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WIDE-RANGE NUCLEAR-MAGNETIC-RESONANCE DETECTOR USING INTEGRATED CIRCUITS

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16. Abstract
This report describes the electronics developed for sensing nuclear magnetic resonance over a wide range of magnetic fields (0.1 to 18 T). The system was designed to operate with a long coaxial transmission line between the rf coil and the electronics package, a feature which makes it suitable for use with high field cryomagnets. The instrument is small and portable, and it is constructed predominantly with commercially available integrated circuits. A computer program for the computation of the resonant modes of the coaxial lines is included.

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SUMMARY

Research at this laboratory involving extremely high magnetic fields (up to 18 tesla) necessitated the development of special nuclear magnetic resonance (NMR) techniques. The large physical size of the magnets together with their cryogenic cooling require that the sensing probe be located a considerable distance from the control and demodulating electronics. The high fields require that the system be capable of spanning several hundred megahertz.

The NMR system uses a coaxial transmission line between the radiofrequency coil of the sensing probe and the remote electronics package. By operating the system on the resonant modes of the interconnecting transmission line, the required frequency range of operation is obtained. Included in this report is a computer program for the computation of the resonant modes of the transmission line. The use of integrated circuits to implement the design of the apparatus, resulted in a small, portable, yet highly sensitive detector.

INTRODUCTION

Recent advances in magnet technology have made available facilities that are capable of producing steady magnetic fields approaching 18 tesla (180 kG) (ref. 1). These high fields are attained in cryogenically cooled solenoidal magnets wound of either a superconductor or a high purity metal such as aluminum. Previously, fields of this magnitude could be obtained only in a pulsed fashion, and then in relatively small volumes. Microsecond field pulses were typical. Obviously the pulsed nature of such fields is a severe limitation. In the area of magnetic resonance, the pulsed magnets are not particularly useful.

Superconducting magnets, on the other hand, are able to maintain a desired field virtually indefinitely. The normal-metal cryomagnets are capable of peak field operation extending over periods currently of the order of minutes. At lower fields the period can be considerably longer.

Along with their stable high-field capabilities, the new cryomagnets possess another desirable quality: field homogeneity. Homogeneities on the order of one part in 10^4 over central volumes of approximately 6 cubic centimeters are readily achieved as a consequence of the sheer size of these magnets. Over smaller volumes, on the order of 2 cubic centimeters, homogeneities of one part in 10^5 are possible. With the addition of trim coils, homogeneities of one part in 10^6 are possible.

At this time, nuclear magnetic resonance appears to be the most reliable means of obtaining accurate field calibrations at these high fields. Field measuring techniques that rely on the transport properties of conduction electrons, for example, magnetoresistance, Hall effect, and de Haas-van Alphen effects, cannot be confidently extrapolated to these uncharted high fields. Alternatively, field measuring techniques based on the use of inductive coils, such as, snatch coils, rotating coils, and integrating coils, cannot with precision be extended to fields that are generally a minimum of 10 times that at which they were calibrated. Furthermore, it is difficult to assure the physical stability and orientation of the coils in the large cryogenic environment of the magnets. Nuclear magnetic resonance, however, does provide a simple means of accurate calibration that does not suffer from these drawbacks.

Unfortunately, the new generation of high-field magnets poses somewhat of a problem in implementing an NMR measurement. Chiefly because of three factors, (1) the huge size of the magnets, (2) their cryogenic environment, and (3) their large fringing fields, active components such as transistors, diodes, etc., cannot be located near the sample-bearing coil as is the common practice. Instead, they must be separated from the sample-bearing coil by perhaps as much as 10 to 20 meters in order to remove them from the influence of the cryogenics and fringe fields. Yet, separating the coil from the other electronics should not limit the frequency range (and hence the field range) over which the system can operate. Rather, in order to reach the higher fields, the frequency range of operation must necessarily be far greater than is commonly employed.

This report describes an NMR system that circumvents the need for active elements in the probe head. The design is based on the single rf (radiofrequency) coil type of detector sometimes referred to as the "Q-meter" detector. Connection between the sample-bearing rf coil and the control electronics is made by a coaxial transmission line. Wide-band operation is obtained by operating the transmission line on its resonant modes.

SYSTEM DESIGN

The phenomenon of nuclear magnetic resonance is based on the fact that a nucleus with nonzero spin, when placed in a magnetic field, precesses about the field direction. The rate of precession depends both on the magnitude of the field and on the characteristics of the nucleus itself (its dipole moment). For each nuclear specie there exists a simple linear relation between the precessional frequency f and the field strength H:

$$f = \frac{\gamma}{2\pi} H \tag{1}$$

The parameter γ, commonly called the gyromagnetic ratio, has a unique value for each nuclear specie and has been determined for all with great precision. For protons (H^1), for example, the quantity $\gamma/2\pi$ has the value 42.577 megahertz per tesla, and for aluminum nuclei (Al^{27}) in the metallic state $\gamma/2\pi$ is 11.112 megahertz per tesla. Therefore, a determination of the precessional frequency f gives a direct measure of the magnetic field H experienced by the nuclei.

In practice the precessional frequency is determined by subjecting a sample containing the nuclei to electromagnetic radiation such as that produced by an rf coil. When the frequency of the electromagnetic radiation is equal to the precessional frequency, a resonant condition exists wherein an exchange of energy is induced between the nuclei and the radiation field. The net effect is a minuscule loss of energy from the radiation field. This energy loss can be detected as a slight increase in the loading on the rf coil. A measurement of the frequency at which the resonance is produced thus provides a direct determination of the magnetic field strength.

It should be noted that when NMR is used as a magnetic-field measuring device, the degree to which the resonant condition registers in the detection electronics has no effect on the accuracy of the field measurement. The quantity that is ultimately measured is the rf frequency, not the signal produced by the resonated nuclei. One need only be able to recognize that a resonance does in fact occur and to note the frequency in order to assign a value to the field strength. The precision of the measurement is dependent only on the frequency determination and on the degree to which the gyromagnetic ratio is known, which is usually five significant figures.

The primary design considerations for an NMR detector compatible with the high-field magnets are as follows: First, the sytem must be capable of a very wide frequency range of operation. In order to cover a field range of 18 tesla (180 kG) a system must span 720 megahertz if protons are to be the sample nuclei, or 200 megahertz if a nuclear sample such as aluminum is used. Second, the system must be highly sensitive to the modulation of the rf carrier induced by the nuclei so that the weak signal variations produced by small-volume samples can be detected. This necessarily implies the need for a low noise detection system. It should be noted that the use of small samples is in general unavoidable since the field inhomogeneity over the sample volume must not exceed the internuclear dipole-dipole field (approx. 10^{-3} T or 10 G). Third, the sample bearing probe must be located a considerable distance from the control and demodulating electronics. The great size of the magnets together with their strong, far reaching fringe fields and cryogenic environment require a departure from the conventional system design. Unlike many conventional designs, the use of rf tuning at the sample-bearing probe and/or the need for interchanging of narrow band probes is to be avoided. When positioned in the magnet, the probe head becomes highly inaccessible. Schemes to trim it by mechanically tuning are prohibitively complex. Remote tuning using solid-state devices such as varactor diodes is also precluded because of the magnetic materials generally used in the construction of these devices. Furthermore, it is desirable to have the option of operating the probe directly in the cryogenic bath. Thus, the use of solid-state devices is undesirable not only for trim controls but also for amplifiers, demodulators, switches, and the like.

