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WINTER COLLEGE ON

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(BASIC SPECTROSCOPY INSTRUMENTATION)

SPECTRAL FILTERS, DETECTORS AND SIGNAL PROCESSING

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BASIC SPECTROSCOPIC INSTRUMENTATION : K. S. LOW

LECTURE 3 : SPECTRAL FILTERS, DETECTORS AND SIGNAL PROCESSING

3.1. Spectral filters : spectrometers, band pass filters and sharp cut filters.

3.2. Detectors : photomultipliers, photodiodes, diode array, photon drag, pyroelectric and calorimeters.

3.3. Signal Processing : photon counting, lock-in amplifier, boxcar.

3.1. Spectral filters

- to be able to pick up signal of a specific wavelength, blocking unwanted signals

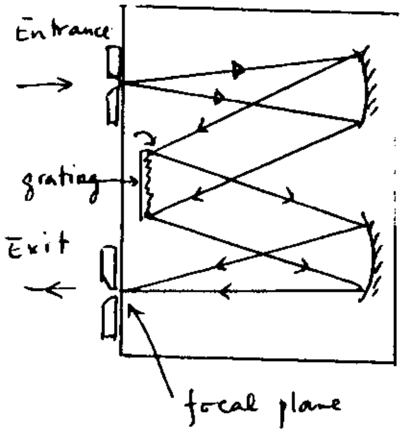
1. Spectrometers : gratings mounted on stepper motor controlled sine drive can be easily interfaced to microcomputers

-resolutions fepend on the number of grooves of the grating illuminated and the size of the gratings

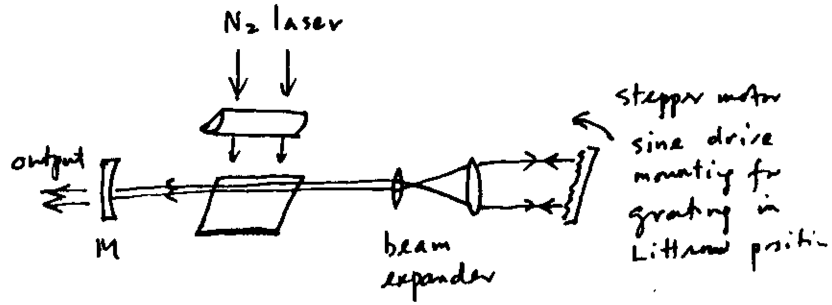
-normally a single detector placed at the exit slit for single channel operation

-if an array of detector placed at the focal plane of exit slit, simultaneous detection of spectra as a optical multi-channel analyser (OMA)

-By rotating a slit placed at the focal plane, an OMA is essentially obtained for dc signals.



-spectrometer like devices can be assembled into dye laser system for wavelength tuning purposes.



2. Band pass filters

-narrow band pass interference filters

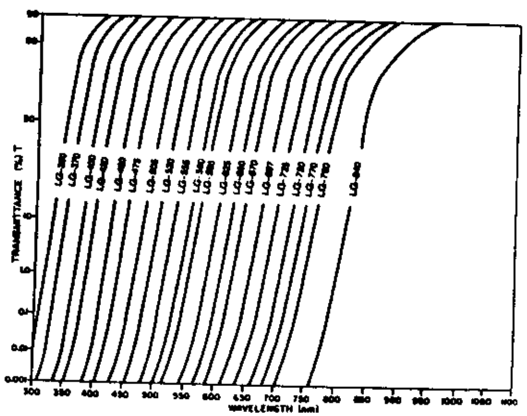
-multi-layer dielectric coated

-to 5 nm bandpass with 20 to 50 % transmission

3. Sharp cut color glass filters

-color filter glass are inexpensive for cut off of signals at the shorter wavelengths

