I. INTRODUCTION

Nuclear magnetic resonance (NMR) spectroscopy is widely recognized as a powerful analytical technique with major applications in chemistry, material science, biochemistry, and medicine. Applications of NMR spectrometers in such fields typically require state-of-the-art instrumentation, which is costly to procure and equally costly to maintain. Yet there are a number of potentially important uses of NMR spectroscopy that do not necessitate such sophisticated instrumentation, but rather are limited in practical terms by constraints such as cost, portability, and other considerations. Examples of commercial applications involve industrial quality control functions and process control analysis. Such investigations typically generate a large throughput and may require several units in parallel or units measuring at different stages of the processes operating with minimal user assistance. Moreover, there are scientific applications which often demand custom engineering or adaption of analytical instruments; examples include NMR spectroscopy, NMR field cycling spectroscopy, microwave spectroscopy, electron spin resonance (ESR) spectroscopy, and logical considerations. Other scientific applications involve data acquisition in the field, e.g., geology and archeology, where the use of state of the art NMR instrumentation is impractical. Finally, an important contribution is that accessibility to low cost practical NMR instrumentation may open up teaching possibilities at the college or even secondary school level. The goal of developing such a personal computer (PC) based NMR standard is facilitated by existing technologies including logic cell arrays, direct digital frequency synthesis, use of PC-based electrical engineering software tools to fabricate electronic circuits, and the use of permanent magnets based on neodymium-iron-boron alloy. Utilizing such an approach, we have been able to place essentially an entire NMR spectrometer console on two printed circuit boards, with the exception of the receiver and radio frequency power amplifier. Future upgrades to include the deuterium lock and the decoupler unit are readily envisioned. The continued development of such PC-based NMR spectrometers is expected to benefit from the fast growing, practical, and low cost personal computer market.
available for personal computers at affordable cost. Advances have also been made in frequency generation utilizing direct digital synthesis (DDS) which can produce digitized samples of sine waves capable of driving a digital-to-analog (DAC) converter. Although the alternative strategy of employing an analog frequency synthesizer has the advantage of generating higher frequencies than DDS and is in widespread use, analog technology is more expensive, requires far more space, and is intrinsically more complicated and thus, far more expensive.

In this work a personal computer-based NMR spectrometer has been designed and fabricated utilizing the above breakthroughs in digital design logic and digital signal generation. The substantially reduced cost and size opens up the applicability of NMR methodologies to environments beyond that of a typical research or industrial laboratory. The present instrument provides for ease of installation and operation of radio frequency control, signal detection, data acquisition, and data processing. Such a personal computer-based NMR spectrometer can be applied to a variety of scientific fields where cost, flexibility, and portability are essential, as well as engineering applications where quality control functions are required. Future applications are readily envisioned including the development of low cost instrumentation for field cycling NMR spectroscopy and magnetic resonance imaging.

II. EXPERIMENT

The pulse programmer and DDS/modulator printed-circuit boards were fabricated for use with an existing 0.47-T aluminum-nickel alloy permanent magnet. Digital design of the pulse programmer and the modulator were produced with use of electrical engineering design software (Visionics). By utilizing logic configured gate arrays (LCA) (XILINX) the majority of the digital logic could be placed into the arrays. The printed circuit board information was then converted to standard Gerber protocol for photoplotting purposes, and then fabricated by a local printed circuit manufacturer (Cadtek, Tucson, AZ). Electrical schematics and board layout prints exist for each printed circuit board, and as well the external receiver and amplifier. The operation of the PC-based NMR spectrometer was initially tested using the 0.47-T aluminum-nickel permanent magnet. In preliminary studies the preamplifier, receiver, and rf amplifiers were used from another NMR spectrometer. To accommodate asphalt samples of 4-in. diam a novel permanent magnet based on neodymium-iron-boron alloy was developed utilizing a magnetic dipole technique. For this new magnet a receiver system was fabricated and interfaced with the pulse programmer and DDS/modulator so that the receiver gain could be controlled directly by the microcomputer. Additional optical isolation of the amplifier and receiver from the microcomputer yielded improved sensitivity and eliminated artifacts produced by the computer. A 100-W rf amplifier was fabricated to drive a 1000-W rf amplifier boost (Henry Radio, Los Angeles, CA).