The system shown in figure 1 circumvents the need both for trim adjustments at the probe head and the interchanging of numerous narrow band probe heads. Furthermore, no active elements are required in the probe head. Figure 2 shows the complete instrument and probe.

Basically the system is of the single rf coil type (ref. 2), the nuclear sample being located within the rf coil. The system is similar to that used originally by Rollin (ref. 3) in that a steady rf voltage, supplied by an external oscillator, is converted to a proportional rf current. This current then is supplied to the tank circuit, which consists of the probe coil, the interconnecting coaxial transmission line, and the tuning capacitor located in the main electronics package.

Also contained in the sensing head is a small Helmholtz coil which provides a weak alternating perturbation to the magnetic field. By driving the Helmholtz coil with a sinusoidal current derived from an internal 220-hertz oscillator, the field can be made to repeatedly sweep through the nuclear resonance. Thus, with the rf oscillator and the tank circuit tuned to resonance, small power losses, such as those that result from the absorption of energy by the nuclear spins, produce minute changes in the amplitude of the rf voltage across the tank circuit. The effect is a weak 220-hertz modulation. Subsequently, the 220-hertz component of the tank circuit voltage is demodulated, amplified, and converted to a dc output voltage using synchronous (lock-in) detection.

An alternate output is also provided on a built-in cathode ray tube display. The amplified and detected signal is displayed on a time base phase locked to the modulating signal. The CRT display serves as an aid in detecting resonances that are passed through in a transient fashion, and thus would not register in the output of the synchronous detector.

Resonance of the tank circuit is obtained for a series of frequencies corresponding to the conditions for standing waves along the transmission line at nearly half-wave length multiples. This technique, which was originally used by Hill and Hwang (ref. 4), greatly expands the frequency range over which a given probe coil can be used. In addition, it allows for locating the tuning trimmer in the main electronics package rather than in the sensing head.

The length of the transmission line can be arbitrarily chosen so as to remove the main electronics package away from the magnetic fringe field. Operation at a desired frequency is then obtained by inserting a short length of line, appropriately cut, to bring the tank circuit into resonance. Additional details concerning the basis of operation of long-line probes as well as a computer program, which is useful for predicting resonant line modes, is described in the appendix.

Note that the output of the computer program is intended only as an aid in selecting the operational parameters for the system and in predicting the resonant modes of the transmission line. The actual calculation of the field strength is made using equation (1) with f being the actual frequency of operation at the time of nuclear resonance.

The various signal processing stages are discussed in detail in the following sections.

CIRCUIT DESIGN

Radio-Frequency Circuits

A minimum of rf circuitry is used in this detector system which tends to make it more versatile. In particular, aside from the resonant tank circuit no tuned rf stages are used making the rf circuitry usable from approximately 1 to 250 megahertz. These circuits are shown in figure 3(a).

Operation of the rf portion of the system is as follows. An external oscillator provides the rf input at a 50-ohm impedance level. This is matched to the Motorola MC 1110 high-frequency amplifier by a step-up transformer. This amplifier was chosen because of its low feedback capacitance which enhances stable wide band performance. The output is taken directly from the second-stage collector. This provides the requisite high impedance (current source) drive to the probe coil. An rf output level control is provided by varying the voltage applied to pin 5 of the amplifier, by the gain control circuit shown in figure 3(b).

The probe coil is resonated with the 5 to 75 picofarad tuning capacitor. The rf output across it is detected by the 1N916 diode and the demodulated signal passed to the amplifier chain.

Amplifier and Phase Detector

The amplifier sections of this instrument are conventional, consisting of a low-noise preamplifier, a band-limited amplifier with variable gain, and a sharply tuned amplifier. This last amplifier drives the phase detector which is followed by an RC integrator and buffer amplifier.

Low noise is the prime requirement for the preamplifier. This was achieved by using high-gain silicon planar transistors selected for minimum noise at an operating current of 10 microamperes. Noise and ripple from the power supplies were minimized by using active transistor ripple filters along with heavy RC decoupling.

The preamplifier shown in figure 4 is dc coupled throughout and has a dc gain of nearly unity. This makes it possible to drive a rf level meter circuit, with logarithmic response, directly from its output. This meter facilitates tuning the system to resonance at the external oscillator frequency. Potentiometric feedback is provided around the amplifier by resistors R_1, R_2, and R_3. At dc the gain is therefore

$$\left(\frac{R_1 + R_2 + R_3}{R_1 + R_2}\right)$$

or approximately 1.1. As the frequency is increased, C_1 bypasses R_2 so that the gain approaches $(R_1 + R_3)/R_1 \cong 150$ at 220 hertz.

Following the preamplifier is a band-pass amplifier with variable gain built around a Motorola MC 1439G integrated amplifier. It provides gains from 2 to 200 within a pass band centered around 220 hertz. This is followed by a narrowband amplifier using a twin T network in the feedback loop. A Q of about 25 and a gain of 50 are realized in this stage. Together, the two band-limiting amplifiers reject sufficient noise outside the frequency band of interest to prevent saturation of the detector by noise even using the full gain of one-half million to this point. This signal is fed to an oscilloscope to give a fast-response qualitative display.

The amplified signal is also monitored by an overload detector. It gives a visual indication if for any reason the signal exceeds that which the phase detector can handle without distortion. The circuit is built around a Motorola SC 4026 integrated amplifier-trigger circuit. This circuit contains a differential amplifier which is used as a level detector and is referenced to an internally stabilized voltage. Also included in the same integrated circuit is an SCR which is used as a lamp driver.

PHASE DETECTOR

The design of the phase detector is based on that of Faulkner and Harding (ref. 5). It is implemented using a single integrated circuit differential amplifier with current source. Figure 5 shows the basic configuration. Transistor Q_3 and Q_5 are alternately saturated by the 220-hertz clipped (reference phase) waveform derived from the modulation oscillator. Clipping the positive peaks is necessary to prevent the reference signal from driving the saturated transistor more positive than its most negative excursion allowed by the current source.

The input signal to be detected modulates the current source. It, therefore, appears alternately across the load resistors R_6 and R_9 depending on which is saturated. Differentially summing the two outputs as shown in the actual schematic (fig. 6) produces a full-wave phase-detected signal. The circuit is quite simple to implement primarily since it requires so few components and particularly no transformers. This feature would make it attractive for both wide-band or high-frequency phase detection.

A passive RC integrator, followed by a buffer amplifier, conditions and buffers the phase detected signal for meter readout or driving an external plotter, etc.

Low-Frequency Oscillator and Drive

Provision for modulating the magnetic field at 220 hertz is provided in this instrument. The oscillator uses an operational amplifier with a parallel T feedback network as the frequency determining element and is shown in figure 7. This configuration is nearly identical to the narrow band amplifier used in the signal channel providing good frequency tracking with temperature.

The oscillator output is buffered and inverted to provide two reference signals 180° out of phase. These are the two signals that drive the phase detector, the scope trigger, and a variable-phase shift network. The variable-phase shift network is provided to compensate for whatever phase shifts occur in the complete NMR system so that proper phasing between the reference and input signals at the phase detector is possible. Signal levels are 5-volt peak throughout this part of the system.