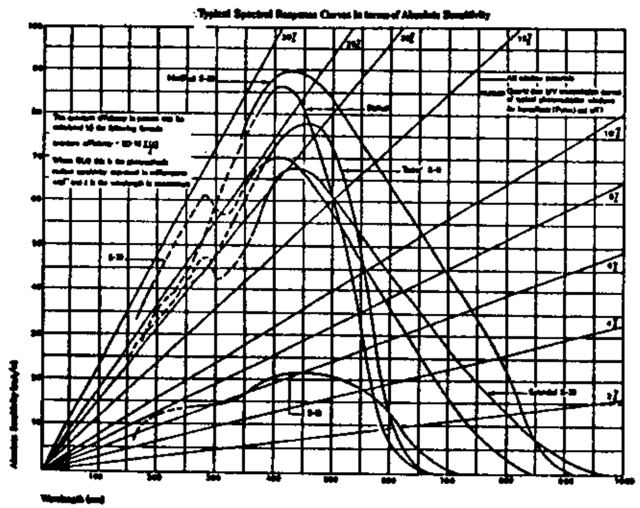
-useful for fluorescence works



3.2. Detectors :

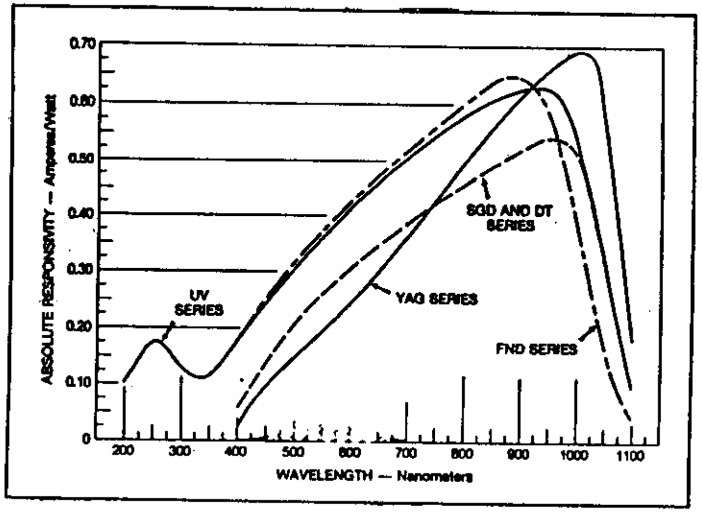
-two types : quantum or thermal types

1. Photomultiplier : most important linear transducer for measuring photons.
   - based on production of primary electrons due to photoelectric effects when photons is incident on the photo-cathode
   - electrons multiplied at secondary electrodes (dynodes)
   - amplified many times before arriving at the anode
   - spectral response dependent on the cathode materials, see Fig. 1. mainly in the visible and some UV and IR response
   - very high response for single photon counting
   - cooling of PMT for lowering of noise level



2. Photodiodes based on semiconductor materials
   - normally 2 types - photovoltaic (PV) as in solar cells or photoconductive (PC) for faster response
   - PV require no external voltage biasing, creation of carriers in one material that diffuse across a junction between two semiconductor materials resulting in a voltage, when exposed to radiation. Simple to use and inexpensive.

   - PC normally operates with a reverse biasing across the junction of the two semiconductor materials. A change of conductivity occurs when exposed to radiation due to creation of carriers.
   - both the output of the PV or PC diodes can be readily amplified with op amps. Some are even produced with amplifiers built into the chips.
   - usable from UV, visible to far IR (with cooling).
   - typical response curve below as Fig. 2.



3. Diode arrays for optical multi-channel analyser
   - an array of small photodiodes few microns apart, typically 512 or 1024 elements
   - normally placed at the focal plane of the exit slit of a spectrograph to capture the entire spectrum of the signal as an optical multi-channel analyser as compared to the single channel nature of a spectrometer system. Require sophisticated data acquisition system.
   - could also include microchannel plate image intensifier tubes to amplify signal.
   - presently still an expensive equipment to acquire.

4. Photon drag detectors

-based on the momentum transfer between photons and electrons and holes in a semiconductor materials (normally germanium). These carriers are dragged along with the photon beam resulting in an emf across the two end plates.

-normally used for far IR laser pulse measurements as in the TEA-CO2 lasers.

5. Pyroelectric detectors

-thermal detectors

-some crystals have permanent electrical polarisation which depend strongly on temperature e.g. LiNbO3.

-when temperature of crystal changes rapidly, a rapidly changing surface polarisation results in differences in surface charge distribution.

-mainly for IR lasers.

6. Joule calorimeters

-conversion of heat differences across thermoelectric junctions, normally as an array in thermopiles

-very rugged and useful across a wide spectrum

-slow response and poor detection limits

-normally for measurement of laser power output and not for detection of spectroscopic signals.

