PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A
MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

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J. W. Brault

Phil. Trans. R. Soc. Lond. A 1982 **307**, 503-511
doi: 10.1098/rsta.1982.0125

Phil. Trans. R. Soc. Lond. A **307**, 503–511 (1982)
Printed in Great Britain

Fourier transform spectrometry in relation to other passive spectrometers

By J. W. Brault
Kitt Peak National Observatory, 950 *North Cherry Avenue*,
P.O. Box 26732, *Tucson*, *Arizona* 85726, *U.S.A.*

The relative merits of Fourier transform spectrometers and alternative passive spectrometers are explored qualitatively with emphasis on the quantity, quality, and cost of information flow. This includes a brief look at throughput, detector considerations and spectral coverage; resolution and accuracy in intensity and wavelength; and cost of construction and data reduction. Finally, the possibilities of multiple detectors and extensions of the technique to the vacuum ultraviolet by means of all-reflecting wavefront division interferometers are mentioned.

1. INTRODUCTION

What follows is intended to be a brief exploration of the relative merits of the Fourier transform spectrometer (F.t.s.) and its alternatives in different spectral regions, especially in view of recent developments in detector and instrument technology. It is by no means an impartial review, but more nearly a testament by a devoted advocate of the F.t.s. technique. The introduction of a personal point of view is not as inappropriate as it may seem in a scientific journal, for the element of style plays a larger role than we would like to admit, even in questions of instrumentation. The strangeness of observing the Fourier transform of a spectrum rather than the spectrum itself may be one of the major blocks to widespread acceptance of this technique; the fact that wavenumber rather than wavelength is the natural output scale may be another.

An evaluation of the usefulness of any tool must begin with a clear understanding of the task it is expected to perform. This simple truth is as applicable to complex scientific instruments as it is to, say, the tools of a woodworker. Let me therefore begin by defining our area of interest as passive spectrometry; that is, we expect to be given a source of light, and we wish to analyse it without being able to affect it. This immediately excludes some very interesting and powerful techniques that rightly occupy the attention of a number of other speakers at this Discussion: opto-galvanic and photo-acoustic spectrometry, laser diode absorption spectrometry, and two-photon laser spectrometry, to name a few. There is, of course, some overlap between passive and active techniques, especially in the field of gas absorption spectra; this comparison has been dealt with briefly in an article by Wijntjes (1979). But by and large, active and passive techniques are more complementary than competitive (or at least should be). Laser diodes, for example, have high power output and superb resolution, but the absolute accuracy of their wavelength scale is poor, and they are worthless as survey instruments. Excessive resolution for a given task is usually a mistake because it must be paid for in reduced signal: noise ratio or free spectral range – imagine trying to read a line of this text by observing it with a microscope.

The far infrared (including microwaves) and far ultraviolet will also be excluded from this review as being outside the expertise of the author. What remains is primarily something that can be characterized as general-purpose spectrometry, in the spectral region between 2000 Å†

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† 1Å = 10^{-10} m = 10^{-1} nm.

and 20 μm. In practice, this field is dominated by only three techniques: the grating spectrograph, the Fabry–Perot interferometer, and the Fourier transform spectrometer (F.t.s.). Of these, the grating is by far the most common, and most of the comparisons will be with this technique. Comparisons will be more qualitative than quantitative; there are excellent references available for those who wish a more detailed discussion of some of the technical issues involved. (See Guelachvili (1981), Connes (1970), Vanasse & Sakai (1967), and the references cited in those works.)

2. Comparative information flow in passive spectrometers

The job of the passive spectrometer is to gather spectral information from a source as rapidly and accurately as possible. Hence, to evaluate the three techniques we will consider in turn three aspects of information flow: the quantity of information per unit time; the quality of that information; and some vague sense of the cost of the information.

(a) *Quantity*

The magnitude of information flow through a spectrometer may be thought of as the product of two quantities, one determined by the spectrometer itself and the other by its detector:

$$\text{information flow} = (\text{optical throughput}) \times (\text{detector acceptance}).$$

The optical throughput may be defined in several equivalent ways; we shall choose here the product of the area A of the entrance aperture and the solid angle Ω subtended there by the collimator, further multiplied by the optical efficiency ϵ_0 of the system:

$$\text{optical throughput} = A\Omega\epsilon_0.$$

Because they have an axis of symmetry, the F.t.s. and Fabry–Perot have an $A\Omega$ product very roughly 10^2 greater than that of a grating instrument (a typical interferometer might accept an $f/25$ beam from a 5 mm aperture); this fact alone often justifies their use. In practice, grating instruments also show significantly lower overall efficiencies than the 0.1–0.5 attainable with interferometers. Grating efficiency is rising as ruling techniques improve, but the grating is still a poor third in throughput.