The phase shifted signal is finally buffered and amplified by the power amplifier to provide in excess of 1 ampere to drive a low impedance coil. High output current simplifies the winding of the Helmholtz coils by requiring fewer turns; output impedances of 0.5, 1.3, and 2.3 ohms are provided to facilitate matching to various coils.

Sweep and Blanking

When using this type detector, it is advantageous to monitor the amplifier output just before it is phase detected. Monitoring at this point makes possible recognition of transient signals that would last an insufficient time to appear at the integrated output. Several things were done to facilitate recognition of the modulation signal amid the inevitable noise. First, the sweep was locked to the reference phase signal and timed to last exactly four full cycles. This makes it easy to see the phase reversal of the signal as it passes through resonance. In addition, narrow blanking pulses were inserted once per reference cycle to further aid the operator in distinguishing between the periodic signal and the noise background. These functions were accomplished by the circuit shown in figure 8. The input signal, selected from either of the reference phase signals, feeds a comparator. The reference signal to the comparator is a variable dc level, selectable so that the comparator transition will occur at any desired level on the input waveform. A blanking signal 3 milliseconds wide is derived from the positive going comparator signal. Its width is determined by R_1 and C_1 and its position relative to the reference signal by the comparator reference. It is thus possible to position the blanked reference at zero crossing or at nearly any position of the reference waveform. This, therefore, provides a visual phase comparison of signals.

Generation of the sweep voltage is done using a constant current source (Q_3) (fig. 8) to charge capacitor C_2. Transistor Q_4 discharges the capacitor at the end of the sweep. Positive synchronization after exactly four cycles is provided by the MC 663P dual flip-flop wired as a divide-by-four circuit. It provides a negative pulse every fourth cycle via capacitor C_3 to turn on Q_4 and end the sweep. An additional feature of this circuit is that a sweep will always be produced even if no input signal is present.

Note that these circuits provide an output ranging from a fraction of a volt to a 5-volt peak. Since this is not a sufficient voltage swing to drive a cathode ray tube (CRT) directly, a commercial miniature CRT indicator unit with built-in x and y amplifiers was provided to give the required small additional gain and gain control.

PERFORMANCE AND OPERATIONAL CONSIDERATIONS

Currently, the NMR system as described is being used to measure and calibrate the high-field cryomagnets at this laboratory. The nuclear sample used for these purposes is a composition of finely divided (-325 mesh) aluminum suspended in an epoxy matrix. Being a metallic sample, the aluminum must be in a powdered state to allow the ac fields to significantly penetrate. This increases the number of nuclei exposed to the rf field and eliminates large scale eddy current losses. Suspending the powder in epoxy serves not only to bind the particles together, but also to insulate the metallic particles one from another. In addition, the protons contained in the epoxy resin are available as an alternate nuclear specie. By utilizing the H^1 resonance in low fields and the Al^{27} resonance in the higher fields, a single probe can be used over a very broad field range. The calibration constants $\gamma/2\pi$ for the H^1 and Al^{27} nuclei are 42.577 and 11.112 megahertz per tesla, respectively.

The aluminum-epoxy sample was fabricated in cylindrical form 6 millimeters long and 3 millimeters in diameter. A three-turn rf coil was wound directly onto the surface of the cylinder and secured with epoxy. This gave an rf coil of approximately 0.3 microhenry inductance which could be used over a 30- to 200-megahertz range. With 12 meters of coaxial transmission line between the probe coil and the resonating capacitor, the operating (resonant) modes are approximately 9 megahertz apart.

Signal-to-noise ratios for this system are typically greater than 10 to 1. Several factors influence the signal-to-noise ratio, principal among them the noise level of the rf oscillator, the Q (quality factor) of the rf coil, line losses in the transmission line, and the homogeneity of the ambient field. The noise level in the amplifier section is less than 1 microvolt referred back to the input at the rf detector. When driven by the rf oscillator, the noise level is raised to several microvolts.

The other factors (a low Q rf coil, line losses, and insufficient field homogeneity) all serve to degrade the system's sensitivity. For a discussion of those factors affecting spectrometer sensitivity the reader is referred to a paper by Wind (ref. 6). However, aside from the general considerations discussed therein, one should be aware that the choice of the number of turns and the dimensions of the coil are crucial in preserving a high Q for the intended frequency range of operation. Since the Q of a coil exhibits a maximum at some frequency, the choice of coil parameters should be made to locate that maximum within or to span the frequency range of interest.

The choice of transmission line length has two effects. The longer the length of line, the smaller the frequency interval between operating modes. However, line losses increase with line length. Thus, the choice of line length must be a compromise between the number of operating modes desired for a given frequency range and the signal-to-noise ratio to be tolerated.

Field homogeneity, or the lack of it, is likely to be the limiting factor in the application of an NMR system. Here again, a compromise must be struck. The sample volume must be small enough to ensure that the field differential over that volume is not so great as to broaden the resonance to the point of obscurity. This requires that the field differential over the sample by typically less than 0.001 or 0.002 tesla (10 or 20 G). Yet the sample volume must not be so small that it contain an insufficient number of nuclei to generate a detectable signal. Measurements with this system indicate that sample volumes as small as 0.01 cubic centimeter can be used. The ability of this system to use such small sample volumes extends its use to many solenoidal magnet applications or other small volume, high field, magnets.

CONCLUDING REMARKS

The circuit design and a discussion of the operation of a highly sensitive, portable, nuclear magnetic resonance detector has been presented. In addition, a method and computer program for calculating the resonant modes of a probe cable of arbitrary length is included.

The operation of this NMR detector as a magnetometer in very high fields and at low temperatures is indicative of the versatility that can be achieved with the basic Rollin circuit in combination with the long resonant line. With signal-to-noise ratios of 10 to 1 and greater, as attained by this system, no difficulty is experienced in recognizing the occurrences of the nuclear resonances. Thus, the system's sensitivity is more than adequate for magnetometer service since one need only be able to identify the presence of a signal, regardless of the signal-to-noise ratio.

The resonant transmission line technique not only makes it possible to remove sensitive electronic components from the influence of the high fields and cryogenic environment, but also serves as the basis for extending the usable frequency range of any given probe coil. One consequence of this technique, however, is that operation is limited to the resonant frequencies of the transmission line. This need not be a severe limitation, however, since it is possible to achieve operation at any desired intermediate frequency merely by the addition or removal of an appropriate length of line.

The ability of the system to produce high signal-to-noise ratios with small sample volumes suggests a much broader range of applications. The possibility exists, for example, of applying the system to very high-field NMR spectrometry. It might also be applied to situations in which close proximity between the rf coil and the other electronics is not possible due to such factors as physical, thermal, or radiation conditions.

Alternately, it might be used in situations wherein the probe coil need not be remotely located with respect to the demodulating electronics, but which require a system having low-noise detection such as when working with dilute or small volume samples. The system is limited only in that it is not amenable to a swept-frequency operation. The use of a separate external oscillator, however, is really an advantage because it eliminates the need for critical circuit adjustments in order to excite a desired mode of the transmission line.

For any of these applications, the compact portability of the system can be an advantage as well as a convenience. The use of integrated circuits allows for a compact design and one that can be readily duplicated.