Photon Drag Detector Response

Photon Drag: Normalised Responsivity vs. Wavelength
(solid curves are the measured values)

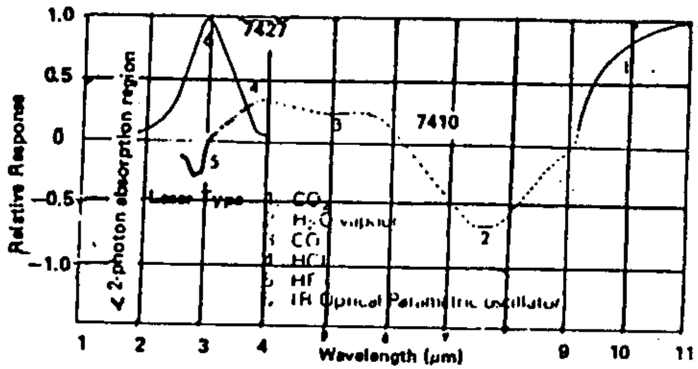


FIG. 1

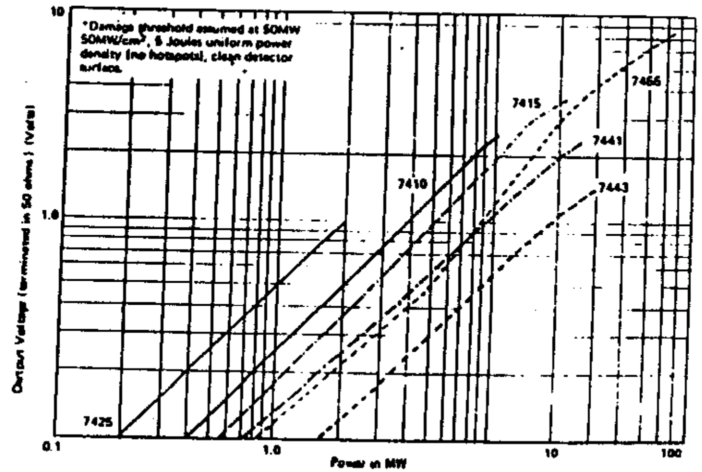


Fig. 2 RESPONSIVITY OF PHOTON DRAG DETECTORS

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3.3. Signal Processing : Photon Counting, Lock in amplifier & Box car averaging

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J D W ABERNETHY

Signal recovery methods

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Suppose that one were given the task of measuring the magnetism of a rock sample in the presence of the unavoidable and much larger magnetic field of the earth, or of measuring a weak infrared signal in a warm laboratory. In both cases the signal of interest would be obscured by a large background signal which will be referred to as 'interference' and which would make the measurement valueless unless its effect could be suppressed. One way of doing this might be to introduce some sort of coding into the signal to make it recognizably different from the interference.

In the examples above, and in an enormous number of other similar situations, the signal is coded by introducing into it, but not into the interference, frequency information. For example the rock sample may be spun at a known frequency so that the output of the magnetometer would consist of two parts, a large zero frequency component due to the earth's magnetic field and a small component at the spinning frequency whose amplitude would be the desired quantity. A high pass filter could now be used to suppress the interference while transmitting the signal to a suitable measuring instrument such as an amplifier, rectifier and smoothing circuit.

In practice the situation is seldom as simple as this, there being additional sources of interference such as hum pick-up, amplifier generated noise, *etc*, and these become significant whenever the signal is very small. In particular some of these additional interferences are likely to contain random noise whose frequency spectrum covers the modulation frequency initially used to code the signal. When this is the case the signal to noise ratio is frequently so poor that ultra narrow band filtering is necessary to make a useful measurement possible. Tuned systems of sufficiently high Q are impracticable for reasons of stability and instead a synchronous detector, often called a lock-in amplifier, may be used.

The invention of the lock-in amplifier is credited to Professor R H Dicke who in 1947 described a novel microwave radiometer. Previously in such radiometers the smallest measurable signal had been limited by noise indistinguishable from the input signal and generated in the radiometer's microwave amplifier. Dicke coded the desired signal by mechanically switching the input of the amplifier back and forth between the actual aerial and a dummy of known temperature, so that, after RF detection, the output of the system consisted of a small square wave obscured by noise. The amplitude of the square wave was a measure of the temperature difference between the objects seen by the actual and dummy aerials. The real originality of the system lay in Dicke's use of a phase sensitive detector (PSD) to measure the amplitude of the squarewave. The PSD is the heart of the lock-in amplifier and its basic action will therefore be considered in some detail below.

