

B-164

FINAL SUMMARY REPORT

on

RESEARCH GRANT NSF G-7361

SUPPORT OF THE RICH ELECTRONIC COMPUTER CENTER AND
BASIC RESEARCH REQUIRING DIGITAL COMPUTATION

Rich Electronic Computer Center
Engineering Experiment Station
Georgia Institute of Technology
Atlanta, Georgia

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SUPPORT OF THE RICH ELECTRONIC COMPUTER CENTER AND BASIC
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Research supported in part by this grant has been carried out on sixteen different projects. Several of these projects are continuing and are being expanded. Some will be continued as additional time and funds become available. Others have provided assistance in various ways to continuing efforts of research on the part of our graduate students and faculty members of Georgia Tech.

The grant has been instrumental in increasing the level of research on the Georgia Tech campus. One indication of this increase in research effort is that the Annual Sigma Xi list of Georgia Tech faculty publications made in June of 1959 for the period March 15, 1958 through March 14, 1959 contained ninety-six entries. The similar report made in June of 1962 contained 140 entries. Another interesting point is that during the last three years well over half of the Sigma Xi awards for research to Master of Science and Doctor of Philosophy candidates and to the faculty have been to investigators who have utilized computers.

An indication of increased computer activities is shown in the fact that at the end of 1958 we were using a little over one shift on the IBM 650, and one shift on the UNIVAC SCIENTIFIC (ERA 1101). The IBM 650 was returned in 1961 in anticipation of up-dating our equipment. Now we are using three shifts on a Burroughs 220 with six tapeunits and one shift on the 1101 modified by the addition of a 1103A core memory and a card read-punch unit. Of course, this increase in computer use has not all been due to research but also due to the increased class and instruction use. Additional evidence is contained in the fact that our non-credit computer seminars on the use of our two computers have been increasing in size. This quarter approximately 300 students and faculty people are enrolled in the seminars. Over ninety of them will be employing the compiler developed for the 1101 under the partial sponsorship of this grant. As a consequence of

this increased usage of the computers, plans are being made to up-date and expand our facilities.

Several reprints of papers resulting from research work associated with this grant are included and listed in the bibliography. Also included in the bibliography is a listing of papers which have been prepared for publication. Additional papers for publications are in process. As they become available they will be forwarded to the National Science Foundation.

A considerable amount of statistical work has also been developed, some of which will eventually find its way into the literature and some of which is useful only to local researchers. Several people who have aided in research work carried out by this project are now involved in research projects elsewhere.

A number of internal publications have also resulted from this research. These include documentation for a complete library of subroutines for the 1101 which was developed after the addition of the core memory to the 1101 in September of 1959. It also includes a write-up of our algebraic compiler for the 1101. Complete circuit diagrams and maintenance instructions for the card input-output unit addition to the 1101 have also been developed. Since there are only two other 1101's in existence and since ours is considerably different from the other two, this material has not been made available elsewhere.

A brief report on each of the sixteen individual projects is given on the following pages.

Project B-164-1 - Restricted Random Walk Research

Principal Investigator: Dr. I. E. Perlin

The object of this investigation has been to study one type of restricted random walk, which can be described as a two-dimensional, two-choice, 90° restricted random walk, in an effort to obtain exact analytical methods for predicting the total number of walks existing at n steps.

Specifically, the problem can be described in the following manner. Let a rectangular cartesian coordinate system be set up in a plane. Starting at the origin, a step of unit length is taken in the x-direction. Then a second step is taken in the y-direction to be followed by a third step in the x-direction, etc. After n steps, only those paths which do not intersect themselves are to be considered.

Problems of this type have been investigated by King¹, Teramoto², Rosenbluth and Rosenbluth³, and Wall, et al⁴⁻⁹. Most of these investigations have been statistical in nature and have led to empirical or semi-empirical relations for predicting the number of existing paths after n walks.

The line of attack taken during this investigation has been to subdivide the various types of paths into classes such as paths not closing on four consecutive steps, twelve consecutive steps, sixteen consecutive steps, etc. Formulae have been obtained for predicting the number of paths which do not close on four consecutive steps, those which do not close on four or twelve consecutive steps, and those which do not close on four, twelve, or sixteen consecutive steps.