Lewis Research Center,
National Aeronautics and Space Administration,
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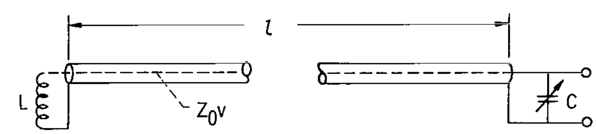
720-03.

APPENDIX - RESONANT MODES OF LONG LINE NMR PROBES

The ability to operate the rf sample coil of an NMR detector at distances considerably removed from the rf source and the demodulating electronics is a consequence of the nature of wave propagation in the interconnecting transmission line. The technique is based on the fact that the voltages and currents established along a transmission line exist with a periodicity. That periodicity is governed both by the characteristics of the line and by the impedances terminating each end of the line. Since there is this periodicity in the voltage and current, it follows that the point-by-point impedance along the line must also vary with the same periodicity. Hence, it is possible to establish a resonant condition for a series of frequencies such that the inductive reactance presented by the transmission line to the tuning capacitor will equal the capacitive reactance. The conditions for resonance can be developed analytically as follows.

Sketch (a) shows the elements that comprise the rf tank circuit: (1) the sample coil of inductance L, (2) the tuning capacitance C, and (3) the interconnecting transmission line of length l. The transmission line is also characterized by an impedance Z_0 and a velocity of propagation v.



(a)

It can be shown (ref. 7) that the actual impedance of the coil Z_L when seen at the capacitor end of the line is transformed by the line to an apparent impedance Z_L' according to the relation

$$Z_L' = Z_0 \frac{\left(\dfrac{Z_L}{Z_0}\right) \cosh \sqrt{Z_1 Y_1}\, l + \sinh \sqrt{Z_1 Y_1}\, l}{\cosh \sqrt{Z_1 Y_1}\, l + \left(\dfrac{Z_L}{Z_0}\right) \sinh \sqrt{Z_1 Y_1}\, l} \tag{1}$$

The quantity Z_1 is the series impedance per unit length of the transmission line ($Z_1 = R_1 + j\omega L_1$), and Y_1 is its shunt admittance per unit length ($Y_1 = G_1 + j\omega C_1$). Here R_1, L_1, G_1, and C_1 are the distributed resistance, inductance, leakage, and capacitance, respectively, for the line. Ordinarily for the frequency range of interest

$\left(R_1/\omega L_1\right)^2 << 1$ and $\left(G_1/\omega C_1\right)^2 << 1$. When these conditions prevail, the propagation constant $\sqrt{Z_1 Y_1}$ is essentially an imaginary quantity of magnitude $\omega\sqrt{L_1 C_1}$. And since $v = \left(1/\sqrt{L_1 C_1}\right)$, equation (1) can be reduced to

$$Z_L' = Z_0 \frac{\left(\frac{Z_L}{Z_0}\right)\cos\left(\frac{\omega l}{v}\right) + j\sin\left(\frac{\omega l}{v}\right)}{\cos\left(\frac{\omega l}{v}\right) + j\left(\frac{Z_L}{Z_0}\right)\sin\left(\frac{\omega l}{v}\right)} \tag{2}$$

The condition for resonance is that $(Z_C)^* = Z_L'$, or

$$\frac{-1}{j\omega C} = Z_0 \frac{\left(\frac{j\omega L}{Z_0}\right)\cos\left(\frac{\omega l}{v}\right) + j\sin\left(\frac{\omega l}{v}\right)}{\cos\left(\frac{\omega l}{v}\right) + j\left(\frac{j\omega L}{Z_0}\right)\sin\left(\frac{\omega l}{v}\right)} \tag{3}$$

which reduces to the form

$$\tan\left(\frac{\omega l}{v}\right) = \frac{Z_0 C}{Z_0^2 C + L}\left(\frac{1}{\omega C} - \omega L\right) \tag{4}$$

For a given set of values of the parameters Z_0, l, v, C, and L, this equation is satisfied by a series of frequencies - the resonant modes of the system. The individual modes can be designated by the quantity m which can take on integer values ranging from 1 to infinity and are included explicitly in equation (4) as

$$\tan\left[\frac{\omega l}{v} - (m - 1)\pi\right] = \frac{Z_0 C}{Z_0^2 C + L}\left(\frac{1}{\omega C} - \omega L\right) \tag{5}$$

$$m = 1, 2, 3, \ldots$$

In using this expression it seems most useful to consider a given probe (i.e., coil inductance L) in conjunction with a given transmission line, and ask what are the frequencies of the resonant modes to be expected with a specified tuning capacitance C and line length l. However, solving the equation for ω is not straightforward since it is a transcendental equation. It can be readily solved, though, by machine calculation in an iterative fashion. The equation can be rewritten in form $\omega = f(\omega)$

$$\omega = \left(\frac{v}{l}\right)\left\{(m - 1)\pi - \arctan\left[\frac{Z_0 C}{Z_0^2 C + L}\left(\omega L - \frac{1}{\omega C}\right)\right]\right\} \tag{6}$$

$$m = 1, 2, 3, \ldots$$

and can be solved to within a preselected error of the correct value for ω by an iterative process similar to that of the Newton-Raphson method.

The digital computer program listed in this appendix is a FORTRAN IV program that can be used to generate solutions to equation (6) by the iteration technique. The input to the program is via four data cards. The first contains the coil inductance, in microhenries, of the sample-bearing coil, and a probe designation number for future identification. The second card contains the tuning range, C_{MIN} and C_{MAX} in picofarads, of the tuning capacitor. Two values of C are specified in order that the frequency range over which the system can be tuned for each mode might be determined. A third card contains the parameters for the transmission line: its cable number (used for identification purposes), its relative velocity of propagation in percent, and its characteristic impedance Z_0 in ohms. The fourth card is used to specify a series of line lengths. Beginning with the shortest length specified, the program calculates the resonant modes for that length, then proceeds in incremental steps to the longest length. Values for the minimum and maximum lengths and the increment in feet are provided by the data card.

The resonant modes for each line length are printed on individual pages. Table I is a typical printout for one particular line length. This printout is a tabulation of both the tunable frequency range of each resonant mode and the corresponding magnetic fields for which resonance of the H^1 and Al^{27} nuclei occur.

Built into the program, and subject to modification, are the following. First, the calculation of resonant modes at any particular line length ceases and advances to the next line length when either 50 modes are attained or the frequencies exceed 320 megahertz. Second, the error for closure of the iteration process is set at 1 kilohertz. This is well below the setability of the rf oscillator and is, therefore, negligible when searching for resonances. Closure of the iteration process to within this error is rapid, requiring usually only two or three cycles.

TABLE I. - TYPICAL TABULATION OF THE RESONANT MODES OF A LONG-LINE NMR PROBE CALCULATED USING THE COMPUTER PROGRAM

[The tunable frequency range and corresponding resonant fields for the H^1 and Al^{27} nuclei are listed consecutively. The calculations are for a 35 foot length of transmission line with a 0.05 μH coil and a 5 to 75 pf capacitor.]