The remainder of the story, however, may be quite different. Let us for the moment combine the effects of detector quantum efficiency and noise into a useful hybrid, the effective quantum sensitivity, q, defined by:

$$q = \{(S/N)_{\text{observed}}/(S/N)_{\text{ideal}}\}^2$$

where $(S/N)_{\text{ideal}}$ is the signal:noise ratio that would result from a perfect detector (no noise, unit quantum efficiency). By using this concept, the detector acceptance may be defined as:

$$\text{detector acceptance} = (\text{quantum sensitivity}) \times (\text{number of detectors}) = qn.$$

The second factor is obvious; the first may be more usefully written as:

$$q = NQ^2/(NQ+N_{\text{d}})$$

where Q is the actual quantum efficiency of the detector, N is the number of photons per measurement interval incident on the detector, and N_{d} is the number of detected photons per measurement interval that would produce the observed detector noise. (Note that for $NQ \gg N_{\text{d}}$,

$q = Q$, but for $NQ \ll N_d$, $q = (NQ/N_d)Q$, and this 'effective quantum efficiency' depends on all three quantities (but especially strongly on the quantum efficiency, which most manufacturers of infrared detectors do not usually specify).

Now, N is proportional to the optical throughput, and also, for the F.t.s. only, to the number of spectral elements m falling on the detector (which may be in the range 10^3 to 10^6 – the so-called multiplex advantage if $NQ < N_d$). It is often true that for an F.t.s. $NQ \gg N_d$, while for a single-element scanning Fabry–Perot or grating observing the same source, $NQ \ll N_d$; in this case, although we do not speak of a multiplex advantage for the F.t.s., it might be appropriate to speak of a non-multiplex disadvantage for the other techniques! Alternatively, the single-element scanners may be forced to use detectors such as photomultiplier tubes, which show very low values of N_d but also have relatively poor quantum efficiency (0.001–0.2) and limited spectral response.

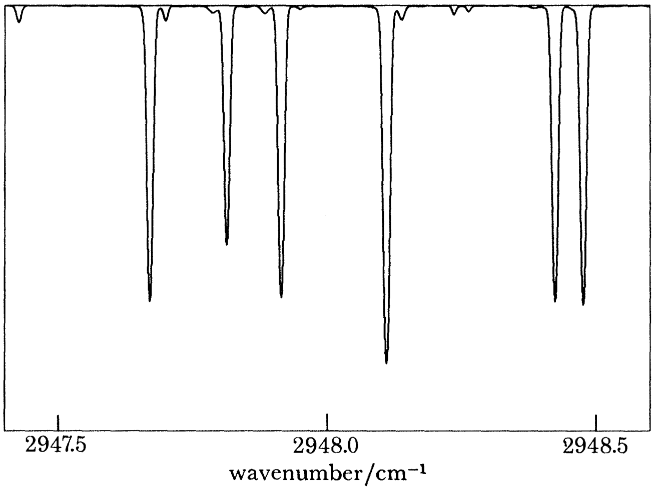

Figure 1. A very small portion of the ν_3 band of methane in absorption at room temperature and low pressure, taken with the Kitt Peak solar F.t.s.

For the grating, there are yet two rays of hope. The first involves the time-honoured photographic plate, for which q is poor (perhaps 0.001–0.01) but n can be 10^3 to 10^5. Then $qn \gg 1$, which roughly cancels the low throughput. The second possibility, and the one that is having a great impact in astronomy, is the silicon array detector (see Boksenberg, this symposium), for which $q \approx 0.5$ and n is 10^2 to 10^3, again cancelling the effects of low throughput.