The predicted number of paths have been checked against the results obtained by the UNIVAC SCIENTIFIC (ERA 1101).

¹

G.W.King, Natl.Bur.Standards, Appl.Math.Ser. AMS,
12 (June 11, 1951).

²

Teramoto, Kurata, Chujo, Suzuki, Tani and Kajikawa,
J.Phys.Soc. (Japan) 10, 953 (1955).

³

Rosenbluth and Rosenbluth, J.Chem.Phys. 23, 356 (1955).

⁴

Wall and Hiller, Ann.Rev.Phys.Chem. 5, 267 (1954).

⁵

Wall, Rubin and Isaacson, J.Chem.Phys. 27, 186 (1957).

⁶

Wall, Hiller and Wheeler, J.Chem.Phys. 22, 1036 (1955).

⁷

Wall, Hiller and Atchison, J.Chem.Phys. 23, 913 (1955).

⁸

Wall, Hiller and Atchison, J.Chem.Phys. 23, 2314 (1955).

⁹

Wall, Hiller and Atchison, J.Chem.Phys. 26, 1742 (1957).

Project B-164-2 - Computer Program Library Research

Principal Investigators: Messrs. K. B. Dunham, D. H. Hay, E. R. Austin,
Drs. J. C. Currie and Wm. F. Atchison

The major piece of work accomplished was the completion of an ALGOL-like compiler for the UNIVAC SCIENTIFIC (ERA 1101) for which no compiler of any type was previously available. Seminars on the use of this compiler have been held for the students and faculty. Consequently, the compiler is now being productively used for faculty and student research and for classroom purposes. Research is continuing in the perfection of compiler construction techniques.

A very considerable amount of 'subroutine work for the UNIVAC SCIENTIFIC has been done. Much of this was done in perfecting the ALGOL-like compiler including the various input-output problems associated with adding the new card read-card punch unit to the computer. The remaining subroutine work was done in connection with and after the addition of the 1103A core memory unit to our 1101 about three years ago. This required essentially rewriting all of our program library.

Project B-164-3 - Computer Capability Research

Principal Investigator: Mr. S. P. Lenoir, Jr.

This project began with the acquisition of a Bull Controlled Reproducer and associated control circuitry that was designed to operate with the UNIVAC SCIENTIFIC 1103 computer. After studying the problems involved in attaching this card reader and card punch to the ERA 1101 computer, it was decided to convert the original design into a transistorized version which would be more versatile and require less maintenance. The system design was then outlined and work was begun designing the transistor logic circuits.

The transistor circuitry decided upon included the normal logic circuits of AND's, OR's, timing circuits, flip-flops, and inverters. Since the system required a small memory unit, transistorized full-set and half-set magnetic core current drivers were designed. Each of the transistor circuits was thoroughly tested for reliability. During these tests a general purpose transistor circuit tester was designed and constructed.

The final system design was completed in February of 1961 and wiring was begun shortly thereafter. The check-out of the system indicated that

Project B-164-3 - Computer Capability Research (cont'd)

an electrical simulation of the mechanical system would be desirable. Additional circuitry was provided which simulated to a great degree the entire mechanical system; this has reduced maintenance time considerably.

The completed system, which is now operational, reads cards at the rate of 120 cards per minute. The transfer of the contents of a card from the reproducer system memory to the computer memory required 400 microseconds. The card punch also can operate at the rate of 120 cards per minute. The transfer of the contents of a card from computer memory to the reproducer memory requires 250 microseconds. When the system operates at its maximum speeds of 120 card per minute, it provides the fastest and most flexible input-output device available on the ERA 1101 computer.

The system has also been provided with the extra capability of off-line card reproduction. This can be accomplished by simply changing the operating mode selection on the reproducer control panel. The cables connecting the computer and the reproducer need never be removed once put in place. Certain maintenance features were designed into the system for the quick analysis of troubles. A maintenance mode has been provided in order that the operator may reproduce a deck of cards and see the contents of each card as it is read. The simulation mode allows the technician to view the system waveforms on an oscilloscope at either five or ten times normal card reading speed.