PROBE NO. AL-815 *3*   RG 58/U COAX   LENGTH = 35 FEET

MODE	TUNING RANGE (MEGAHERTZ)	PROTON RES. (KILOGAUSS)	ALUMINUM RES. (KILOGAUSS)
1	4.24 - 4.53	1.00 - 1.05	3.82 - 4.08
2	12.75 - 13.59	3.00 - 3.19	11.48 - 12.23
3	21.33 - 22.65	5.01 - 5.32	19.19 - 20.38
4	29.99 - 31.71	7.04 - 7.45	26.99 - 28.54
5	38.73 - 40.77	9.10 - 9.58	34.85 - 36.69
6	47.54 - 49.84	11.17 - 11.71	42.79 - 44.85
7	56.42 - 58.91	13.25 - 13.84	50.77 - 53.02
8	65.35 - 67.99	15.35 - 15.97	58.81 - 61.19
9	74.31 - 77.07	17.45 - 18.10	66.87 - 69.36
10	83.31 - 86.16	19.57 - 20.24	74.97 - 77.54
11	92.33 - 95.25	21.68 - 22.37	83.09 - 85.72
12	101.37 - 104.35	23.81 - 24.51	91.23 - 93.91
13	110.44 - 113.46	25.94 - 26.65	99.38 - 102.10
14	119.52 - 122.57	28.07 - 28.79	107.56 - 110.30
15	128.61 - 131.68	30.21 - 30.93	115.74 - 118.50
16	137.72 - 140.80	32.35 - 33.07	123.94 - 126.71
17	146.83 - 149.93	34.49 - 35.21	132.14 - 134.92
18	155.96 - 159.06	36.63 - 37.36	140.35 - 143.14
19	165.10 - 168.19	38.78 - 39.50	148.58 - 151.36
20	174.24 - 177.33	40.92 - 41.65	156.81 - 159.59
21	183.40 - 186.48	43.07 - 43.80	165.04 - 167.82
22	192.56 - 195.63	45.23 - 45.95	173.29 - 176.05
23	201.72 - 204.78	47.38 - 48.10	181.53 - 184.29
24	210.89 - 213.94	49.53 - 50.25	189.79 - 192.53
25	220.07 - 223.10	51.69 - 52.40	198.05 - 200.77
26	229.25 - 232.26	53.84 - 54.55	206.31 - 209.02
27	238.43 - 241.42	56.00 - 56.70	214.57 - 217.26
28	247.62 - 250.59	58.16 - 58.86	222.84 - 225.52
29	256.82 - 259.77	60.32 - 61.01	231.12 - 233.77
30	266.01 - 268.94	62.48 - 63.17	239.39 - 242.03
31	275.21 - 278.12	64.64 - 65.32	247.57 - 250.29
32	284.42 - 287.30	66.80 - 67.48	255.95 - 258.55
33	293.62 - 296.48	68.96 - 69.63	264.24 - 266.81
34	302.83 - 305.67	71.13 - 71.79	272.53 - 275.08
35	312.04 - 314.85	73.29 - 73.95	280.82 - 283.35
36	321.26 - 324.04	75.45 - 76.11	289.11 - 291.62

```
C  THIS PROGRAM LISTS THE RESONANT MODES OF LONG-LINE (LOW LOSS) NMR
C          PROBES.  THE TUNING RANGE FOR EACH MODE IS CALCULATED FOR A
C          SERIES OF LINE LENGTHS.  THE CORRESPONDING NMR FIELDS FOR
C          PROTONS AND METALLIC ALUMINUM ARE COMPUTED.
C
C  INPUT FROM DATA CARDS -
C       1. PROBE DESIGNATION NUMBER, AND COIL INDUCTANCE (UH).
C       2. CMIN AND CMAX (PF) OF TUNING CAPACITOR.
C       3. CABLE TYPE, REL. VEL. OF PROP. (PERCENT), LINE Z (OHMS).
C       4. LINE LENGTHS - MINIMUM, MAXIMUM, AND INCREMENT (FEET).
C
      DIMENSION  PROBE(2), CABLE(2), GAMMA(2), H(2,2), X(2,2), FX(2,2),
     1           A(2), C(2), XSTART(2), FREQ(2)
      REAL  L
      READ(5,500) PROBE, COIL
  500 FORMAT(2A6,2F12.4)
      READ(5,501) CMIN, CMAX
  501 FORMAT(2F12.0)
      READ(5,500) CABLE, VREL, Z
      READ(5,502) LMIN, LMAX, INC
  502 FORMAT(3I6)
C  ADJUST $TCP CARD ACCORDING TO THE NUMBER OF LINE LENGTHS SELECTED.
C
      L=COIL*1.0 E-6
      C(1)=CMAX*1.0 E-12
      C(2)=CMIN*1.0 E-12
      V=VREL*2.99793 E6
      A(1)=(Z*C(1))/(Z*Z*C(1) + L)
      A(2)=(Z*C(2))/(Z*Z*C(2) + L)
      PI=3.14159265
      F=2000.*PI
      GAMMA(1)=42.577
      GAMMA(2)=11.112
C
      DO 8 LENGTH=LMIN,LMAX,INC
      RLGTH=LENGTH
      B=V/(RLGTH*0.3048006)
      XSTART(1)=6.0 E6
      XSTART(2)=6.0 E6
      WRITE(6,602)  PROBE, CABLE, LENGTH
  602 FORMAT(1H1,5X,10HPROBE NO.  ,2A6,6X,2A6,5H COAX,
     1         5X,8HLENGTH =,I3,5H FEET//
     2         6X,4HMODE,7X,12HTUNING RANGE,9X,11HPROTON RES.,9X,
     3         13HALUMINUM RES./
     4         17X,11H(MEGAHERTZ),10X,11H(KILOGAUSS),10X,11H(KILOGAUSS)//)
C
      DO 7 M=1,50
      DO 4 J=1,2
      X(1,J)=XSTART(J)
      N=0
      K=0
      RM=M-1
      FX(1,J)=B*(RM*PI - ATAN(A(J)*(X(1,J)*L - 1./(X(1,J)*C(J)))))
      X(2,J)=FX(1,J)
    1 FX(2,J)=B*(RM*PI - ATAN(A(J)*(X(2,J)*L - 1./(X(2,J)*C(J)))))
      CALL TANDAD(X,FX,E,N,K,J)
      IF(N.GT.20) GO TO 6
      GO TO (1,2),K
    2 FREQ(J)=(X(2,J)*1. E-6)/(2.*PI)
```

```
      XSTART(J)=X(2,J)
      DO 3 I=1,2
    3 H(J,I)=(FREQ(J)*10.)/GAMMA(I)
    4 CONTINUE
C
      WRITE(6,603) M, FREQ, H
  603 FORMAT(7X,I2,3(6X,F6.2,3H - ,F6.2))
    5 IF(ABS(X(2,2)).GT.2.0 E9) GO TO 8
      GO TO 7
    6 WRITE(6,603) M
    7 CONTINUE
    8 CONTINUE
      WRITE(6,600)
  600 FORMAT(1H1)
      STOP
      END


      SUBROUTINE TANDAD(X,FX,E,N,K,J)
      DIMENSION X(2,2),FX(2,2),XX(2),DERFX(2)
      IF(ABS(X(2,J)-FX(2,J)).LT.E) GO TO 2
    1 K=1
      DERFX(J)=(FX(2,J)-FX(1,J))/(X(2,J)-X(1,J))
      XX(J)=(FX(2,J)-X(2,J)*DERFX(J))/(1.-DERFX(J))
      X(1,J)=X(2,J)
      X(2,J)=XX(J)
      FX(1,J)=FX(2,J)
      N=N+1
      RETURN
    2 K=2
      RETURN
      END
```

