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DECUS NO.	8-238
TITLE	EPRSIM, AN ELECTRON PARAMAGNETIC RESONANCE SIMULATOR
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DATE	October 8, 1969
SOURCE LANGUAGE	MACRO-8

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EPRSIM, AN ELECTRON PARAMAGNETIC RESONANCE SIMULATOR

DECUS Program Library Write-up

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ABSTRACT

An electron paramagnetic resonance (EPR) spectrum simulation program has been coded in Macro 8 for the Lab 8 computer. The program will display spectra derived from either a Gaussian or Lorentzian derivative line shape. The horizontal length of the display is 512 locations and is adequate for many simulation problems. A spectrum may either be displayed on an oscilloscope or an x-y recorder.

INTRODUCTION

In order to correctly assign the coupling constants of complex EPR spectra it is usually necessary to simulate the experimental spectra with assumed coupling constants and line shape. Several Fortran programs exist which elegantly perform this task using large digital computers. Unless a terminal is readily accessible the task of assigning a spectrum with a central computer may prove to be inconvenient and time consuming. We have coded a program which will rapidly simulate a first order EPR spectra on a Lab 8 computer with 4096 word memory and plot the spectrum on an x-y recorder. Use of the smaller computer leads to greater user-

computer interaction and in many cases to a more rapid assignment of spectra. The program has the advantage of displaying the spectrum as soon as a coupling constant for one nuclear spin species is entered into the computer. This direct interaction provides an excellent instructional aid for students of EPR spectroscopy.

OPERATION DETAILS

The derivative of a parent Gaussian or Lorentzian line is originally calculated using the floating point arithmetic package (included in the binary tape) and stored in the Display Buffer after it has been transformed to a double precision fixed point number. The Display Buffer addresses correspond to the magnetic field positions and the contents correspond to the intensity of the resonance. The spectrum is generated sequentially by accumulating appropriate multiples of the parent line shape from the Display Buffer and transferring it to the Data Buffer according to the coupling constant and the number of particular nuclear spins. After the spectrum is built up in the Data Buffer its contents are placed back into the Display Buffer and displayed. This procedure takes place as many times as nuclear spin parameters are entered from the teletype.

The actual calculation of the composite line shape proceeds as follows: Addresses are stored in List 1 which differ in value from each other by the coupling constant. The number of addresses equals the number of spin projections of the equivalent nuclei ($2I + 1$ double precision addresses) and the statistical weights for each of the address in List 1 are stored in List 2. The lowest address in List 1 is the bottom address

in the Display Buffer. The calculation proceeds by adding the contents of the addresses in List 1 each multiplied by its corresponding weight in List 2 and placing the results in the bottom double precision location in the Data Buffer. The addresses in List 1 are incremented by two and the process is repeated for the remaining points in the Data Buffer. In this manner the $(2I + 1)$ double precision windows of List 1 are swept through the Display Buffer and the weighted sum of the contents are deposited into one double precision Data Buffer location for each step of this sweep. The Data Buffer contents then replace the Display Buffer contents and are displayed on the oscilloscope.

Several precautions are noted. The total width of the spectrum should not exceed 512 double precision locations. This means that $\sum_i (2I_i + 1)a_i < 512$ where a_i is the coupling constant (in locations) of the *i*th species, and I_i is the total nuclear spin of *i*th species. All data which overflows the buffer area are irretrievably lost. The number of equivalent spin 1 or 1/2 nuclei entered at one time is restricted to three or less. All numbers other than 1, 2, or 3 for the number of equivalent nuclei are ignored.

The display subroutine presents a 9 bit "window" of a 24 bit word in the Display Buffer to the AX08 and the output of the D-A converters is fed to an oscilloscope. This window is rotated to the right or to the left by the expand or contract commands. A stationary point remains on the top or bottom of the screen if the data is expanded out of the range of the display.

REQUIREMENTS

Equipment: PDP-8/I (4K), AX08, Oscilloscope (Lab 8 Computer),
x-y plotter (optional)

Subroutines: Supplied with binary program

EXECUTION

Loading: via BIN Loader

Start: Starting Loc. 5000 for Initial Dialogue

Starting Loc. 200 for display operation; once display
is operating the initial dialogue is destroyed

The initial dialogue consists of the following instructions and
options.