III. RESULTS

A. Overall block diagram

Figure 1 shows a block diagram of the personal computer-based NMR spectrometer. An Intel (Santa Clara, CA) 80386 microprocessor is the sole processor for the entire system and can be easily upgraded to 80486 and subsequent generations. The disk interface is also an item commercially available for personal computers (Everex Systems, Fremont, CA). An ethernet card (3COM, Santa Clara, CA; model 3C503) for transferring the acquired data to other destinations is also part of the hardware configuration. Several graphics interface boards including enhanced graphics adapters (EGA) and very enhanced graphics adapters (VGA) have been successfully tested with this spectrometer configuration. The processing software (PCMR) contains a routine to adjust to a particular resolution of the video interface.

The pulse programmer we have constructed is an 80-bit wide word and 8-K deep programmable memory space. By taking advantage of logic cell arrays one has the flexibility to implement new hardware improvements simply via the software. Hardware changes on the schematic level alter the netlist of the circuit; the newly produced netlist is then converted to XILINX netlist format (XNF). The generic XNF file is converted to a specific Xact LCA file depending on the version and gate density of the logic cell array, which is submitted to the automatic place and route (APR) program for placement and interconnect net routing. The resulting binary code file comprises the actual gate array information which is downloaded by the microcomputer in order to configure the LCA. It is noteworthy that this approach has al-
The radio frequency modulator utilizes a dual direct digital synthesizer (DDS) from Qualcomm (San Diego, CA; model Q2334) for the frequency source. Frequency and phase can be set by the pulse programmer or computer. The phase resolution is better than 1° and the frequency can be set by the pulse programmer or computer. The DDS/modulator board includes virtually all the radio frequency generation needed for the PC-based NMR spectrometer.

A photograph of the pulse programmer and modulator boards is shown in Fig. 2 and illustrates clearly the compactness of the PC-based NMR spectrometer. The two boards are connected by two plastic screws and occupy two slots in the microcomputer bus.

The receiver system has been configured to accommodate fast-free-induction decays with short values of $T_2$ which are needed for solid and liquid crystalline samples. A typical recovery time of 10 $\mu$s can be expected for a carrier frequency of 20 MHz utilizing an Avantek (Santa Clara, CA; model UTO-221) preamplifier. The receiver incorporates components including operational amplifiers having a high slew rate specification (200 V/µs) to facilitate wide line spectroscopy. Special care has been given to achieving optical isolation of all connections to the personal computer in order to eliminate computer frequency noise. A 12-bit digitizer with 1-MHz analog-to-digital conversion rate is used to acquire the data into the PC. The digitizer is commercially available and includes an on-board memory buffer of 1 Mbyte (Keithley Metrabyte Corporation, Taunton, MA; model DAS-50). All of these items are easily installed and fulfill the basic functions of a NMR spectrometer.

A photograph of the pulse programmer and modulator boards is shown in Fig. 2 and illustrates clearly the compactness of the PC-based NMR spectrometer components. The boards occupy two slots on the microcomputer motherboard, and have the rf connections positioned in the standard fashion on the rear side of the computer chassis. The boards can be installed in a manner analogous to that of printed circuit boards in a microcomputer by a suitably qualified specialist. A more detailed description of the pulse programmer and frequency direct digital synthesis/modulator boards is given below.

### B. Pulse programmer board

The block diagram of the pulse programmer is illustrated in Fig. 3. The pulse programmer board consists of 80 K of static memory and two logic cell arrays containing all of the digital logic needed to generate the 32 programmable real time clock (RTC) pulses. (The latter are dc pulses which can be varied in their width and number of repetitions.) In the present case this is done individually for each of the 32 RTC pulses. A provision is made to expand the total number of RTC pulses through introduction of an additional printed circuit board. The input/output (I/O) section is in conformance with the industry standard personal computer bus system. The static memory is divided into the pulse programmer memory and the delay memory. The delay memory contains information about how long a particular instruction lasts (e.g., an instruction to turn on a real time pulse with a pulse width of 10 $\mu$s would have a duration of 10 $\mu$s). The size of the delay memory is 16 bits by 8 K allowing for 8192 different durations. The 16 bit word is loaded into the instruction delay generator, which consists of a 12 bit binary

