error, and dividing by N to get the average. Suppose each spectrum has the same error ΔT_{sys} (by "same", we mean *statistically* the same, not *identically* the same!). From equation 18b, the error in the *sum* is just

$$(error\ in\ sum)^2 = \left[\sum_0^{N-1} (\Delta T_{sys,n})^2\right] = N(\Delta T_{sys})^2 \tag{20a}$$

The average is the sum divided by N, the square of the average is the square of the sum divided by N^2. Similarly, the error in the *average* is just that in the sum divided by N^2, i.e.

$$(error\ in\ average)^2 = \frac{(\Delta T_{sys})^2}{N} \tag{20b}$$

or

$$(error\ in\ average) = \frac{error\ in\ each\ measurement}{\sqrt{N}} \tag{20c}$$

This illustrates the famous, and almost general, rule that the noise decreases as the square root of the number of times that a measurement is repeated. "The noise decreases as root N". In our case this rule is fulfilled by the noise decreasing as $\frac{1}{\sqrt{\tau}}$.

3.2. Application of equation 19a for the cool method

Let's again write equation 13, but for brevity replace $T_{sys} + T_{ant,HI}(\nu)$ by $T_{sys}(\nu)$, where we incorporate the frequency-independent T_{sys} and frequency-dependent $T_{ant,HI}(\nu)$ into a single frequency-dependent system temperature $T_{sys}(\nu)$:

$$T_{sys}(\nu) = \underbrace{\left[\frac{P_j^{ONLINE,CALOFF}}{P_j^{OFFLINE,CALOFF}}\right]}_{the shape} \cdot \underbrace{T_{sys}}_{scaling factor} \tag{21}$$

If we apply equation 19b, we get

$$\delta T_{sys}(\nu)^2 = \left[\left(\frac{\delta P_j^{ONLINE,CALOFF}}{P_j^{ONLINE,CALOFF}}\right)^2 + \left(\frac{\delta P_j^{OFFLINE,CALOFF}}{P_j^{OFFLINE,CALOFF}}\right)^2\right] T_{sys}^2 \tag{22}$$

But the statistical properties of $P_j^{ONLINE,CALOFF}$ and $P_j^{OFFLINE,CALOFF}$ are the same, so we find that

$$\delta T_{sys}(\nu)^2 = 2\left(\frac{\delta P_j^{ONLINE,CALOFF}}{P_j^{ONLINE,CALOFF}}\right)^2 T_{sys}^2 \tag{23}$$

In words: combining the two spectra $P_j^{ONLINE,CALOFF}$ and $P_j^{OFFLINE,CALOFF}$, which have identical noise from the statistical standpoint, increases the noise $\delta T_{sys}(\nu)^2$ by 2, or the noise in $T_{sys}(\nu)$ by $\sqrt{2}$. If you look carefully at the bottom two panels of Figure 1, you will find that this is the only difference.

There is no way around the introduction of this noise unless you can generate a noise-free spectrum of G_j. In practice, nobody can do this.

This brings up the question: because we have to measure both $P_j^{ONLINE,CALOFF}$ and $P_j^{OFFLINE,CALOFF}$ and combine them, what is the optimum ratio of time to spend on each? In particular, doesn't it make sense to spend more time measuring the $ONLINE$ than the $OFFLINE$ spectrum? After all, that's where the signal is!

The somewhat surprising answer: given a fixed total integration time, the best result is obtained by spending *equal time*. From the discussion in this section, you know enough to prove this simple truth; the proof is straightforward.

4. FIGURE 3: REAL LIFE

In reality, the result from equation 16 is imperfect because it contains additional artifacts. These occur because our assumptions are not completely correct. Specifically, G_{RF} is not *exactly* independent of frequency; neither is T_{rcvr}. The most obvious result of these is to make the spectrum have a non-flat "baseline"; the baseline is the part of the spectrum outside the line. In other words, if there were no line, the spectrum would not be flat. The top panel in Figure 3 shows a typical "baseline problem".