OPERATION CODES FOR TELETYPE

- Type 0 for Gaussian function
- 1 for Lorentzian function
- 2 to enter linewidth and total # of spin states
- 3 to enter number of spin one nuclei (≤ 3) and coupling
constants
- 4 to enter number of spin 1/2 nuclei (≤ 3) and coupling
constants
- 5 to contract display
- 6 to expand display
- 7 to creat x-y plot

Program halts with voltage for pen at (0,0); connect x-y plotter;
zero pen, hit continue; disconnect recorder after plot is done, hit
continue.

SAMPLE SPECTRUM SIMULATION

Assume that a spectrum simulation is desired for a spin system of
2 spin one nuclei with coupling constant of 1.3 gauss, 4 spin 1/2 nuclei

with coupling of 1.8 gauss, and 2 spin 1/2 nuclei with coupling of 9.5 gauss. The line shape is Gaussian and the line width is 0.8 gauss. The program will only accept integral numbers for the coupling constants and line width because these numbers will be transferred directly to location numbers in the computed spectrum. It is therefore convenient to multiply all parameters by 10 and generate the spectrum in the following manner.

Type 2 L - Width = : 8 Return

Spin States = : 576 Return

Type 0 (Gaussian line shape)

Line shape will be displayed on oscilloscope in about 20 seconds.