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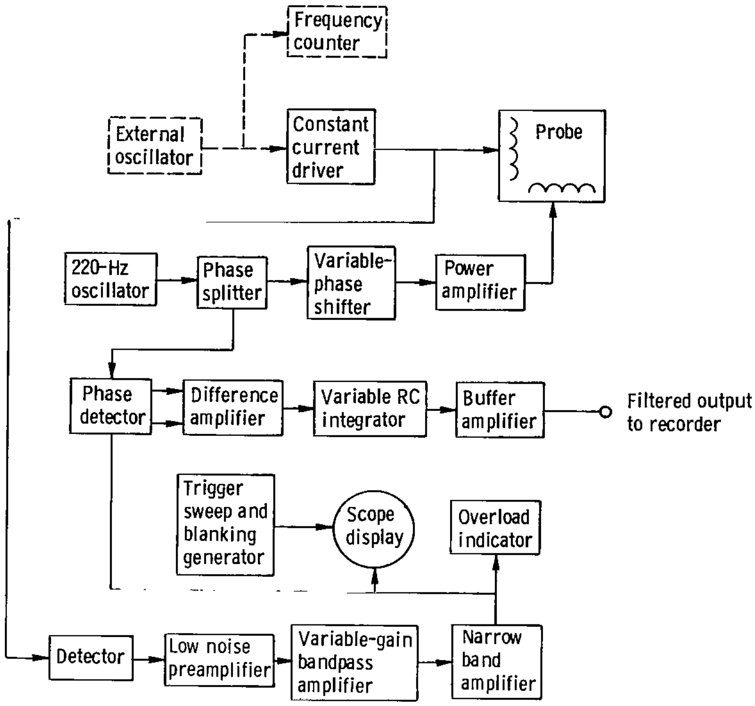

Figure 1. - Nuclear magnetic resonance (NMR) detector system block diagram.

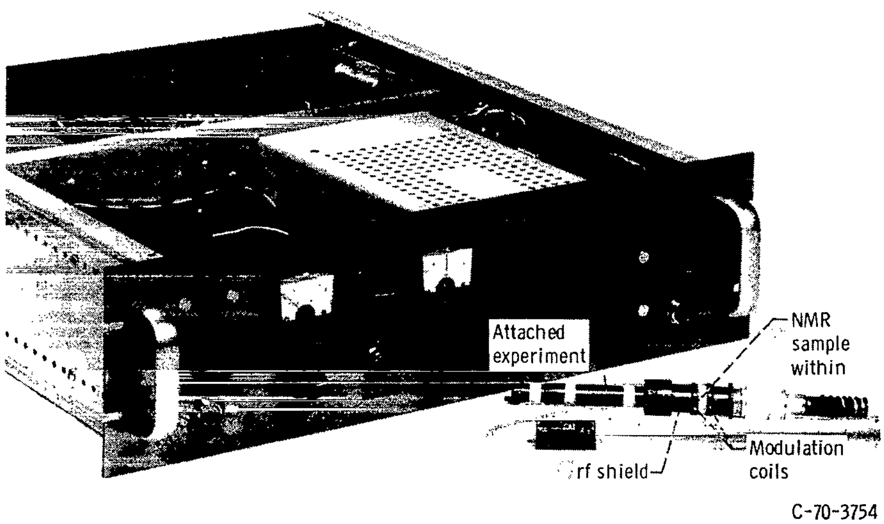

Figure 2. - Nuclear magnetic resonance detector electronics package and probe tip. The lower (left) end of probe is an attached experiment. The NMR sample is located within the rf shield between the Helmholtz modulation coils.

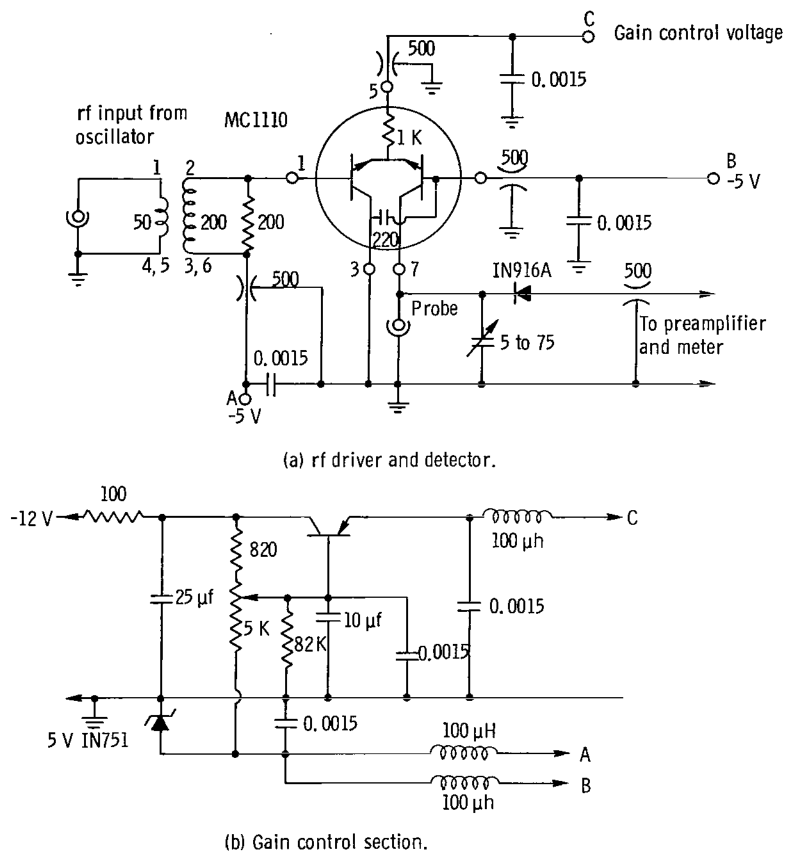

Figure 3. - Radiofrequency drive and control circuits. (Capacitor values less than one are in µF; values greater than one are in pF unless otherwise stated.)