The transistorized version of the control circuitry has reduced the required floor space by almost one-half and has increased the capabilities of the system by twelve times or more. The transistor rack itself is only four and one-half feet high and nineteen inches square. It contains approximately one hundred and twenty-five transistorized logic cards with an average of five logic circuits per card. Also included is a magnetic core memory containing 1420 magnetic cores, the equivalent of forty computer words. Six power supplies are contained in a separate rack.

The service which this system will render in the future will greatly increase the capabilities of this computer and the Rich Electronic Computer Division as a whole. In addition, this project has afforded to many people valuable experience in the design of transistor circuits and systems.

Project B-164-4 - Machine Translation Research

Principal Investigator: Prof. J. Gough, Jr.

A syntactic study has been made of the following seventeen German locative place adverbs:

wo	hier	oben	droben	überall
irgendwo	da	unten	drunten	
	dort	vorne	draussen	
		hinten	drinnen	
		aussen	drüben	
		innen		

The adverbs above are of particular interest, since they belong to the category of indexical symbols called "shifters" (term from Jespersen). They thus possess a dual nature. Like other symbols, the locative place adverbs have a conventionally assigned meaning. For example, the adverb hier means "an dem Ort, wo der Sprechende ist", (English: here = at the place, where the speaker is). In this respect, they may be regarded as constants. On the other hand, these adverbs also possess a variable side, in that their definition in each case depends on the message in which they occur.

Let us consider the following example. The sentence "Ich bin hier" (I am here), said in Germany, has the same basic meaning it would have in America; viz. ich denotes the speaker and hier the place where the speaker is. Yet the general meaning of this statement shifts as the speaker and the country change, i.e., as the shifters assume different values. Thus, we have: "Ich, Hans Müller, bin hier in Deutschland" as against "I, Johnny Jones, am here in America". In both cases the variable or open aspect of the shifters is now defined.

Actually, shifters may be defined extralinguistically or linguistically. In the first instance, one draws on extralinguistic data for his linguistic interpretation of the shifter. However, such an interpretation is possible because of the structural expansion-potential inherent in the shifter. In the second instance, one finds the definition of the shifter within the message itself or in the context of the message, i.e., within the same sentence in which the shifter occurs or in some preceding or subsequent sentence.

We have made a study of locative place adverbs from the point of view that they are shifters. We have restricted this examination to a limited number of kernel sentences, in which these adverbs fulfill a

Project B-164-4 - Machine Translation Research (cont'd)

primary syntactic function, that of predicate complement. This function they fulfill in the same manner as locative elements that are non-shifters. Moreover, the classification of the verb on the basis of its concurrence with a locative complement is examined.

We have also studied the intrasyntax inherent in the locative adverbs as evidenced in their expansion-potential. This amounts to a description of various locative strings (sequences of locative elements) introduced by these adverbs. Such strings are interpreted as definitions of the variable aspect of the shifters. In addition, we have studied the change of locative place adverbs to goal-directed place adverbs in connection with the transformation from static to causative verbs.

Finally, generation rules illustrating the syntactic and intrasyntactic interpretation above have been set up. Plans are made to program these generation rules on the Burroughs 220.

The present study is being written up and will be submitted as a doctoral dissertation to the Department of Linguistics of Harvard University.

Project B-164-5 - Computational Procedures and Other Studies in the Field of Statistical Analysis

Principal Investigator: Dr. J. W. Walker

Introduction

The statistical studies conducted under this grant have been generated with two things in mind: (a) Pursuance of mathematical results, but (b) with special emphasis on the use of high-speed computers both in conceptualizing the studies and in carrying analyses through computational algorithms.

Several of the studies were stimulated by statistical problems which came under the purview of the Engineering Experiment Station for which routine procedures were not already established.

