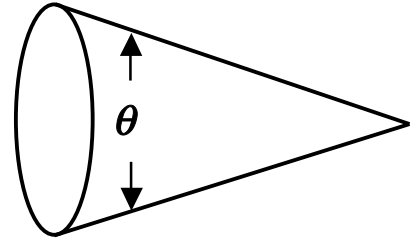


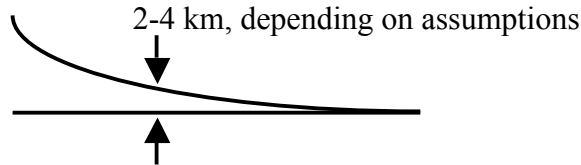
11. Atmospheres and Instruments

Preliminaries

1. Diffraction limit: The diffraction limit on spatial resolution, θ , in radians $= 1.22\lambda/d$, where d is the diameter of the telescope and λ is the wavelength (λ and d are in the same units).



2. Limb advantage:



3. Rough rule of thumb: Spectroscopic information on vertical profiles (*e.g.*, from nadir sounding), as opposed to geometrical information, is limited to ~ 1 atmospheric scale height.

4. Spectral resolution helps in selectivity (another old rule of thumb says that the resolution should be matched to the line width, but I think that more is better), S/N, and a *little bit* in altitude distribution for limb measurements.

- Microwave and IR lines are seldom fully-resolved, except where it doesn't make much difference.

5. The Sampling Theorem

Any waveform that is a sinusoidal function of time or distance can be sampled unambiguously (that is, there is *no* loss of information) with a sampling frequency ≥ 2 times the period of oscillation. Thus, sampling at a certain temporal or spatial frequency will fully sample all frequencies that are ≤ 0.5 times that frequency. Higher frequencies will be *aliased*.

Any spectrum is normally measured in a fashion that limits the ultimate spectral resolution – whether by limitations in the optics (especially the grating or prism) in a spectrograph, the frequency of spatial sampling in a Fourier transform spectrometer (*FTS*, more later), or in sampling and binning in a heterodyne instrument. The sampling theorem states that if a signal (*e.g.*, that will trace out a spectrum or its Fourier transform) is *band-limited*, in the sense that there is a high-frequency cutoff, ω_{\max} , to the information that is detected spatially (in the case of an array detector instrument) or temporally (in the case of a scanned spectrometer or an *FTS*) then, if the spectrum is sampled to twice that frequency, $2\omega_{\max}$, the spectrum is fully and rigorously determined. It may then be re-sampled on another spectral grid, or interpolated to give a smoother display with no loss (or gain, in the case of interpolation) of information. It helps to think

of this as the number of sines and cosines in a series required to expand an arbitrary signal. The factor of two is explained by needing both sines and cosines.

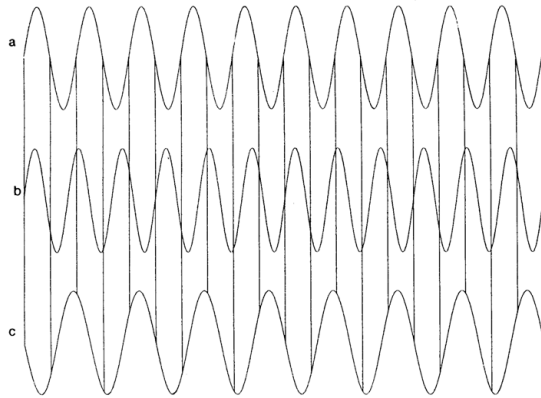


Fig. 2.3. (a) A sine wave sampled at exactly twice its frequency. (b) A higher-frequency wave sampled at the same frequency as in (a). (c) A sine wave of lower frequency than the wave in (a) and sampled at the same frequency. Note that the sampling amplitudes in (b) and (c) are identical.

Griffiths and De Haseth, *Fourier Transform Infrared Spectroscopy*

If a spectrum is properly sampled, it is *Nyquist* sampled. If it is not it is undersampled, with potential dire consequences for understanding the information that is apparently in the spectrum due to *aliasing* of frequencies. **Aside:** The need to fully sample applies to spatial measurements (*e.g.*, astronomical or other images) as well. This is why funny, wavy patterns sometimes occur when a person on television is wearing a pattern of stripes or checks that is not Nyquist sampled at the scanning resolution. It is why stagecoach wheels appear to turn backwards in the movies (the canonical example of aliasing). It is also why digital music must be filtered to reduce frequency content, in comparison with tape, vinyl, or wax.