Finally, there are the separate but related topics of spectral coverage and free spectral range. Some problems may be solved by observing a fraction of a wavenumber, while others require broad coverage: up to tens of thousands of wavenumbers. In the latter case, the amount of spectrum that may be covered without readjusting or changing components becomes a factor in the information flow. Here, it is the Fabry–Perot that ranks a poor third, with the F.t.s. a clear first. For the F.t.s., spectral coverage is limited only by beamsplitter coatings, substrate transmission and detectors. Wavelength ratios of 5:1 are achievable in a single scan, and ratios of 100:1 or more are possible by switching beamsplitters or detectors or both (which may or may not be trivial, depending on the design). Thus, an enormous spectral range is accessible to such an instrument, with a wide free spectral range in a single measurement.

(*b*) *Quality*

Here we are concerned with the resolution and 'cleanness' of the apparatus function, the accuracy of the intensity and wavelength scales, and any possible sources of excess noise. Resolution is determined by the maximum path difference in the diffracted or interfering beams. For the grating, this means it is limited by the physical size of the grating itself, which again puts the grating at the bottom of the list. For the interferometers, resolution limits are similar, although the F.t.s. achieves it through a long single path while the Fabry–Perot uses multiple reflexions on a shorter path. For major research instruments, this effective maximum path difference is typically 1–5 m, corresponding to an unapodized resolution of 0.005–0.001 cm^{-1}. Figure 1 shows a typical application of high-resolution interferometry: a very small portion of the ν_3 band of methane in absorption at room temperature and low pressure, taken with the Kitt Peak solar F.t.s. Many problems, of course, do not require the full resolution of such instruments. For these problems, it is useful to have variable resolution, because excess resolution reduces the signal:noise ratio; the F.t.s. is especially flexible in this regard.

Intensity accuracy is ideally limited only by photon statistics, but in practice there are many systematic effects which degrade performance: scattered light to falsify the zero line; apparatus function smearing effects to distort the shape of spectral lines; nonlinearity and crosstalk in detectors.

Our main concern here is with line shapes in detail, as contrasted with more global properties such as equivalent widths. In the past, spectroscopy has treated its two main variables very differently, being highly quantitative on the wavelength axis and qualitative on the intensity axis, largely because intensity measurements were difficult and unreliable. But accurate intensity information is now increasingly important in many areas: modelling stellar atmospheres; unravelling complex hyperfine structure patterns; ratioing or differencing spectra to see small differential effects in the presence of large systematic effects (e.g. atmospheric transmission); understanding non-Voigtian line shapes, etc. It is with such applications in mind that I shall evaluate the three techniques.

For the grating, scattered light in broad-band absorption spectra is typically a small percentage, and smearing due to the apparatus function is relatively important, since the wings die off only as $1/(\Delta\lambda)^2$. The most severe inaccuracies, however, result from the use of photographic plates as detectors. The photometric difficulties (nonlinearities, threshold effects, adjacency, etc.) are too well known to need discussion here. The photographic plate is really very modern in concept: it is used once and then thrown away (at least as a detector). As a result, there is no way to get a direct photometric calibration, and consistent accuracies better than 5% are rare and painful.

Diode arrays, on the other hand, can be calibrated – which is a very good thing, since each element tends to have a different offset and sensitivity; interference fringes can also be a problem. In the end, however, the limits to accuracy will still be set by the smearing and scattered light of the grating itself. There is a tendency to assume that because the random (photon) noise can be made very small by sufficient integration, the intensity (line shape) accuracy must be very high. Unfortunately, low random noise is necessary but not sufficient for good line shapes, and the systematic effects mentioned above will eventually be dominant. Still, there are many problems for which 1–5% line distortion is perfectly acceptable, and for these problems the grating remains a useful tool.

The Fabry–Perot has by far the worst apparatus function for distorting line shapes: not only do the wings fall off slowly, but their asymptote is not even zero. Furthermore, it is fruitless to attempt to get around the problem by simply increasing the resolution, because the free spectral range then becomes too small to be useful. It is no accident that the most useful results from Fabry-Perot measurements have been wavelengths rather than intensities.

