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DESIGN NOTE

A microcomputer-based data acquisition system for an NMR pulse spectrometer

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Abstract. A data acquisition card is designed and constructed for the Amstrad PC 1512, a low-cost IBM compatible microcomputer. This card is installed in the expansion slot of the microcomputer and the software necessary for nuclear magnetic resonance data acquisition and analysis is developed. This system generates the pulse sequences necessary for a nuclear magnetic resonance pulse spectrometer and acquires data from the free-induction-decay signal for further analysis. The generation of the timing pulses and the capturing of the free-induction-decay signal are done with the help of an assembly language source program.

1. Introduction

The IBM PC and its compatibles are being used in data acquisition applications for the measurement of various physical parameters. These applications involve interface boards which go into the expansion slot of the PC. This system generates the logic necessary for the application and acquires data for the measurement of the desired physical parameter, using proper software.

Tsuneki (1986) has constructed a low-cost pulse generator using a NEC PC 9801 microcomputer for an electron spin-echo spectrometer. His system uses a 12-bit analogue-to-digital converter interface for the above computer, which employs the Intel 8086 microprocessor operating at 8 MHz. Meller (1988) has developed computer-assisted video microscopy for the investigation of monolayers on liquid and solid substrates by interfacing an IBM PC to the fluorescence microscopic monolayer equipment. Shenhing and Patrick (1988) used an IBM PC AT compatible microcomputer to host the interface of a Fourier-transform ion-cyclotron resonance mass spectrometer and carried out the excitation and data acquisition. El-Dhaher *et al* (1988) have used a MAC-86 microcomputer employing the Intel 8086 microprocessor with the 8087 coprocessor for image processing in an electron microscope application. A low-cost real-time data acquisition system for laser and radio frequency spectroscopy employing an IBM PC has been reported by Brenner *et al* (1988). A summary of the use of the IBM PC for interfacing various sensors has been reviewed by Tumpkins and Webster (1988). Puvvada and Escid (1989) have reported a data acquisition system employing the Amstrad PC 1512, a low cost IBM compatible microcomputer for nuclear magnetic resonance (NMR) data acquisition and analysis. The aim of the present communication is to present a data acquisition system for an NMR pulse spectrometer, employing an IBM compatible microcomputer. This system generates all the timing pulses necessary for the spectrometer and captures the free-induction-decay signal for further analysis.

2. Materials and methods

The Amstrad PC 1512, a low-cost IBM compatible microcomputer, employing the Intel 8086 microprocessor operating at 8 MHz, is used in the present application. A data acquisition card (in the form of a printed circuit board) is designed and constructed following the IBM expansion slot configuration (for an XT type of computer) described by Coffron (1987) and is installed in the computer. The circuit diagram of the data acquisition card, as shown in figure 1, consists of a sample and hold (SH) circuit (AD585), an analogue-to-digital (AD) converter (AD574A), a parallel programmable interface (PPI 8255A) and the address decoding logic. This logic facilitates the positioning of the various ports of the PPI in the input/output (IO) address space of the 8086 microprocessor. The address decoding was done in such a way that port A, port B, port C and the control buffer register (ContR) of the PPI are assigned the hexadecimal ad-

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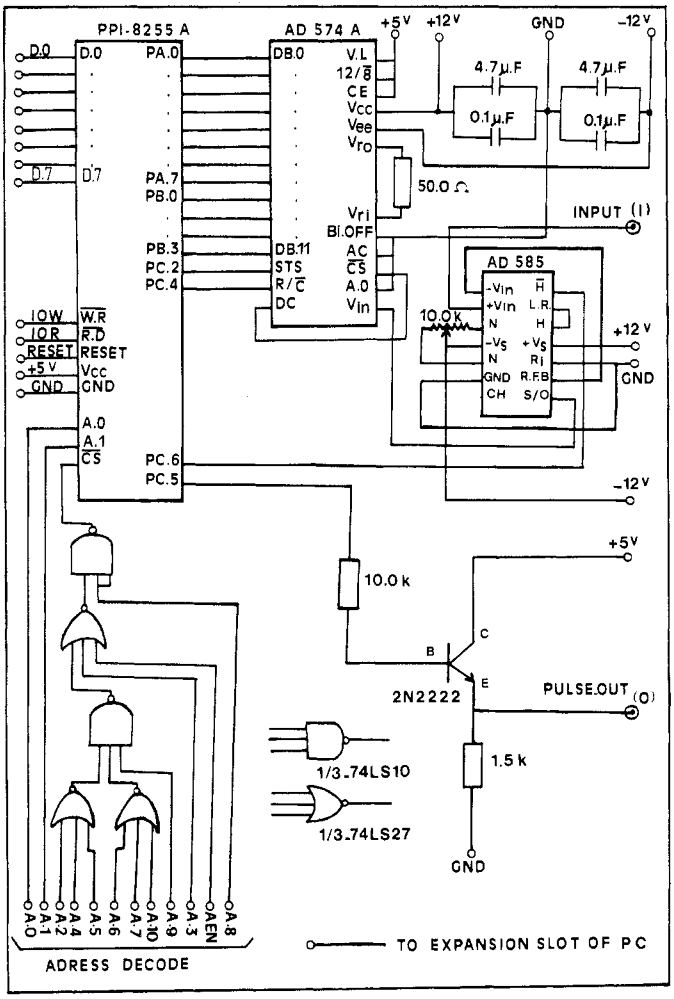