Microwave (μw) and millimeter-wave instruments

Notable examples:

Ground-based CIO measurements from Antarctica

Microwave limb sounder (balloon, UARS, EOS Aura)

- High resolution advantage
- long $\lambda \Rightarrow$ aerosol effects small
- Emission \Rightarrow diurnal variation, global measurements
- “May select temperature-independent lines.” (But watch out, this claim works in most regions where discrete lines are measured; you know how to test for this.)
- (In limb) Pressure height is determined from the measurements themselves. This is important since emission pointing is tough. It is hard to do it directly to better than ~ 1 km on the limb from satellites (better from balloons with sophisticated mechanical pointing).

How are measurements done?

Telescope \equiv *antenna*

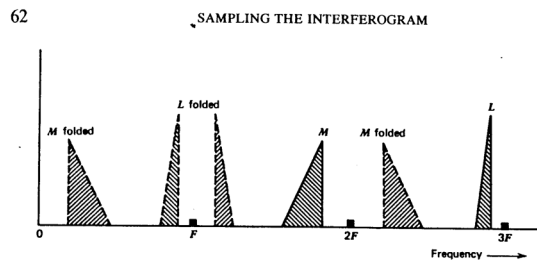
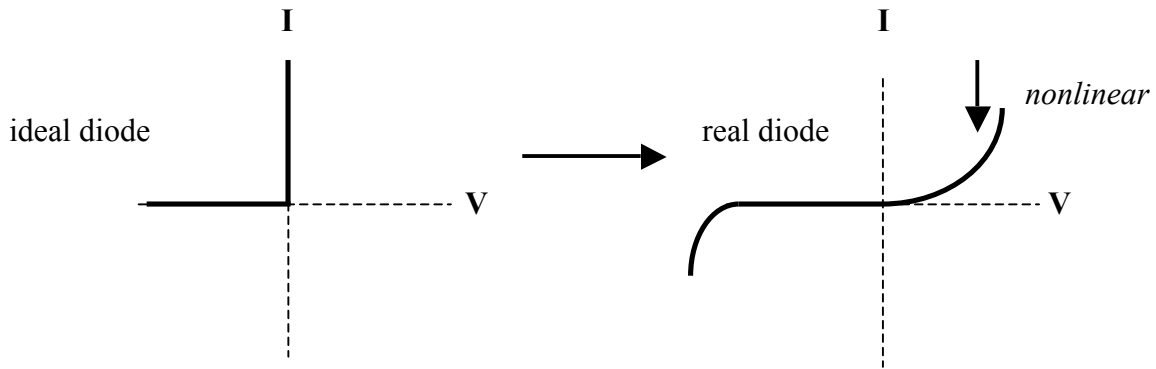


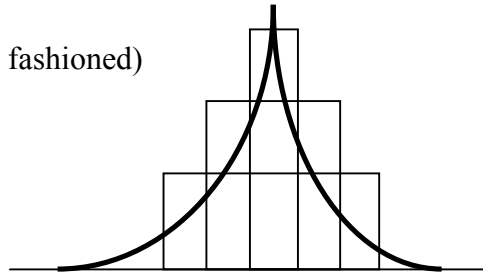
Fig. 2.5. Regions of folding: Two spectral features L and M having frequencies greater than F , the maximum allowable frequency under the sampling conditions, are computed to occur at frequencies less than F . (Reproduced from [3], by permission of Marcel Dekker, Inc.; Copyright © 1972.)

Detector \equiv *mixer*, usually a diode of some sort:



Nonlinear mixing of ω_1 (the *local oscillator*, LO) and ω_2 (our signal) to give $\omega_1 + \omega_2$, $\omega_1 - \omega_2$ (what we want), ... LO in frequency range of interest gives \pm *sidebands* – “heterodyne down-conversion.”

Then we sample: Here with a *filter bank* (old fashioned) or with an *auto-correlator* (modern).