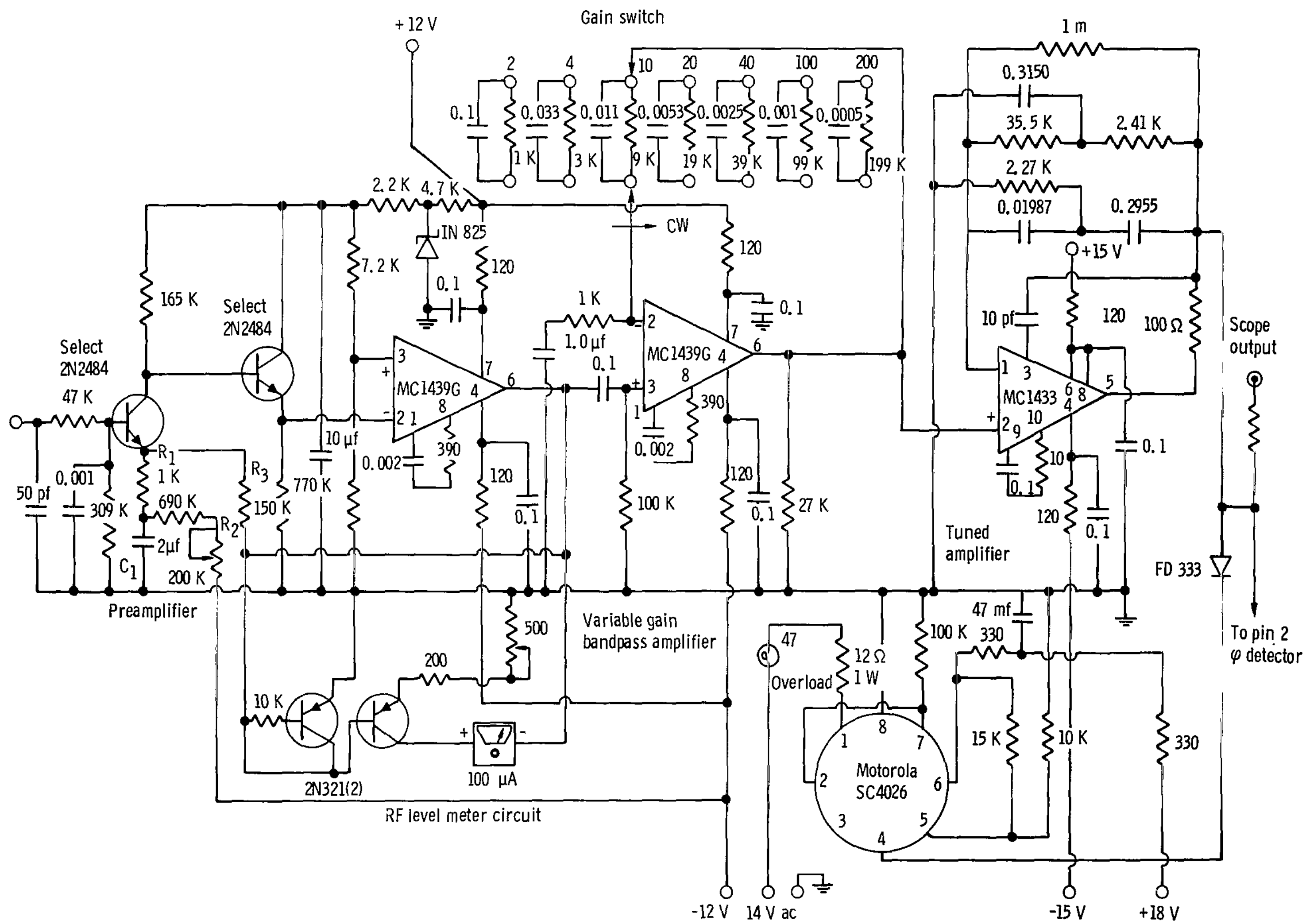

Figure 4. - Signal amplifiers. (Values <1 are in μF and values, >1 are in pF unless otherwise stated.)

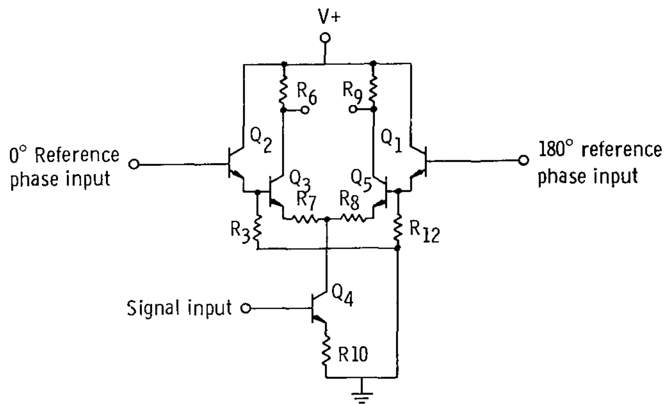

Figure 5. - Basic phase sensitive detector (RCA CA3001).

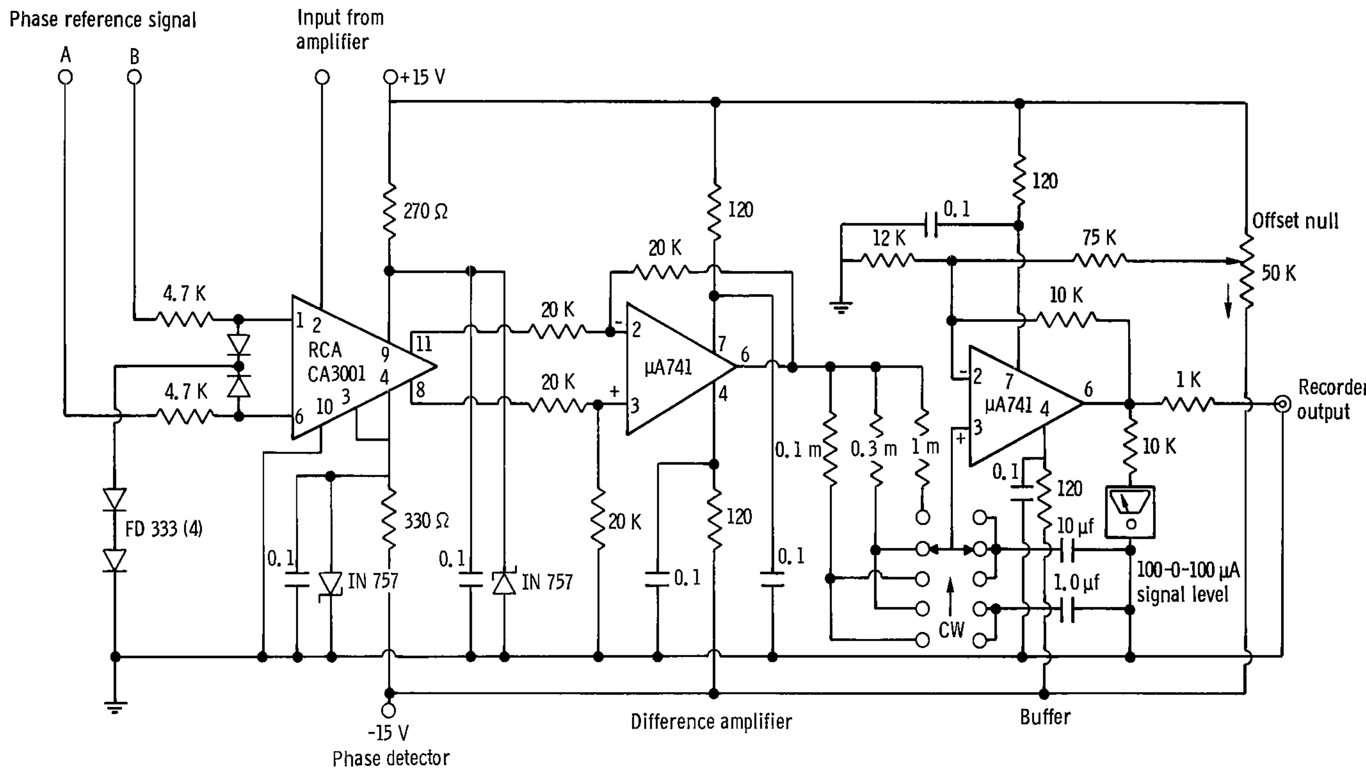

Figure 6. - Phase detector and output stages. (Values <1 are in μF and values >1 are in pF unless otherwise stated.)