Phase sensitive detector

A full wave PSD consists essentially of a phase splitter, a simple *RC* low pass filter and, between the two, a change over switch, operated so that the input to the filter is alternately taken from first one and then the other output of the phase splitter. The switch is electronically controlled and the controlling voltage is arranged to synchronize the switching action with the zero crossings of the signal to be measured. As will be seen from figure 1 this leads to rectification of the signal, giving a DC output from the filter. By contrast noise, except that very close to the signal frequency, gives rise to frequencies outside the pass band of the filter and is therefore rejected.

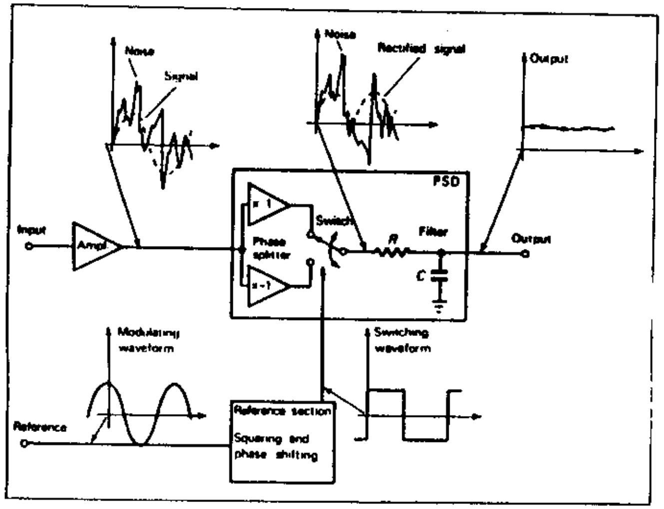

Figure 1 Phase sensitive detector

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The switch controlling voltage, to be synchronized with the signal, must be derived from the same source as the original modulator and PSDs are therefore only of use when such a so called reference is available. Note also that the controlling voltage must be in phase with the signal: in quadrature it leads to zero output.

To give a different viewpoint the PSD may also be considered as a type of special purpose correlator. In switching the noisy signal at the reference frequency, ω_r, it is in effect multiplying the signal by a square wave of that frequency. Decomposing the square wave into its Fourier components gives

$$V_{switch} \propto \cos\omega_r t + \tfrac{1}{3}\cos 3\omega_r t + \ldots$$

so any term in the signal such as $V_s\cos(\omega_r t+\varphi)$ will give, among others, a product such as

$$V_s\cos(\omega_r t+\varphi)\cos\omega_r t$$

which is proportional to

$$V_s\cos\varphi + V_s\cos(2\omega_r t+\varphi).$$

$V_s\cos\varphi$ is a DC term and appears at the output, while the other term is AC and, with a suitable filter time constant T, will be effectively rejected. Thus the PSD gives a DC output for a signal component at the reference frequency (and to a decreasing extent at its harmonics), the DC output being proportional to that component of the signal which is in phase with the reference.

Noise components of frequency near ω_r, say $\omega_r+\delta\omega$, give lower side bands at $\delta\omega$ and their degree of rejection is determined by the low pass filter which has a -3dB point bandwidth of $1/\pi T$. It has a 'noise equivalent bandwidth' of $1/4T$, this being the bandwidth of a notional 'rectangular' filter which will transmit the same noise power as the actual filter in white noise conditions.

The PSD differs from tuned filter-rectifier systems in three significant ways. First such noise as is passed by the PSD is purely AC with zero average. Secondly the PSD is phase sensitive which has the effect that it passes half the noise power of an equivalent phase insensitive filter. Thirdly, its centre frequency is rigidly locked to an external signal, and so in signal recovery applications, where both the signal to be measured and the reference come from the same source, there is no scope for centre frequency drift. It follows that a PSD may have very high Q factors. In fact one commercial lock-in amplifier can have a Q factor of 10^8 at its highest frequency.