In general, higher frequencies give greater emission: $BB + S(\sigma) \Rightarrow \sigma^3$ advantage in peak emission. (See why? look at Rayleigh-Jeans limit and the definition of line intensity.) Hence the general desire in atmospheric and astronomical measurements to develop higher frequency measurements.

Also, note the selectivity with these measurements.

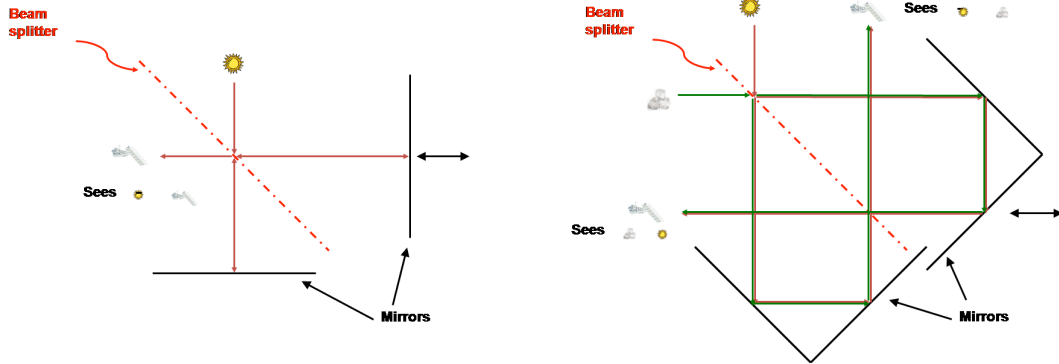
600 GHz is a common upper limit (HCl but not HF)

1.8 THz is lowest atmospheric OH line (now measured by Aura MLS); 2.5 and 3.5 THz are even better (Aura MLS and FIRS-2); note that low frequency OH hyperfine transitions constitute the commonly observed astronomical masers.

Aura MLS target gases: H₂O, O₃, ClO, BrO, HCl (600 GHz), HO₂, HNO₃, OH

Michelson interferometer or Fourier Transform Spectrometer (FTS)

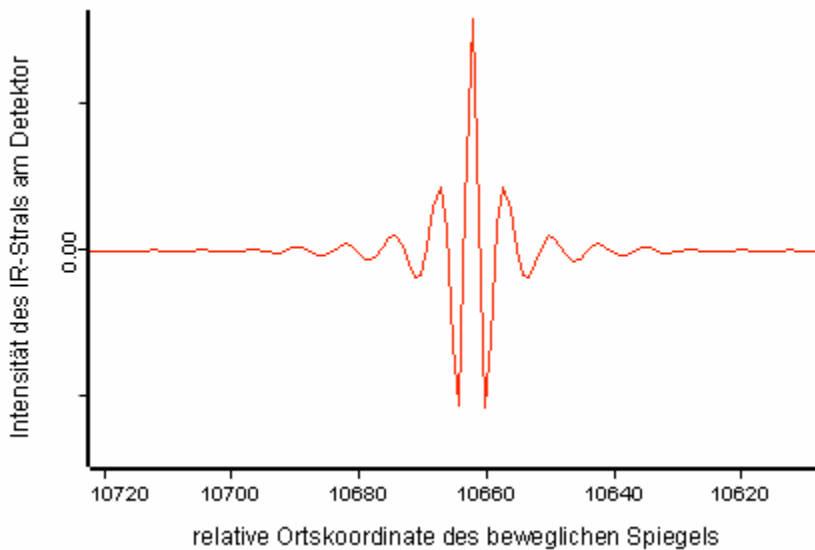
Sketches of instrument variants (single-beam and double-beam/normal or polarization) and an extremely simple interferogram



As the mirror is moved, $I = \frac{I_0}{4} \left(1 + \cos \frac{2\pi\delta}{\lambda}\right)$, δ = twice the mirror movement.

Then, Fourier transform the interferogram, to get a spectrum with a *sinc function* line shape, $\text{sinc}(x) = \sin x / x$, with resolution $1/4L$, where L is the total mirror movement.

Usually scan at constant velocity and sample on fringes from a (mostly HeNe) laser.