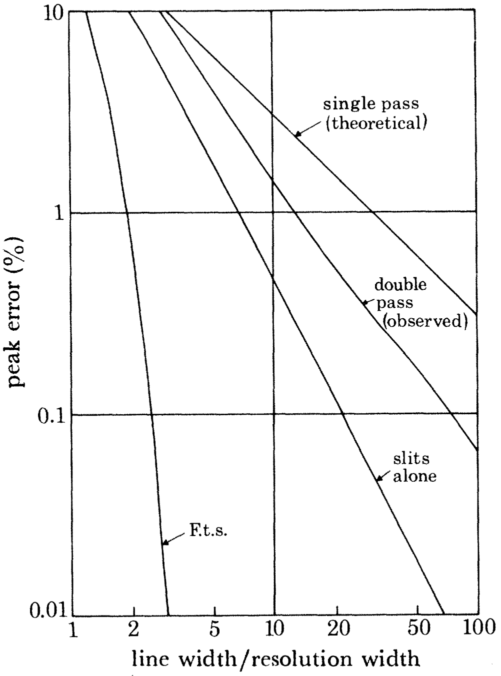

Figure 2. The distortion of a gaussian line by the F.t.s. and a grating in several modes, as a function of resolution relative to the line width.

The F.t.s. has, in principle, the best apparatus function, since its frequency response is essentially flat out to the end of the interferogram, where it drops suddenly to zero. This is shown in figure 2 where the errors produced by an F.t.s. and a grating instrument are plotted as a function of resolution (the curve for a Fabry–Perot would be somewhat above that of the single-pass grating). In practice, it is best not to use the F.t.s. at the low end of this scale if possible, since the oscillatory nature of the F.t.s. error makes it much more visible than an error of the same size produced by smearing with a grating apparatus function.

Wavelength accuracy can also be a large and nettlesome subject. Again, in the best of all possible worlds, it is limited only by photon noise. Under these conditions, the uncertainty in the position of a spectral line is roughly the line width divided by the product of the signal:noise ratio in the line and the square root of the number of samples in the line width. If both resolution and S/N are high, the position uncertainty due to photon noise can be made very small indeed. Figure 3 shows the scatter in the lines of an N_2O band observed with the Kitt Peak solar F.t.s., compared with values calculated from approximate molecular constants. In the R branch (which is free from blending), and in the region where the lines are strong (marked by a horizontal bar), the r.m.s. scatter is only *ca.* 2×10^{-6} cm^{-1}, as expected in a spectrum where the lines are only 0.01 cm^{-1} and S/N is several thousand. Such precision is straightforward (though not common) in modern F.t.s. work. With much greater efforts, the Fabry–Perot can do nearly as well, while the grating lags far behind; the most routine F.t.s. measurements tend to be roughly 10 times more accurate than the most careful grating measurements.

(*c*) *Cost*

Our final concern is with the resources required to perform useful spectrometry with these three techniques, including not just capital outlay, but the time used in understanding and becoming familiar with the equipment, maintaining and extending it, and handling the data that justify the whole apparatus in the first place. It is quite impossible to give general rules about, say, the cost per bit of information for an F.t.s. or grating. There is a widespread feeling that grating instruments are cheap and simple and that an F.t.s. is complex and expensive, and to some extent this is true – but the instruments being visualized when such comparisons are made are usually vastly different in power. The most challenging problems are handled not with, say, a 1 m Ebert–Fastie with photographic recording, but with 10 m class multiple-passed scanning gratings; not with a simple single Fabry–Perot etalon, but with multiple etalon systems such as Pepsios. However it is accomplished, high-precision spectrometry is expensive – in the time of experts, if not in capital. Today's grating instruments are the result of decades of invention by a large number of talented instrumentalists. By comparison, the development of F.t.s. has been carried out by a handful of believers, and there has simply been not enough time for simple, cheap designs to emerge. The next 5 years should see a dramatic change in this direction.

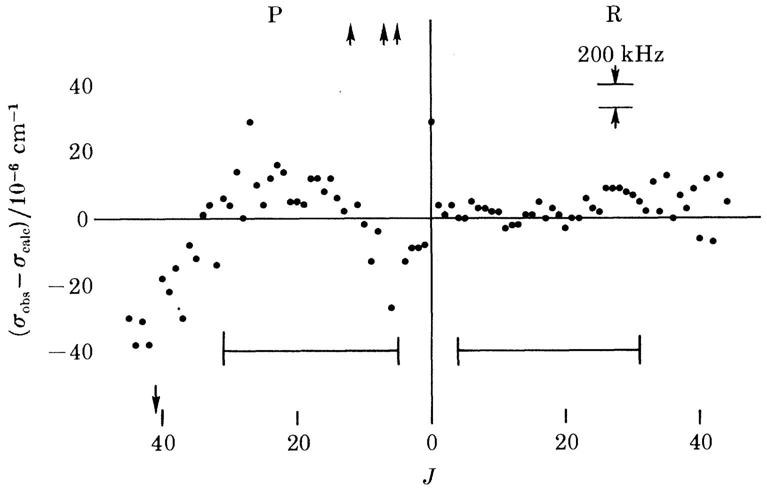

FIGURE 3. The scatter in wavenumbers σ of the lines of an N_2O band (00^02–00^00) observed with the F.t.s., compared with values calculated from approximate molecular constants. Note especially the strong lines of the blend-free R branch (solid bar). Arrows represent points off the scale.