These baseline problems plague spectral line observers and there is no bulletproof solution. Accordingly, one fits an empirical smooth curve to the baseline (the off-line portions of the $ONLINE$ spectrum). One usually does this with a polynomial least squares fit[2]. The dashed line in the top panel of Figure 3 shows this fit; the bottom panel shows the result minus the fit, in which the curvy baseline is removed.

This fixed-up profile looks good. The baseline fit automatically subtracts out the system temperature, so we are left with the a 21-cm line profile coming from a zero baseline.

However, this procedure camouflages possible discoveries! For example, in the top panel of Figure 3 the whole spectrum is displaced upwards relative to the ideal one in the bottom panel of Figure 2. Is this upward displacement an artifact, *or it is it real?* It could be that our line sits on top of a very broad, weak line whose emission is removed by the baseline-fitting procedure! But the baseline fit subtracts out all this, making the implicit assumption that it's an artifact.

[2]Use either my *polyfit* or IDL's *poly_fit*.

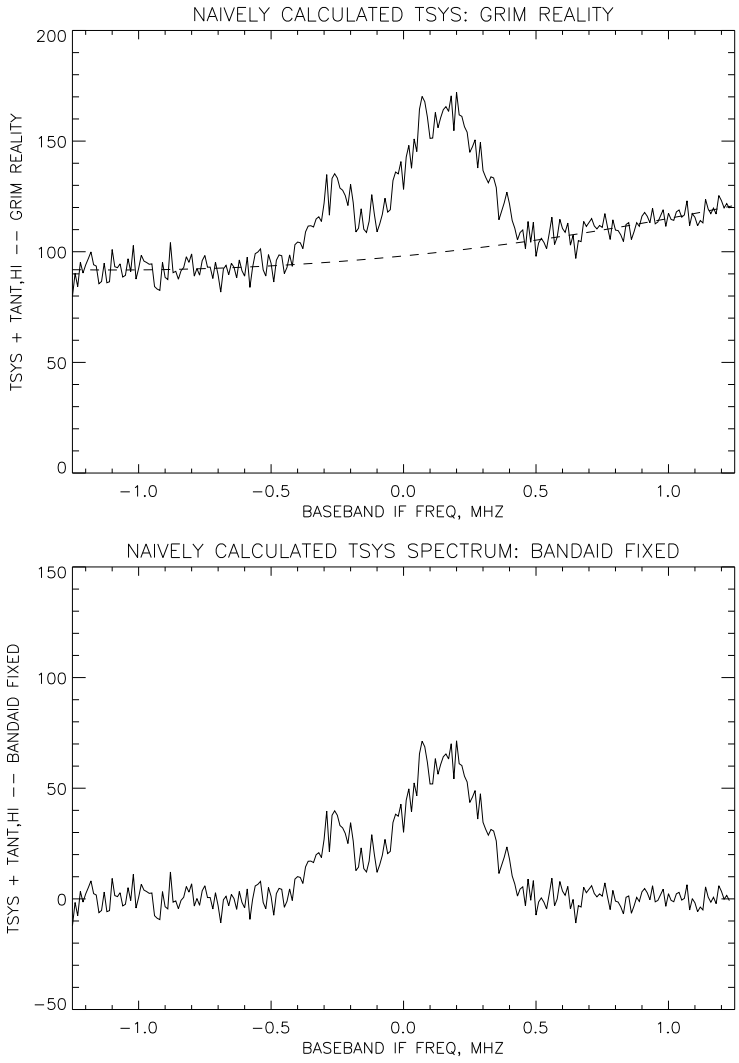

Fig. 3.— The grim reality in spectral line measurements. Departures from our ideal assumptions produce curved, displaced baselines, shown in the top panel. Fitting a polynomial baseline with least squares and subtracting it produces the apparently perfect spectrum im the botom panel.