Figure 1. Circuit diagram of the data acquisition card.

dresses 0300, 0301, 0302 and 0303 respectively. This was done in the user reserved IO address space of the 8086 microprocessor, following the criteria imposed by Intel (Amstrad 1986).

The SH circuit takes about 3 μs for acquiring each data point and goes into the hold mode before passing the analogue value into the input of the AD converter. The AD converter takes about 35 μs to convert this analogue value into a 12-bit digital word. This 12-bit output available on the data bus of the AD converter, is passed into the memory space of the 8086 microprocessor through ports A and B of the PPI, in the form of two bytes. Pin 6 of port C (PC6) of the PPI is used to generate the logic necessary to activate the SH circuit. Pin 4 of port C (PC4) is used to command the conversion cycle of the AD converter. Pin 2 of port C (PC2) is used to test the end of conversion. Pin 5 of port C (PC5) is used to generate the pulse sequences necessary for the NMR pulse spectrometer. This output is buffered and is made available to the transmitter through a BNC connector. The analogue input to the data acquisition card is also made available through a BNC connector. The data acquisition card is energised with the help of the power supplies +12 V, −12 V and +5 V, available on the expansion slot of the PC 1512.

```
                TITLE                 ACQUI12.ASM
COMMENT         * Program to generate the 90 degree transmitter
                pulse and to acquire 40 data points from the free
                induction decay signal using a 12-bit AD
                converter. Data starts at 2000:400h. Runs as a
                COM file*
portA           EQU  0300h
portB           EQU  0301h
portC           EQU  0302h
contR           EQU  0303h
code            SEGMENT
                ASSUME CS:code,DS:code
                ORG 100h
start:          CLI                   ;clear all interrupts
                MOV DI,400h           ;starting address of data for
                MOV BL,40             ;40 data points (2 byte each)
                MOV DX,contR          ;initialisation of the PPI. portA
                MOV AL,93h            ;and portB in input, portC inf.
                OUT DX,AL             ;in input and
                                      ;portC sup. in output
                MOV AL,0Ah
                OUT DX,AL             ;set PC5 low
                MOV AL,04h
                OUT DX,AL             ;set PC2 low
                MOV AL,09h
                OUT DX,AL             ;set PC4 high
                MOV AL,0Ch
                OUT DX,AL             ;set PC6 low
                MOV AL,0Bh
                OUT DX,AL             ;set PC5 high
                MOV CX,0015           ;to generate the 90 degree
acq1:           LOOP acq1             ;transmitter pulse
                MOV AL,0Ah
                OUT DX,AL             ;set PC5 low
                MOV CX,0010h
acq2:           LOOP acq2             ;saturation recovery
acq3:           MOV DX,contR
                MOV AL,0Dh
                OUT DX,AL             ;set PC6 high for sampling
                MOV CX,05
acq4:           LOOP acq4
                MOV AL,0Ch
                OUT DX,AL             ;set PC6 low, end of sampling
                MOV AL,08h
                OUT DX,AL             ;set PC4 low to command
                MOV CX,05             ;AD conversion
acq5:           LOOP acq5
                MOV AL,09h
                OUT DX,AL             ;set PC4 high
                MOV DX,portC
acq6:           IN AL,DX
                TEST AL,04h           ;test if PC2 is low for the
                JNZ acq6              ;end of AD conversion
                MOV DX,portB          ;high byte of data
                IN AL,DX              ;in through portB
                AND AL,0Fh            ;make high nibble 0
                PUSH DS
                MOV DX,2000h          ;define the data segment
                MOV DS,DX
                MOV [DI],AL           ;store high byte
                INC DI                ;prepare for next data byte
                MOV DX,portA
                IN AL,DX              ;low byte through portA
                MOV [DI],AL
                INC DI
                POP DS
                DEC BL
                CMP BL,00             ;for the required data points
                JNZ acq3
                STI                   ;set all interrupts
                MOV AH,4Ch            ;return to DOS
                INT 21h
code            ENDS
                END start
```

Figure 2. Assembly language program.