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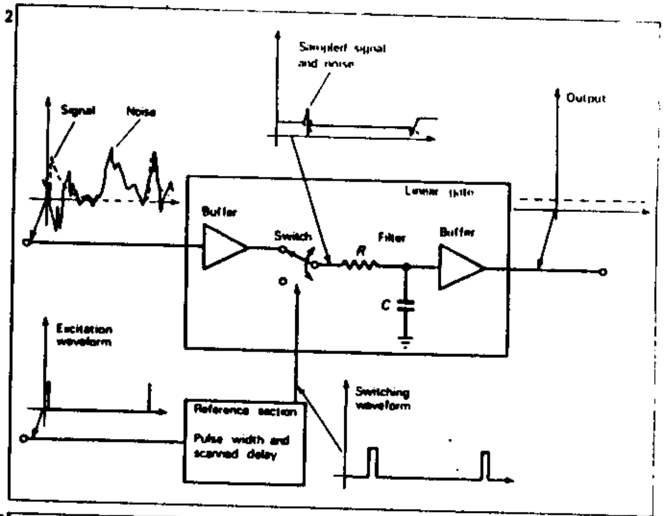

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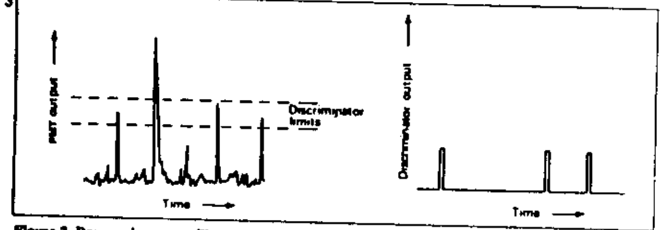

Figure 2 Boxcar detector **Figure 3** Photon counting pulse trains

Lock-in amplifier

The lock-in amplifier (LIA) consists of three main parts: a PSD, an amplifier and a reference section. The amplifier is normally necessary to increase the magnitude of the noisy signal to a level just below the input overload level of the PSD. Some early LIAs included tuned filters in the amplifier section which served the purpose of helping PSDs with poor overload capability. In the last few years the advent of high quality PSD circuits has led to the partial abandonment of tuned systems with their attendant disadvantages of amplitude and phase instability. They are retained as options for special purposes. Instead the modern LIA has simple high and low pass *RC* filters which can be set so that they contribute no appreciable phase shift at ω_r.

The LIA is also likely to have a line frequency reject filter since line frequency noise is the most frequently encountered large interference. The reference section converts the reference input to the desired switching waveform (a symmetric square wave). In the last three years it has become universal for LIAs to have semi-automatic reference sections which will trigger off almost any input wave form and provide a variable calibrated phase shift whose value does not change with reference frequency.

Performance

The criterion by which the performance of the LIA is judged is its ability to provide an output of better signal to noise than that of the input. There are three dominant sources of output noise, the first fundamental and the other two practical. First consider an LIA recovering a small signal from white noise of bandwidth ΔF. If the equivalent noise bandwidth of the PSD is δF, the ratio of input to output noise powers is $\Delta F/\delta F$ and so the ratio of input to output noise voltages is $(\Delta F/\delta F)^{\frac{1}{2}}$. In a typical setting ΔF might be 10 kHz and T might be 10 s ($\delta F = 1/40$ Hz), giving an improvement in signal to noise ratio of 600. In practical cases the noise seldom is white, often being largely contributed by hum and flicker noise, and in these cases where a smaller proportion of the noise power falls within δF a higher figure is obtained.

Secondly, thermal drifts in the PSD circuit give rise to spurious very low frequency outputs which contribute to output noise. Referred to maximum input level this effect may give an output as low as 1 ppm/°C in modern equipment.

Thirdly, even order, nonlinear effects in the PSD circuit provide a slight degree of rectification and this, in the presence of large noise signals, can give an appreciable erroneous DC output. This effect is measured in terms of 'out of phase rejection', and referred to maximum input level typically is about 10 ppm.

In cases where the noise is preeminently random the first, 'correct' noise output is likely to be dominant. In these circumstances the LIA is operating as well as is theoretically possible. In cases where the noise is discrete the last two sources of output noise are likely to be dominant, giving a limit to the LIA's performance.

More complex waveforms

The LIA is suited to the recovery of continuous signals, such as sinusoids and square waves, buried in noise. Sometimes the signal is a pulse, resulting from pulsed excitation of the experiment. Examples occur in crack detection in metals, radar, *etc*. While an LIA could be used in such measurements it would clearly be inefficient the more so as the ratio of 'off' to 'on' periods is increased. Instead it is normal to use a boxcar detector (BD) to measure such pulses. It operates by sampling and averaging the noisy pulse during the duration of the pulse only, and by holding readings between pulses. In such applications the BD is said to be operating in the 'single point mode'.