![Block diagram of the pulse programmer board showing how instruction cycles can be varied to generate real time clock pulses (see text). The RTC pulse controls the time intervals for the rf pulse width, receiver gating, acquisition interval, and other parameters. The architecture of the pulse programmer is comparable to that of a microcomputer. The pulse programmer can execute simple operations, e.g., branching to another location; moreover, one can program the duration of each instruction which can have different values during the pulse program. With this approach, all the parameters of the pulse (e.g., the pulse width and interval between pulses) can be varied individually, so that the user can implement any pulse sequence or experiment with new pulse sequences.](image)
C. Modulator board

A block diagram of the DDS/modulator board is illustrated in Fig. 4. The DDS generates the radio frequency which is modulated (e.g., turned on or off by the pulse programmer signals). The modulator can be controlled both by the PCMR software through the PC bus or by the pulse programmer using the real time pulse; a multiplexer combines the two sources. Radio frequency pulse shape and phase are, in general, controlled by the pulse programmer, with a phase resolution of $1^\circ$. The frequency and amplitudes are in general set by the processing software, the frequency resolution is 1 Hz and the amplitude switching time is 10 $\mu$s. For testing purposes software control over the modulator is extremely helpful. The gate array from Qualcomm (model Q2334) contains two independent direct digital synthesis circuits which can generate independent frequencies and phases for both circuits. Radio frequency sine waves are generated by the digital to analog converter (Sony, El Segundo, CA; model CX20202A). The two radio frequencies are then doubled and split into a total of four outputs (channels 1–4). The amplitudes of channel 1 and channel 4 are controlled by an attenuator (Mini-Circuits, New York, NY; model PAS-3); subsequently all four channels are gated by ring modulators (RM) (Mini-Circuits; model TSM-1) which are controlled by the pulse programmer. (Ring modulators are frequency mixers in which the radio frequency is mixed with dc pulses so that the output is on or off corresponding to the dc pulse level being high or low.) The two 12 bit digital to analog converters (Burr Brown, Tucson, AZ; model No. DAC1201) drive the two attenuators (e.g., channels 1 and 4) and can be set by either the computer or directly by the pulse programmer. By including an additional frequency mixing unit the range can be extended to reach proton ($^1H$) frequencies corresponding to the highest commercially available NMR magnetic field strengths (as high as 750 MHz). Each channel has two independently modulated outputs where one of them includes a voltage controlled attenuator to enable pulse amplitude control and pulse shaping. The other output has a fixed amplitude which makes it suitable as a reference frequency source, which is needed for phase detection in the receiver system.

D. Receiver

Figure 5 depicts the receiver block diagram, in which both the preamplifier and the receiver are external units and are connected to the computer via coaxial cable. The preamplifier is powered with a 12-V dc source which is supplied by the receiver. The receiver includes frequency demodulation and quadrature phase detection. Quadrature detection improves the sensitivity by a factor of $\sqrt{2}$ and also enables phase cycling, which minimizes baseline offsets of the free induction decay (FID) and averages inequalities of the two quadrature channels (e.g., 90° phase shift and gain differences). The preamplifier consists of two wideband cascadable amplifiers (Avantek; model UTO-221). Each amplifier has a bandwidth ranging from 5 to 200 MHz and a noise figure of less than 2 dB and gain of 24 dB. During the radio frequency pulse period of a NMR experiment two antiparallel diodes protect the preamplifier against high voltages. The limiter (Avantek; model UTL-1001) prevents the transients due to the transmitter from being passed into the receiver, which would increase the recovery time. (The recovery time or dead time of a receiver is the period between the radio frequency pulse and the first undistorted data point of the FID.) A short dead time is required for short values of $T_2$ or fast decaying free induction decays which are

![Diagram](image-url)
FIG. 5. Block diagram of the receiver and preamplifier circuits. With such a compact approach the receiver and preamplifier modules can be easily utilized for new applications without any further modifications.