A summary description of those studies considered significant is included below. Detailed writeups, with derivations, references, statements of unsolved problems, etc., have been completed and are available in

Project B-164-5 - Computational Procedures and Other Studies in the
Field of Statistical Analysis (cont'd)

our files. The material, which has developed according to needs and tastes without benefit of the usual careful pyramid of previous results in the area, has not been completely mined, screened, and cross-checked for publication. The completion of the writeups, alluded to above, makes this latter project feasible now.

1. Partitions of sets and integers

(a) A computer program has been developed to list all the decompositions of a finite set into a finite number of subsets.

(b) It has been shown that the number of partitions of a positive integer N into m parts can be expressed in general as

$$\sum_{x_1=1}^{f_1} \sum_{x_2=1}^{f_2(x_1)} \dots \sum_{x_{m-1}=1}^{f_{m-1}(x_1 \dots x_{m-2})} 1, \quad ,$$

where the upper limit functions explicitly depend on which of several kinds of partitions is being enumerated. The formula provides a fairly easy algorithm for computer programming. Also, asymptotic relationships have been developed connecting the number of unordered partitions to the number of ordered partitions. Some unsolved problems are listed.

Manipulations of partitions constitute important collateral problems in combinatorial aspects of statistics, which have arisen especially in working with multivariate multinomial distributions.

2. A computational scheme for testing the difference between two population means when the variances are unequal

The procedure devised has been used repeatedly with very satisfactory results. It has the advantage of simplicity, and it does not rely on the use of any of the approximate Fisher-Behrens tables.

The method consists in constructing the likelihood ratio test and employing the asymptotic distribution of that test statistic (under the null hypothesis).

The test statistic becomes

$$(2.1) \quad n_1 \ln \left[1 + \frac{(\bar{x}_1 - \hat{\mu})^2}{s_1^{*2}} \right] + n_2 \ln \left[1 + \frac{(\bar{x}_2 - \hat{\mu})^2}{s_2^{*2}} \right],$$

where n_i ($i = 1, 2$) are sample sizes, \bar{x}_i sample means,

$$s_i^{*2} = \frac{\sum_{j_i=1}^{n_i} (x_{ij_i} - \bar{x}_i)^2}{n_i},$$

and $\hat{\mu}$ satisfies the equation

$$(2.2) \quad \mu = \frac{n_1 \bar{x}_1}{n_1 + n_2 g(\mu)} + \frac{n_2 \bar{x}_2}{n_1 g(\mu) + n_2}, \quad g(\mu) = \frac{s_1^{*2} + (\bar{x}_1 - \mu)^2}{s_2^{*2} + (\bar{x}_2 - \mu)^2},$$

Equation (2.2) lends itself to iterative methods quite readily, but it can also be expressed as a cubic in μ to be solved. The statistic (2.1) has an asymptotic chi-square distribution with one degree of freedom.

Although no difficulty has arisen in practice, it remains to prove that (2.2) has a unique solution and under what condition the iterative procedures converges.

3. Testing for equality of error variance, coincidence, and parallelism among regression planes for several groups of data

The standard tests here are those derived by Gulliksen and Wilks (Psychometrika, V.15). What was not explained in the Gulliksen-Wilks paper was how the regression estimates are distributed under the several alternative hypotheses.

If the common error variance hypothesis is acceptable, it is possible to represent the data of the several groups in a single regression model. Using this model, it is possible to resolve the questions which arise about distributions of estimates. It is also possible to define a statistic (in generalization of the multiple correlation coefficient) which measures the simultaneous fit of the several regression planes and whose distribution (under the null hypotheses of zero regression coefficients) is essentially an F distribution.

However, the main effort in this study was devoted to the development of a computer program for handling, at the option of the research worker, intercorrelations, regression problems, and/or Gulliksen-Wilks problems. This was accomplished in a program which is not restricted by the number of observation vectors, or the number of groups to be studied simultaneously. The number of regression variables may be as large as fifty.

The program was an experiment in which we attempted to combine the following:

- (a) Without loss either of computer efficiency or simplicity of input structure, to write a program handling the complex of problems involving intercorrelations, regressions and Gulliksen-Wilks tests;
- (b) Full range of options on printout;
- (c) Something akin to testbook format;
- (d) An editing feature sufficiently flexible to describe the output in a logical textual report.