It is easy to ignore the cost of data reduction, but this can be a real mistake: an instrument is (one hopes) built once, but used many times to obtain data. The natural output of an F.t.s. (after a straightforward numerical transform) is a set of digital numbers representing the intensity (on a linear scale) at a set of points equidistant in wavenumber. There has already been considerable development of computer programs that operate directly on such records, producing plots and lists of spectral line parameters almost automatically, and making it possible to deal with spectra of quite remarkable complexity. The importance and value of such a capability cannot be overemphasized.

3. SUMMARY

Each of the three systems occupies a useful niche in the overall scheme of things.

(i) Broadband spectra of modest quality are most cheaply obtained by the grating with photographic recording, at least in the visible and u.v.; this system is also the most tolerant of source variation.

(ii) High resolution and good portability are the strong points of the Fabry–Perot, though it is restricted to problems that need only a small free spectral range, and are tolerant of apparatus function smearing.

(iii) The F.t.s. is the system of choice in the infrared under almost any conditions (with or without multiplex advantage), and in the visible and u.v. when high accuracy is required in either intensity or wavelength.

4. EXTENSIONS OF THE F.T.S.

In spite of the apparent long history of the F.t.s., the technique is still in its infancy: more than half of the high-resolution interferograms ever taken have been obtained in the past 5 years. Many significant improvements and extensions obviously still lie ahead. Let us now consider briefly two extensions that appear to have some promise.

(a) *Multiple detectors*

In the discussion on information flow, we noted that the grating spectrometer still qualified by virtue of its ability to make use of multiple detectors to compensate for low throughput. Clearly, if multiple detectors could be used on a high throughput system like the F.t.s., we would have a very superior system. This is in fact possible in principle, although the implementation may be expected to involve a considerable amount of high technology.

In brief, the output beam is dispersed (probably by a prism or grating!) and allowed to fall on a detector array instead of a single detector; 100 to 200 elements seems feasible. Each element then receives the interferogram of only a fraction of the spectrum. Most importantly, the noise from the remainder of the spectrum is excluded, and again the detector acceptance goes up as the number of detectors. The extension is thus very simple in principle; the practical problems are mainly concerned with the digital techniques required to handle all the detectors in real time.

(b) *The all-reflecting (u.v.) F.t.s.*

Another interesting possibility is the extension of F.t.s. techniques to the far u.v. where no suitable transmitting substrates exist. The idea that operation at, say, 1000 Å would require impossible tolerances is completely fallacious. The effect of errors in optical figure and position control is only proportional to wavenumber. The Kitt Peak system operates very comfortably down to 2000 Å; errors would only be twice as large (and still acceptable) at 1000 Å. The main difficulty is in finding a suitable design that operates with all-reflecting optics. The following concept was worked out in conjunction with R. C. M. Learner & A. P. Thorne of Imperial College.

The proposed design is, as so often happens, an old idea (the Rayleigh interferometer) with a new twist: the addition of a grille instead of a slit as the entrance aperture, with a matching grille in the exit plane (figure 4). This simple modification raises the throughput of the Rayleigh interferometer to a value that may approach one-half that of the corresponding F.t.s. The operation of the interferometer may be understood by reference to figure 5, which shows the intensity distribution in the exit plane, due to a monochromatic line source at the entrance, for (*a*) an even, or (*b*) an odd number of half waves of path difference between the two halves of the wavefront at recombination. Most of the modulation takes place over the central angle $\Delta\theta = \pm\lambda/2W$, where W is the full width of the beam, but a periodic grille, with λ/W as half period, would clearly work nearly as well. The use of the periodic grille at the exit, however, allows us to use a series of line sources of equal period at the input, thus raising the throughput considerably. If the line sources are narrow compared with the grille spacing, the modulation efficiency exceeds 60 % but the throughput is low; widening the input spaces improves the throughput but reduces the modulation somewhat.