Sometimes the outputs of pulsed experiments are signals of unknown but interesting waveform, for example in fluorescent decay studies. To recover these from noise it would be possible to use, say, 100 BDs in parallel, each recovering one segment of the waveform. This is, in effect, what a class of instruments called signal averagers does. Another approach is to use one BD and control it to measure 100 points on the waveform sequentially, when it is said to be operating in the 'multi-point mode'. Both approaches are widely used. The signal averager is more efficient than the BD in that it does not discard 99% of the input information but the BD can operate with waveforms of very much higher frequencies, is typically a quarter of the price of the signal averager and performs better in circumstances of very adverse signal to noise ratio.

The boxcar detector

The boxcar detector consists of two main parts, a linear gate and a reference section; these are not unlike the PSD and reference sections of an LIA.

The linear gate consists of an input buffer, an electronically controlled switch, a simple *RC* low pass filter and an output buffer (see figure 2). The switch either connects the input buffer to the filter, or disconnects them, according to the state of the controlling voltage. The controlling voltage is timed so as to close the switch just for the duration of the noisy pulse (or segment of waveform) to be measured. The only signal which is applied to the *RC* filter is a DC pulse amplitude plus AC noise, so the capacitor charges over a number of cycles towards a DC level representing the pulse amplitude and the noise averages towards zero. During the off periods the capacitor charge, and hence the output, is held steady and for this reason the output buffer is designed to draw negligible input current.

The reference section takes in a sample of the original excitation pulse train and converts this into a train of switch controlling pulses which can be varied in width and delay, the latter being fixed when in the single point mode. In the multi-point mode the switch controlling pulse width is set to be just less than the required resolution of waveform detail. The reference unit automatically scans the delay, very slowly, across the unknown waveform; in practice this is done continuously rather than in discrete steps as implied earlier. The result is that the BD slowly gives out a cleaned-up version of the signal waveform.

The BD is limited in performance in exactly the same way as the LIA and for the same reasons. However, in practice the BD has to be able to handle pulses as narrow as 10 ns and this design constraint leads to the BDs having a dynamic range around 10 times worse than that of the LIA.

The photon counter

Photon counting is an emergent technique for improving the signal to noise ratio at the output of photomultiplier tubes. As such it is a form of signal recovery, though very different in nature from those described so far.

The output of a photomultiplier tube might look like the first trace of figure 3. It contains three wanted pulses originating from incident photons, a large pulse originating from a cosmic ray interaction, some small tube generated pulses and random noise. If this signal were averaged in an *RC* network the output signal to noise ratio could clearly be very poor, particularly at low incident light levels. When this is the case it is normal to code the signal by chopping the light incident on the experiment and to use an LIA to recover the resultant noisy squarewave.

It is a property of some photomultiplier tubes that the output pulses caused by incident photons are all of approximately the same amplitude and shape and are therefore already coded, that is recognizable, and this property can be used to eliminate most of the tube and amplifier generated noise while passing most of the photon generated signal.

In the photon counting technique the photon counter (PC) takes in the noisy signal which is amplified by a very fast amplifier and is then fed into a discriminator. The discriminator gives out a standard pulse each time an input pulse has a peak within maximum and minimum amplitude limits which are preset to include, as far as feasible, all photon generated pulses and no others. The standard pulses are then counted digitally (hence the name photon counter), the count rate being proportional to the light incident on the photomultiplier tube. In this DC mode the PC duplicates the *RC* averager, but gives a better signal to noise ratio. Even with normal photomultiplier tubes which give photon generated output pulses of widely varying amplitudes it is frequently possible to obtain considerable improvements in signal to noise ratio by careful choice of discriminator levels.

So far it has been assumed that all photon event pulses represent a wanted signal but in low level measurements it is likely that many are derived from stray light representing further noise. For this reason also it is usual to chop the light incident on the experiment: the count rate during the 'dark' periods is wholly due to noise while that during the 'light' periods is due to signal plus noise. High performance PCs, such as the Brookdeal 5C1, count alternately into two counters, A and B, synchronized by the chopping waveform, so that the difference $A-B$ is a measure of the signal. In this mode the PC is digitally duplicating the LIA from a frequency filtering point of view, but with the added advantage of amplitude discrimination. In cases of unsteady excitation, that is fluctuating signal amplitude, a second photomultiplier tube may be used to observe the signal source directly, its output being counted into a third counter, C, so that the normalized output $(A-B)/C$ may be computed ■