Note the symmetry:

The interferogram is a series of sine/cosine functions ($4L$ of them = 2Δ of them, in units of the sampling distance; why do we need both sines and cosines?): The spectrum of a δ -function spectral line (like from a very good laser) is a sinc function, but it is not normally sampled exactly on the grid (*i.e.*, where $x = 0$). Digital transformation of an N -

point interferogram gives an N -point spectrum where each point represents the intensity of a continuous sinc function centered at that position.

Highest frequency = $N/4L$ (cm^{-1}), where there are $2N$ samples ($\pm N$).

The spectrum must be band-limited to only allow light frequencies $\leq N/4L$ (why? how?) Since the spectrum is fully-sampled (Nyquist sampled), it can be interpolated without loss of information. It may also be apodized in order to improve the looks of the spectrum. These operations normally commute, at least for the most common apodization techniques. Simple apodizing examples include Hamming (0.23, 0.54, 0.23) and the von Hann (0.25, 0.5, 0.25) smoothing. There are many other techniques. Each has a spectrum and an interferogram equivalent.

Fourier Transform infrared (FTIR) gives a vast array of molecules (but no HO_x : remember $d\mu/dr$ of OH; HO_2 vibrational transitions are also weak.) FTIR may be used in emission (at sufficiently long wavelengths, determined by the blackbody curve) and in absorption of sunlight. Limb scattering is too weak because of the $1/\lambda^4$ of Rayleigh scattering.

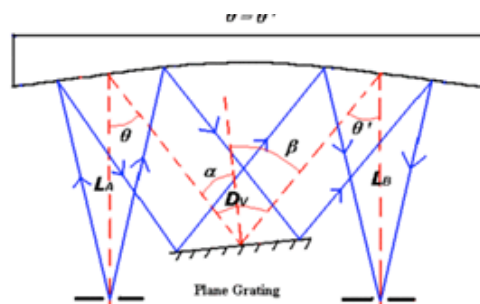
The far infrared gives HO_x (OH and HO_2 , and also the reservoir species H_2O_2). It is normally used in emission where, like the microwave, diurnal variation and global measurements are possible.

Why use an FTS instead of a dispersive instrument? (*cf.* Bell, Introductory Fourier Transform Spectroscopy)

- Bigger $a\Omega$ possible
- Better spectral resolution for its size
- Measure all frequencies at once compared to a scanning spectrometer \Rightarrow better S/N. However, a non-scanning, array-based instrument may have superior S/N.

Grating instruments

Example: A **Fastie-Ebert** [usually Ebert-Fastie] instrument consists of one large spherical mirror and one plane diffraction grating. A portion of the mirror first collimates the light which will fall upon the plane grating. A separate portion of the mirror then focuses the dispersed light from the grating into images of the entrance slit in the exit plane.



It is an inexpensive and commonly used design, but exhibits limited ability to maintain image quality off axis due to system aberrations such as spherical aberration, coma, astigmatism, and a curved focal field. (From <http://www.horiba.com/us/en/scientific/>).

The Optics of Spectroscopy: A Tutorial by J.M. Lerner and A. Thevenon

<http://www.horiba.com/us/en/scientific/products/optics-tutorial/?Ovly=1>

Spectrum of wavelengths is “time like.” Still need to Nyquist sample: higher frequency information will alias down. Example: GOME (SCIAMACHY, OMI) – Doppler shift encountered during irradiance (*i.e.*, I_0) measurements, plus temperature variation of instruments make I and I_0 have different wavelength grids \Rightarrow *undersampling*, which adds apparent noise to the spectrum. Fortunately, most of it can be eliminated by using a Fraunhofer reference spectrum to mimic the undersampling, at least in favorable parts of the spectrum.

UV/visible satellite instruments: GOME, SCIAMACHY, OMI, OMPS, SAGE-3.

Molecules: O_3 , O_2 , O_2-O_2 , NO_2 , SO_2 , H_2O , H_2CO , $C_2H_2O_2$, BrO , ClO , IO , $OCIO$

Need enough spectral resolution to

- avoid interference;
- resolve O_3 Huggins bands (T-dependence, tropospheric ozone).

Also notable:

- BUV (Singer and Wentworth, 1957)
- TOMS (especially 317.5 nm)
- BUV/SBUV

All these latter three have ~ 1 nm bandwidth, close to triangular bandpass