The report writing is accomplished by combining phrase-capsules, into sentences and paragraphs, according to the options exercised and the results of computation.

4. Investigations of the normal multivariate integral

Evaluation of the probability "volume" under the p-variate normal density surface over variously defined regions in p-space continues to be an important and frequently disconcerting problem, in spite of the numerous studies which have been made in this area. Our results include:

(a) A generalization of an identity of Karl Pearson's and an application of this to obtain an elementary derivation of a generalized "tetrachoric series" expansion of the multivariate normal integral over the rectangular region $\left\{ (x_1, x_2, \dots, x_p): 0 \leq x_i \leq \xi_i \right\}$. M. G. Kendall

has previously indicated this result, appealing to a Fourier inversion formula in $\bar{3}$ -space, and suggesting the generalization. We have developed the series in enough detail to enable us to flowchart a computer program, except that control of truncation error remains (for $p \geq 3$) an open problem.

(b) In the case where the region is $\left\{ (x_1, x_2, x_3): 0 \leq x_i < \infty \right\}$

(in generalization of a result of Sheppard's), a closed form of the integral has been noted. It is a simple function of the Arcsines of the three correlation parameters.

(c) In generalization of a result of Polya's, in the case when the region is $\left\{ (x_1, x_2): 0 \leq x_i \leq \xi_i \right\}$ a single-term elementary

function has been determined which approximates the bivariate integral and a bound on the relative error is obtained. The bound is approximately 1.5%.

(d) The value of the bivariate normal integral over a region bounded by certain hyperbolas has been evaluated in a series of Bessel functions.

5. Estimation of parameters of truncated normal distribution

A general sampling model has been developed which covers all the truncation cases for the normal distribution. In this model a part of the domain of the normal density function may be censored (i.e., unavailable for sampling) and the remainder of the domain may be decomposed into subsets in one of which exact observation is possible, but in the other subsets of which it is only possible to determine that an observation is either in the subset or not.

Following the method of maximum likelihood, a pair of equations was obtained (for the general model) whose solutions theoretically must yield estimates of μ and σ^2 , the normal parameters.

Iterative methods, to be used in conjunction with a computer, are proposed for extracting these solutions.

Project B-164-5 - Computational Procedures and Other Studies in the
Field of Statistical Analysis (Cont'd)

For certain special problems under the general problem proofs have been obtained guaranteeing convergence of the iterates to a solution.

In making these proofs several interesting and tight inequalities have been established which involve the standard normal probability density function and its integral.

6. A criterion for grouping of data into a finite number of subsets

In this problem a single unknown parameter in a continuous-type distribution is to be estimated, but on the basis of information derived from a sample each observation of which is known only to fall in one of a finite number of subsets in a decomposition of the real line. Estimates of this type occur in practice; for example, the tetrachoric estimate of correlation is based on such "grouped" data.

In his doctoral thesis (U.N.C., 1957) the principal investigator has shown that it is possible to define a decomposition with optimum information (for fixed sample size and fixed number of subsets in the decomposition).

With this optimum decomposition thus defined theoretically, it is conceptually possible to study the relative efficiency of such standard grouping procedures as the tetrachoric. To carry this out in individual cases generally requires extensive computations and tabulations. Computer programming has been undertaken for certain of these comparisons, especially for estimating the mean parameter in the normal distribution. Computations show the deterioration of efficiency, in departing from the optimal decomposition, accelerates only very slowly.

Only exploratory computations have been made in the more involved tetrachoric problem, because of the presence of disturbing nuisance parameters. In an oversimplified version of the tetrachoric estimation we are able to show its efficiency (compared to the optimal estimation) tends to zero for correlation tending to one.

A sequential estimation procedure has been devised, which permits sampling in blocks with a revision of the decomposition depending on the observed samples. This has been studied empirically in Monte Carlo runs. In these runs the procedure has shown good efficiency.

Little progress has yet been made in extending the general theory to the case of estimating several parameters.