Type 3 Spin 1 nuclei ? : 2

Coupling constant = : 13

Type 4 Spin 1/2 nuclei ? : 3

Coupling constant = : 18

Type 4 Spin 1/2 nuclei ? : 1

Coupling constant = : 18

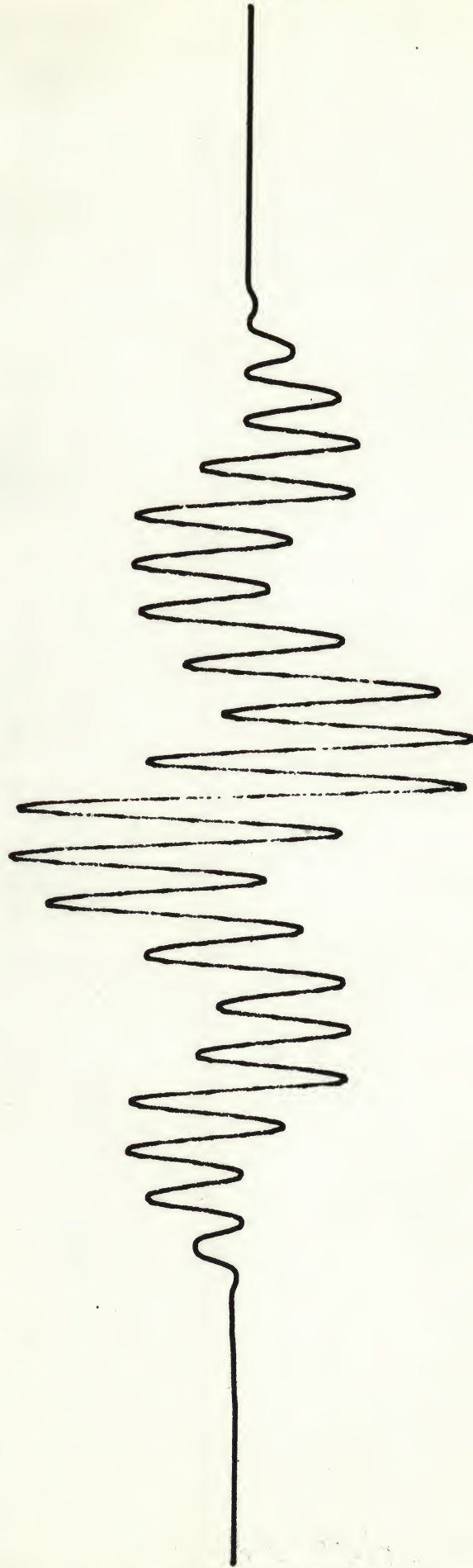
Type 4 Spin 1/2 nuclei ? : 2

Coupling Constant = : 95

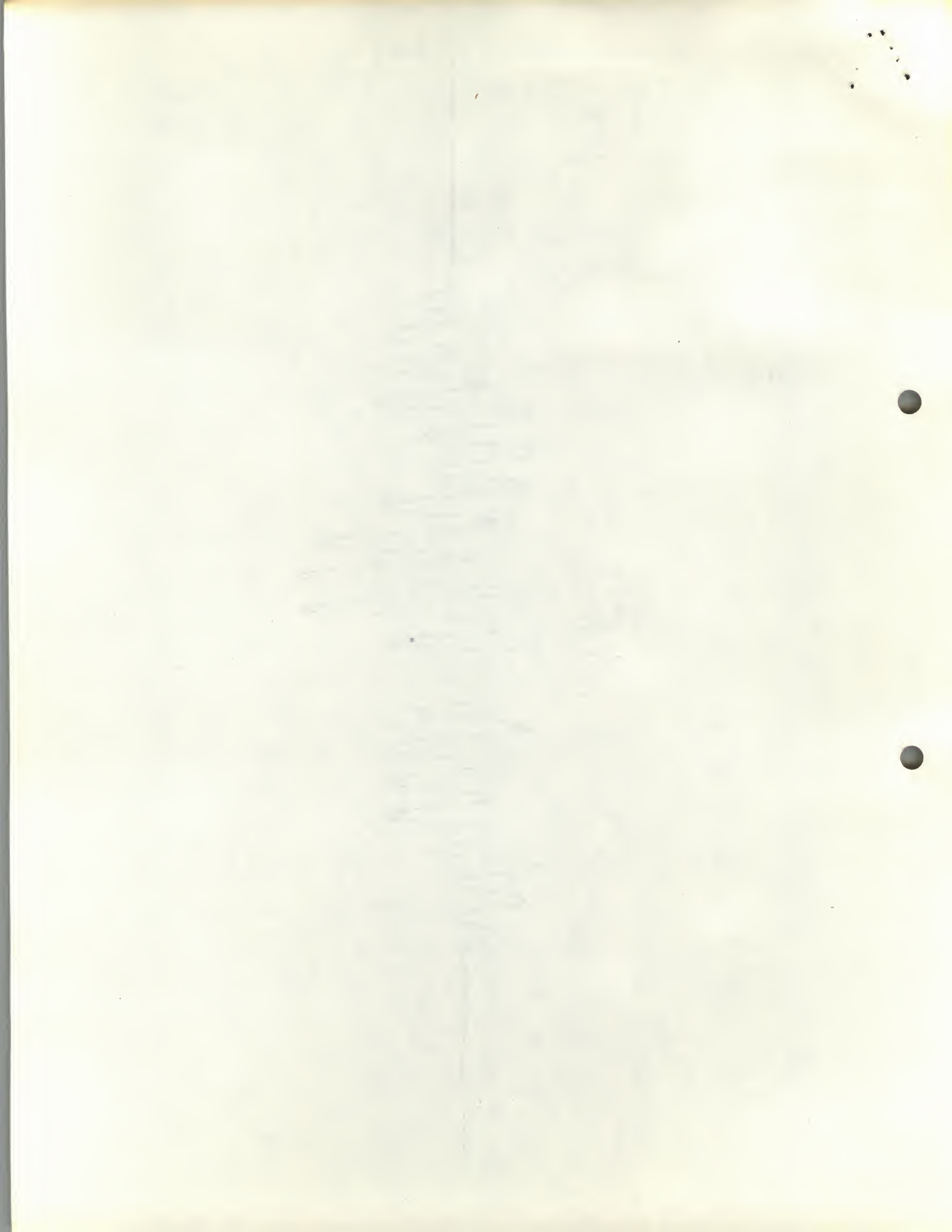
The oscilloscope will display the spectrum as it is built up. Typing a 5 or a 6 will contract or expand the vertical dimension of the display at any time. A photograph may be taken of the oscilloscope screen or if an x-y plotter is available the x and y inputs may be taken from the oscilloscope x and y leads and a plot made according to the instructions in the operation codes. Location 105 stores the negative number which controls the time delay between x-y points. The number 7700 is equivalent

to approximately one second per point. The program is initially set to 7770 which is about $1/8$ second per point.

After the spectrum has been recorded the procedure must be started anew. The initial line shape is destroyed in the spectrum generation. The line width and total number of spin states, however, are not destroyed and the initial line shape may be recalculated by typing, respectively, a 0 or 1 for a Gaussian or Lorentzian line.



Sample Spectrum



ADDENDUM TO DECUS NO. 8-238

The locations 1-1577 are used for the program proper, with 5000-5401 containing the initial dialog. This initial dialog is typed if SA 5000 is used and suppressed if SA 200 is used. After generation of the waveform, the dialog is destroyed. Subsequent starts must be made at SA 200. It is to be noted that use of the program requires floating point package #1 to be loaded first, as the FEXP as written in this program requires modification of location 6553 in floating point package to 1415, the starting address of FEXPO, the floating exponent.

The display buffer, which contain the information shown on the scope is stored in location 1600 to 3577. The calculations take place in location 3600-5577. Information read into the display buffer from an external source can be processed as if it had been calculated there, and no internal pointers need to be set in the program.

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