typical of solids and liquid-crystalline samples. The achievable dead time for a 20-MHz carrier frequency is on the order of 10 μs. Both the UTO-221 amplifiers and the limiter are mounted on a printed circuit board (Avantek; model TB-4) and shielded by an aluminum enclosure (Avantek; model TC-4X) to ensure optimal performance. The amplified NMR signal is then routed into the receiver and further amplified by two wideband hybrid amplifiers (Motorola, Phoenix, AZ; model MWA130). A voltage controlled attenuator (Mini-Circuits; model PAS-3) with a range from 0 to 40 db attenuates the receiver gain. The attenuator is controlled by the computer via optical isolators (Motorola; model 6N137) and an 8 bit digital-to-analog converter (Burr Brown; model DAC08). The overall gain of the preamplifier and receiver has a range from 70 to 110 dB. Because such microcomputers typically generate a large spectrum of electronic noise, it is desirable to optically isolate all control signals between the personal computer and the receiver. The NMR signal is then transmitted through a low-pass filter following by a splitter and by two ring modulators (Mini-Circuits; model TSM-1) to achieve phase demodulation, i.e., mixing of two frequencies. The frequencies utilized for the phase demodulation of the NMR signal are generated from the reference radio frequency arising from the modulator, which is split into two rf signals in the receiver with phase shifts of 0° and 90° to obtain quadrature detection. Utilizing the ring modulators as mixers produces an output signal which contains the sum and the difference of the two frequencies. In the case of phase demodulation the difference of the two frequencies is required and the sum is filtered by a low-pass filter. Following transmission via the low-pass filter two operational amplifiers and 50-Ω line drivers (National Semiconductor, Santa Clara, CA; models LH0024 and LH0004) further amplify the two phase detected NMR signals to a maximum of 10 V. The signal is then routed to the digitizer via a 50-Ω coaxial cable. The receiver is mounted in an aluminum enclosure (15 ×20×3 cm) which ensures optimal shielding.

E. Broadband radio frequency amplifier

In Fig. 6 we present the design of a practical low cost 100-W amplifier which represents a useful alternative to commercial sources. The amplifier has three stages. The first stage consists of a wideband amplifier module (Motorola; model MHW592) which has a range from 5 to 200 MHz and an output power of 2 W. The subsequent two stages utilize rf power metaloxide semiconductor field-effect transistors (MOSFET) (Motorola; models MRF150 and MRF153). These field effect transistors (FET) are suitable for broadband operation due to the relatively small frequency dependent input impedance. (Note that care must be taken because the FETs can be easily damaged.) The rf power FETs are biased by a dc pulse prior to applying the rf to ensure a fast rise time. The bias pulse is required because the field effect transistors cannot be turned on continuously which would result in overheating. By contrast, the radio frequency pulse cannot turn on the FET fast enough to generate an acceptable rise time. Consequently, a dc bias pulse of 10 μs is applied prior to the rf pulse to achieve a rise time of less than 1 μs. The third and final stage consists of a power field-effect transistor (Motorola; model MRF153) which amplifies the rf pulse to 100 W. The unique aspect of this amplifier is that it can be fabricated locally for a small investment (total cost for parts is approximately $250) and still maintains good rf pulse
amplification over a range from 5 to 50 MHz. The cost of a typical commercial rf amplifier having the same capabilities would currently be $2000–$5000.