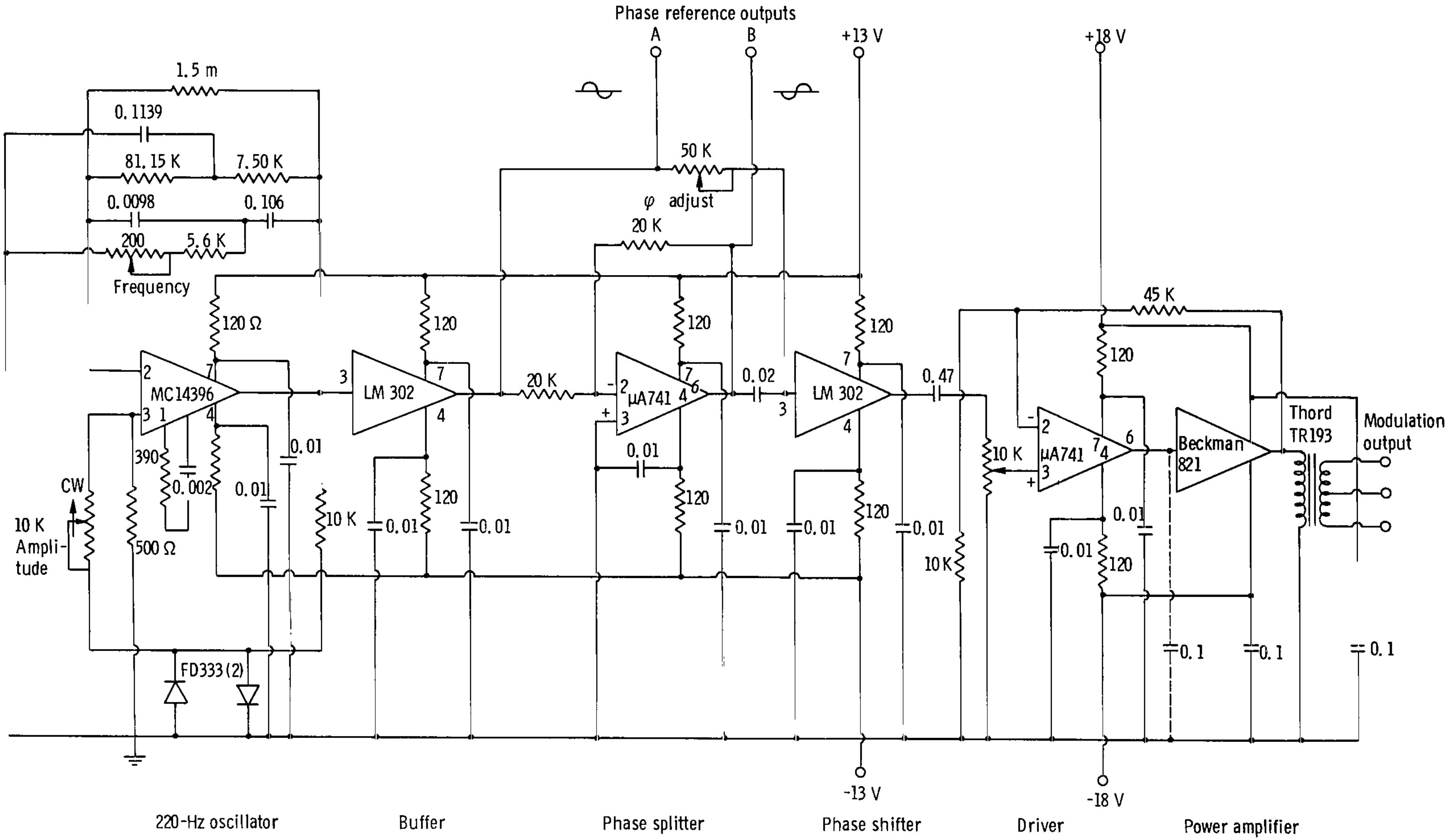

Figure 7. - Oscillator reference driver. (Values <1 are in μF; values >1 are in pF unless otherwise noted.)

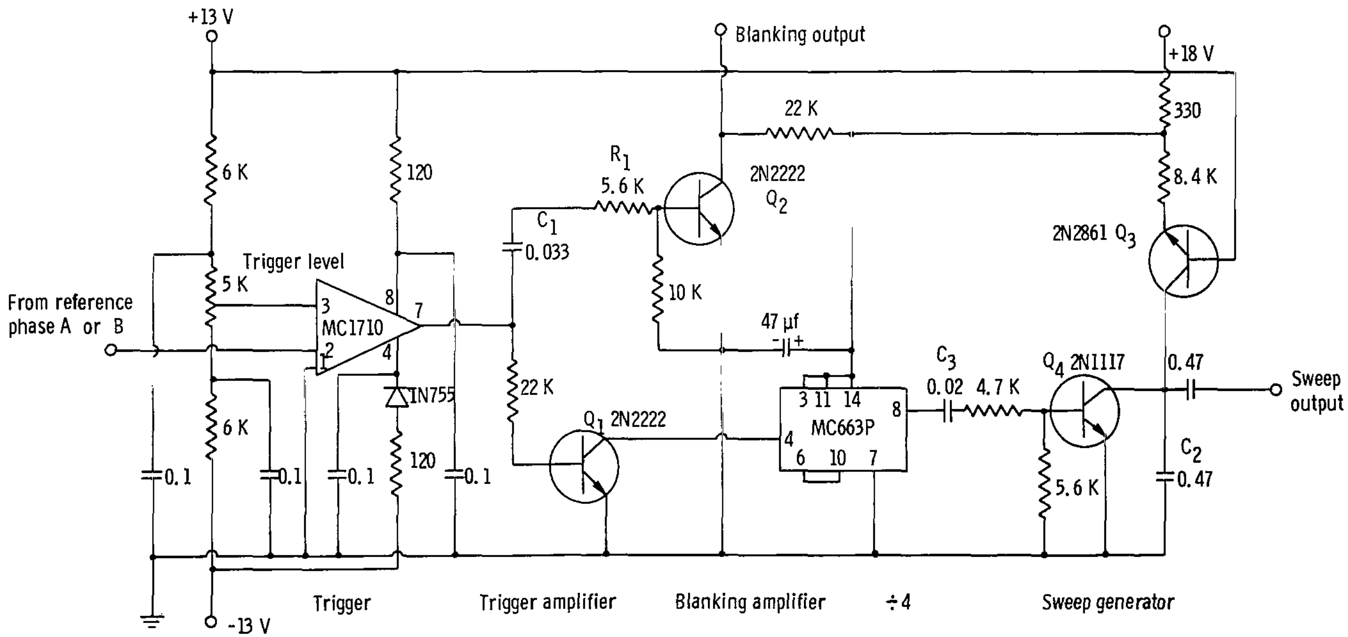

Figure 8. - Sweep generator and trigger. (Values <1 are in µF and values >1 are in pF unless otherwise stated.)

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