An assembly language source program is prepared and is converted into a COM file following the procedure described by Miller (1987). This COM file is used to capture the free induction decay (FID) signal of water protons, by interfacing the data acquisition system to a home built NMR pulse spectrometer, operating at 5 MHz. The assembly language source program, as presented in the listing of ACQUI12.ASM (figure 2) firstly initialises the PPI of the data acquisition card so that port A, port B and the lower half of port C are programmed as input and the upper half of port C is programmed as output. Then the program generates the 90° transmitter pulse and waits for a few microseconds so that the NMR receiver recovers from the saturated state. Then it activates the SH circuit to sample the first data point of the FID signal. After a few microseconds of sampling, the SH circuit is put in the hold mode and the AD converter is activated to convert the analogue value into a 12-bit digital word. The end of conversion is sensed through the STS (status) pin of the converter going low. Now the data available as two bytes at the ports A and B is transferred into the memory space of the microprocessor starting from 2000:400 hex address. Then the program repeats the data acquisition cycle to acquire 40 data points (80 bytes) from the FID signal. The chronogramme representing the various events in acquiring each data point is presented in figure 3. The FID signal of water protons obtained from the data acquired is presented in figure 4.

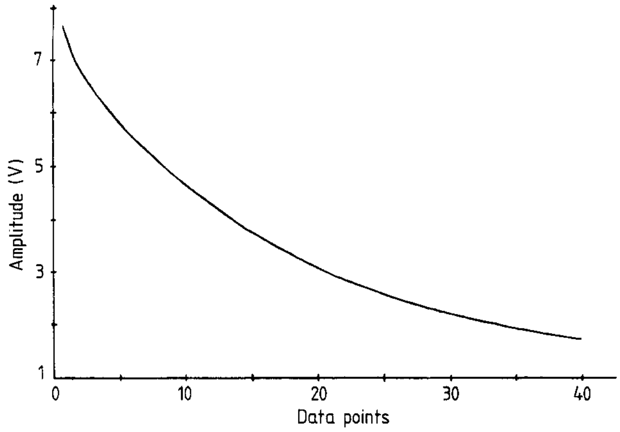

Figure 4. FID signal of water protons.

3. Results and discussion

The data acquisition card has been constructed and tested using the assembly language program presented, to acquire the FID signal of water protons. Work is in progress to develop software for performing the Fourier transform analysis of the FID signal to facilitate the spectral analysis. Also programs are being developed to determine the proton spin–lattice (T_1) and spin–spin (T_2) relaxation times, using the data acquisition system described.

We have especially chosen a 12-bit AD converter to optimise between speed and cost. 8-bit converters are less precise but are the fastest. 16-bit converters are highly accurate in data acquisition but are very slow. Fast 16-bit converters are prohibitively expensive. So one has to find a compromise between precision, speed and cost while realising a data acquisition system, necessary for a specific application (Clayton 1984). One can easily modify the card to use a 16-bit AD converter, if the application demands more precision. We find that this card is quite satisfactory for many applications in NMR data acquisition and analysis.

Acknowledgments

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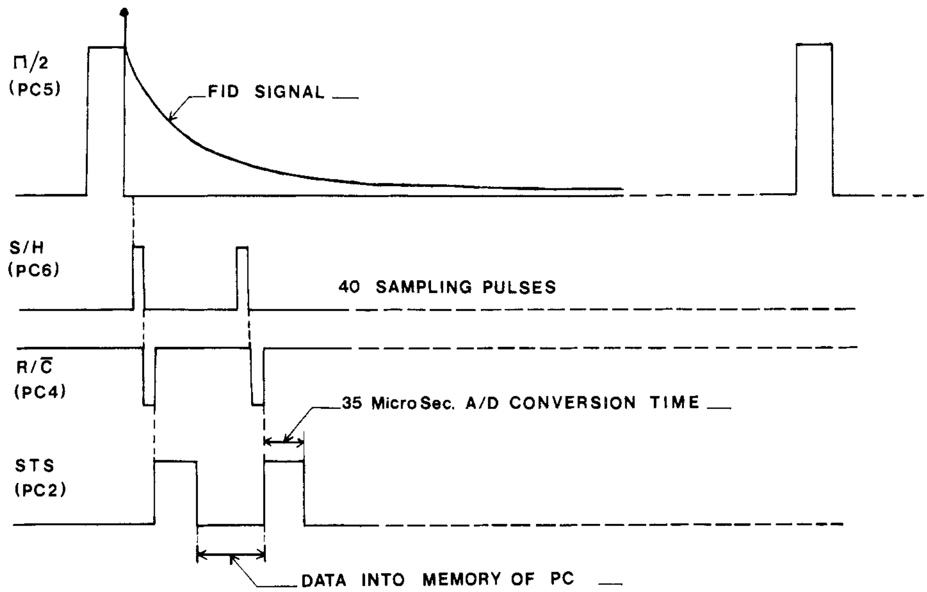

Figure 3. Data acquisition sequence from the FID signal.

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