Project B-164-6 - Scheduling Research

Principal Investigator: Dr. I. E. Perlin

The problem under investigation can be described as follows:

Given a list of courses with instructors, number of weekly sessions, time duration of each session, maximum number of students per course specified. Further, the number of hours of instruction per day, the number of classrooms, and the minimum number of students required in order that a course be offered is prescribed. Each student makes a selection of courses that he desires to take. It is required to produce a master schedule specifying time and classroom for each course together with the assignment of students to each course such that the number of conflicts has been held to some acceptable level.

Preliminary investigations have been made and several methods of attack have been investigated. A promising technique appears to be that of setting up an interference matrix showing which courses interfere with each other (courses having students in common). The entries in the matrix indicate the intensity of interference, e.g., five students in common, 20 students in common, etc. The analytical procedure would be to process the interference matrix subject to the restrictions prescribed, such that the total number of interferences would be within the acceptable level.

Some small scale experiments have been made utilizing this technique, and the results were extremely satisfactory.

Project B-164-7 - Business Simulation Research

Principal Investigator: Dr. J. L. Fulmer

This project concerned preparation and testing of a Management Decision-making Business Simulation. Its purpose is to train students in the School of Industrial Management and executive groups in the decision making process.

The specifications for the Business Simulation Game have been written, converted to mathematical formula, and programmed on both the IBM 650 and the Burroughs 220 computers. A non-computer version of the game has also been prepared.

Project B-164-7 - Business Simulation Research (Cont'd)

An Instructor's Manual entitled, "The Theory and Practice of Management Decision-making with Business Simulation Games" was published in May 1961 by the Engineering Experiment Station (144 pages plus iii).

The Business Simulation has been employed in the following training programs:

1. Conference of Southern University Professors on Management Decisions, June 21-23, 1961.
2. Public Utility Executives Course, Management Decision-making Exercise, August 18-19, 1961.
3. The Georgia Society of Certified Public Accountants, Management Decision Simulation for Executives, December 18, 1961.
4. School of Industrial Management Seniors, Management Decision Laboratory, Winter and Spring Quarters, 1962.

Other activities in connection with the project are as follows:

1. A short article, "Test of State Per Capita Income Model with County Per Capita Income", was published in the Southern Economic Journal, October (1960), pp.137-38.
2. The author participated in a data processing conference at the University of Alabama May 19-20, and made a luncheon talk on "Using Business Simulation for Management Training". This has been published in Proceedings for the Fifth Annual Electronic Data Processing Conference, University of Alabama, Extension News Bulletin, Nov.(1960), pp.47-56.

Project B-164-8 - Biela's Comet Research

Principal Investigators: Mr. E. L. Davis, Jr. (and Mr. R. B. Southworth of Harvard College Observatory)

This project was undertaken in connection with Harvard College Observatory to study the orbit of Biela's Comet and the meteors which resulted from its breakup.

Project B-164-8 - Biela's Comet Research (Cont'd)

The orbit of Biela's Comet has been computed forward from 1826 to 1960, and backward from 1826 to 1772. Various initial conditions were used in order to obtain a "best" fit to observations. Data on coordinate position and velocities have been transmitted to the Harvard College Observatory.

Project B-164-9 - Coulomb Effects in Beta Decay

Principal Investigators: Dr. H. R. Brewer, Mr. D. H. Hay, Dr. D. S. Harmer

The calculations required for an investigation of Coulomb Effects in a Beta Decay are similar to those needed for the computation of internal conversion coefficients. In fact, Project B-164-9 is an expansion of a previously initiated internal conversion calculation also sponsored by the National Science Foundation. These two projects, Internal Conversion and Beta Decay, have been complimentary both in personnel and effort. For the above reasons, a summary of the progress in each will be presented.

Beta-Decay

The transition probability in beta decay depends on both the nuclear and electron-neutrino matrix elements. In order to compute electron-neutrino matrix elements the continuum electron wave functions must be known. For realistic extra-nuclear potentials, analytic solutions of the Dirac equation are not known and the Dirac equation must be evaluated numerically.