F. Application software

An overview of the PCMR program is provided in Fig. 7, which is written in IBM PC assembly language and compiled and linked utilizing the Microsoft (Seattle, WA) macroassembler (MASM). The setup subprogram consists mainly of routines which facilitate the preparation of the acquisition parameters. These include automatic resonance adjustments, single phase or quadrature detection, frequency selection, dwell time, and data size. The pulse programmer editor enables the user to program a specific pulse sequence. There are 8192 programmable steps and an additional 4096 individual delays are available. Further adjustable parameters are the rf phase, rf amplitude, frequency, and the external real time clock pulse which can be used for triggering the digitizer, biasing the rf transmitter, and so forth. The acquisition subprogram controls the data flow through the analog-to-digital converter (ADC) into the computer memory, and from there into the video memory where data are displayed after each scan. The data are accumulated as 32 bit integer words, and data points are interleaved between quadrature channels A and B. The processing subprogram includes evaluation routines for longitudinal $T_1$ and transverse $T_2$ relaxation measurements, with routines that facilitate the evaluation of data obtained using the Carr–Purcell–Meiboom–Gill (CPMG) sequence. The file system predominantly interfaces with the disk drive and stores data in integer, floating point, or ASCII format; it stores and retrieves specific pulse sequences and parameter lists. Finally, the help screen provides a short user-friendly description of each available command. Commands to perform a certain task consist of two letters which is similar to commercially available NMR programs. The start of the PCMR program initially resets all acquisition parameters, and downloads the LCA file which contains the hardware logic produced during the fabrication phase by the XILINX system into the logic cell arrays. After a successful completion, the program awaits for further instructions from the user. The user can then load a previously created pulse program from the disk and display it by the pulse programmer editor, or start the pulse program in a setup mode. In this routine the user has the option to change the observation frequency until the free induction decay is on resonance by toggling the up/down arrows. Five step sizes are available, e.g., 1 Hz, 10 Hz, 100 Hz, 1 kHz, and 10 kHz to facilitate this task. Analogously the user can change the rf phase of the receiver by toggling the left and right arrows. Again five step sizes are available, e.g., 1°, 3°, 5°, 10°, and 30°. Such frequency and the phase adjustments are necessary for implementation of multiple pulse sequences such as the CPMG sequence. The user can determine the 90° pulse by changing the rf pulse width, which can be done in the foreground without activating the pulse programmer editor. Once the 90° pulse width is determined the user can begin the data acquisition. For multiple pulse sequences additional parameters need to be set accordingly; a help screen is available by executing the help command. After the acquisition is completed the user can store the data in...
IV. DISCUSSION

We have designed and constructed a basic data acquisition instrument which is inherently modular in design and can be easily adapted to evolving scientific or industrial applications. Ideally the instrument design specifications include (i) portability, (ii) low weight, (iii) low cost, (iv) minimal maintenance, and (v) capability of future expansion with downwards compatibility with regard to both software and hardware. This low cost basic data acquisition and control system utilizes recent advances and breakthroughs in microcomputers and microelectronics. Moreover, the present technology when used with permanent magnets can reduce the cost of the NMR spectrometer substantially. The entire cost of constructing the microcomputer-based NMR spectrometer (about $20,000) is a fraction of the cost of an equivalent commercially available NMR console. Such systems are broadly applicable to (i) scientific research where cost and space are of concern, (ii) engineering quality control and process control, and (iii) educational projects at the college and possibly the secondary school level.

The approach of generic instrument development is essential for penetrating new fields and areas as well as for new applications of existing technology. Our instrument is founded on personal computer-based technology, and therefore is ensured of benefiting from the continuing progress of faster and more powerful hardware and software having full downwards compatibility. It suggests the concept of having all NMR spectrometers one day based on personal computer technologies in contrast to the present situation. Presently, NMR manufacturers utilize third party computers (e.g., Silicon Graphics; San Diego, CA) for which downwards compatibility is an issue of increasing concern. The unique aspect of this fabrication is that the entire radio frequency generation, direct digital frequency synthesis, radio frequency phase control, radio frequency pulse control, and radio frequency pulse shaping are realized on two printed circuit boards. The receiver system is located in a small external enclosure which is optically isolated and connected via three coaxial cables and one ribbon cable to the printed circuit boards. The radio frequency amplifier is connected to the modulator board by a single coaxial cable. A person familiar with installing printed circuit boards on a personal computer is of such simplicity that an electronics specialist could easily reproduce the printed circuit boards as well as modify them for specific tasks. For process or quality control, where several units are needed, this can have a major impact on cost, space, and maintenance.