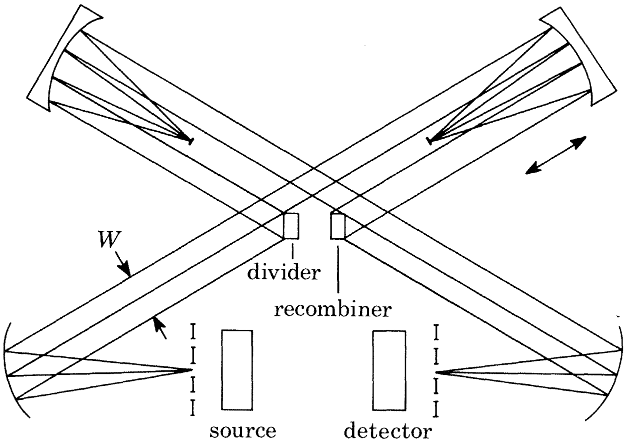

FIGURE 4. Schematic design of an all-reflecting wavefront division F.t.s.

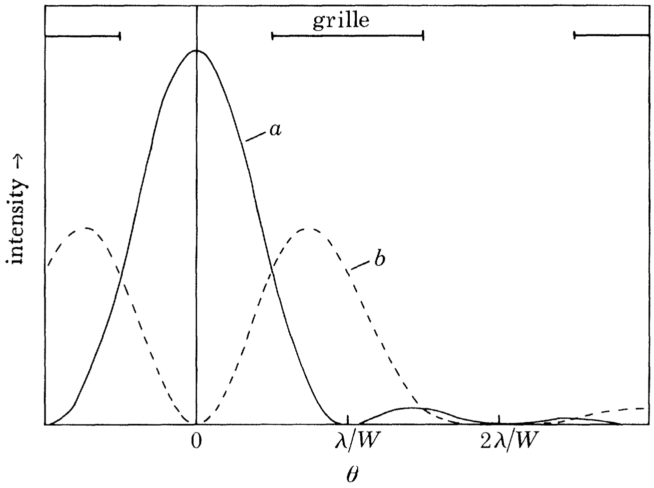

FIGURE 5. Intensity distribution in the exit plane due to a monochromatic line source at the entrance. Path difference is (*a*) an even number of half waves and (*b*) an odd number.

Considerably more work remains to be done to optimize the design of this interferometer, but it is clear that a device could be built that shares (in a lesser degree) all of the major advantages of the F.t.s. while operating with all-reflecting optics. Throughput might be lower than that of a normal F.t.s. by a factor of 2 or 3, and modulation efficiency perhaps only 50 %, but the remaining advantage is still great. Since the optimum grille spacing is wavelength-dependent, efficiency considerations would limit operation to an octave or less, but that is about the range (800–1600 Å) over which such a device might be used in any event.

As shown in figure 4, the interferometer has only one input and one output. It can be very conveniently converted to a completely symmetrical dual input – dual output device by replacing the grilles with a matched pair of low-angle reflexion gratings, as shown in figure 6. By adjusting the focal length of the collimator and camera mirror, one of the common gratings in the 75–300 lines mm^{-1} range can be easily used. Many other variants of the optical arrangement are clearly possible, and one with fewer reflexions would certainly be desirable.

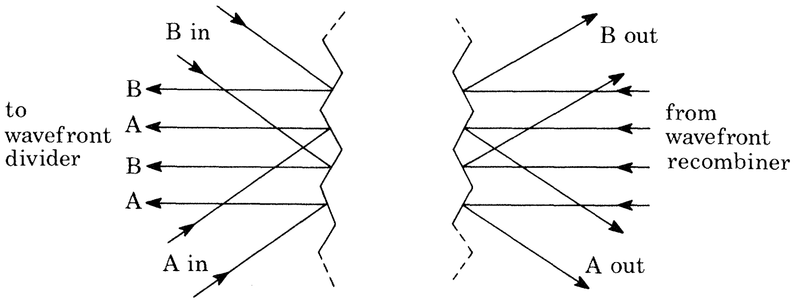

FIGURE 6. Illustrating the use of low-angle gratings instead of grilles at the entrance and exit to permit symmetrical operation.

Kitt Peak National University is operated by the Association of Universities for Research in Astronomy, Inc., under contract with the National Science Foundation.

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