Most NMR spectrometers in operation today involve high resolution applications to liquids and utilize high-field superconductive magnets. Wide line NMR spectrometers are also employed and are primarily utilized for studies of mo-

G. Applications

Representative free-induction decays obtained from samples of corn and oak hardwood using the personal computer-based NMR spectrometer are shown in Fig. 8. Both samples were measured with a one pulse sequence, parts a and c, and with a CPMG sequence, parts b and d, utilizing a 0.47-T aluminum-nickel alloy permanent magnet. In the latter case, each echo generates one data point in the free-induction decay; in practice 20–40 echoes are sufficient to produce enough data for accurate determination of the relaxation time T2 from the decay envelope. Use of the CPMG sequence is essential because the echo envelope represents the true T2 relaxation time of the compound.10,12 The value of T2 is, in general, limited by the inhomogeneity of the applied magnetic field, which is compensated by the CPMG sequence. Fast-Fourier transformation of the FID is accomplished by separate processing software, e.g., Felix (Biosym).

FIG. 8. Representative experimental data obtained using the personal computer-based NMR spectrometer. 1H NMR results are shown for a kernel of corn and a sample of hardwood (oak) exposed to excessive moisture. In both cases the deadtime of the receiver was 10 μs. Free induction decays (FID) were acquired using a one pulse sequence, and further data were obtained using a Carr–Purcell–Merriam–Gill sequence [90°, π, 180°, π, (echo), π, 180°, π, (echo), ...]. (a) FID obtained for a single kernel of corn; (b) corresponding result of applying CPMG sequence to the same kernel of corn; (c) FID of the hardwood sample; (d) corresponding result for hardwood sample using CPMG sequence. The fast decaying component in the FID (parts a and c) represents the bound water, and the slower decaying component is due to free water in the corn and wood sample. In the CPMG results (parts b and d) the envelope of the series of echoes represents the true T2 of the free water present in the samples. Note that the resulting T2 relaxation time of corn is longer than that measured for the hardwood sample. The results indicate that relatively sophisticated multiple pulse relaxation time of corn is longer than that measured for the hardwood sample. Use of the CPMG sequence is essential because the echo envelope represents the true T2 relaxation time of the compound. The fast decaying component in the FID (parts a and c) represents the bound water, and the slower decaying component is due to free water in the corn and wood sample. In the CPMG results (parts b and d) the envelope of the series of echoes represents the true T2 of the free water present in the samples. Note that the resulting T2 relaxation time of corn is longer than that measured for the hardwood sample. The results indicate that relatively sophisticated multiple pulse relaxation time of corn is longer than that measured for the hardwood sample.
A number of potential applications of such a personal-computer based NMR instrument exist which can be expected to evolve in the future as NMR technology becomes more widespread. Examples of such applications involve quality control functions and process control analysis in the food industry, including measurement of the moisture content of grains and other foodstuffs;\textsuperscript{14} metallurgy, with determination of the free and bound moisture in aluminum oxide; and additionally the online monitoring of processes in the chemical, petroleum, and coal industries. Potential applications in the pharmaceutical industry includes measurement of the moisture content of medicinal drugs and determination of $T_1$ and $T_2$ relaxation times in the presence of contrast agents as an adjunct to magnetic resonance imaging. With regard to civil engineering, there are a large number of asphalt bridges and highways that are part of the decaying public transportation infrastructure, and need to be inspected periodically for reliability and security reasons and reconstruction purposes; related applications involve quality control in the asphalt and cement industries. In the medical arena the combination of MRI with imaging guided biopsy procedures offers considerable promise in diagnosis and treatment of cancer. Yet another example which could benefit from such a new standard is a mobile ESR spectrometer for geologists and archaeologists to analyze samples and artifacts directly in the field.\textsuperscript{15-17} Finally, in the future such a mobile PC-based NMR spectrometer could be valuable with regard to unmanned or manned space exploration. A possible further upgrade is the utilization of newly available logic cell arrays from XILINX (5000 series) which permit the configuration of static memory inside such logic cell arrays. This would further condense the two boards which now represent the basic NMR console to a single printed circuit board and so further lower the cost and increase simplicity. We are presently adapting this hardware for a field cycling spectrometer where multiple parameters including electrical current, preemphasis of the electrical current, and radio frequency need to be controlled in a highly nonstandard fashion.
11 D. I. Hoult, Prog. NMR Spectrosc. 12, 41 (1978).