Programming of the continuum solutions of electron wave functions for both Coulomb and Thomas-Fermi-Dirac potentials have been completed. The calculation produces solutions for either beta-decay or internal-conversion unbound electrons for nuclear charge, Z , 1 to 92; energy, W , 1.001 to $17 mc^2$; angular momentum quantum number, κ , ± 1 to ± 8 .

The results from the numerical Coulomb solution may be compared with the analytic solution to determine if round-off or truncation error is affecting the results in the numerical evaluation. Since the T.F.D. potential case is calculated by the same numerical process mechanism, except for the modification of the potential, these solutions should be expected to be good to the same degree. This comparison indicated significant errors only for extreme values of the parameters, Z , κ , W . Further study is being made to minimize this error consistent with reasonable calculation time.

Project B-164-9 - Coulomb Effects in Beta Decay (Cont'd)

Comparison of the effect of finite size and screening on the wave functions shows a somewhat different energy dependence of the corrections to allowed beta decay than have been calculated by others. The earlier corrections for finite size and screening were calculated separately. The deviations observed were of the order of a few per cent. This effect is expected to be more pronounced for the forbidden decays.

Additional calculations involving those combinations of wave functions present in beta decay are being planned. A proposal to extend this work has been submitted to the National Science Foundation (P-11101).

Internal Conversion

The internal conversion coefficient is defined as the ratio of the probability of a given excited nucleus decaying by the ejection of an orbital electron to the probability of the same nucleus decaying by the emission of a gamma ray. The calculation of these conversion coefficients requires the computation of both the initial wave function of the bound electron and the final electron continuum wave function which represents the ejected orbital electron. The conversion coefficients are then found by appropriate sums of integrals where the integrands are formed by products of these two electron-wave functions and Hankel functions.

The internal conversion calculation is in the final stage of programming. The Dirac equation has been solved for the bound M-shell electron state with corrections for screening and finite nuclear size. These solutions have been tabulated and stored on punched tape, and also published in tabular form.¹ A comparison of these results to the corresponding Coulomb wave functions has been published.²

The programs for computing the final state continuum solutions as well as the evaluation of the Hankel functions have been written as subroutines. At present the various subroutines are being combined for the final master program which will evaluate the internal conversion coefficients.

¹ "Radial Solution of Diracs Equation for M-Shell Electrons", H.R.Brewer, D.S.Harmer, and D.H.Hay, Document No.6855, A.D.I. Auxiliary Publications Project, Photoduplication Services; Library of Congress, Washington 25, D. C.

² "M-Shell Relativistic Electron Wave Functions", H.R.Brewer, D.S.Harmer, and D.H.Hay, Physical Review Letters, 7, 319 (1961).

Project B-164-10 - Monte Carlo Studies

Principal Investigator: Dr. J. H. MacKay

The problem considered is that of determining the frequency of a periodic signal buried in band-limited white noise. Digital observations at the Nyquist rate were used for studies of the maximum likelihood and cross-correlation estimates. The likelihood and cross-correlation functions both peak near the true frequency of the periodic signal, and in both cases the peak apparently becomes much higher and narrower as the number of observations is increased.

For low signal-to-noise ratios these two estimates were observed to behave very erratically, at least for moderate sample sizes. For large sample sizes the numerical values of the estimates are difficult to determine without some a priori information about the true frequency. This suggests that some sort of sequential estimation method might be economical and efficient, although time did not permit the search for a suitable method to be carried out.

Project B-164-11 - Ternary Equilibrium

Principal Investigator: Dr. R. Techo

The problem as outlined in the Annual Progress Report, NSF G-7361 has been completed. The results have been published in a doctoral dissertation entitled, "Liquid-liquid Phase Equilibria". A paper entitled, "An Accurate Method for Testing the Thermodynamic Consistency of Isothermal Binary Vapor-Liquid Equilibrium Data" has been prepared and submitted for publication in the Journal of Chemical Science. It is currently being reviewed. The abstract to this paper is quoted in its entirety below.

The area of thermodynamic consistency of vapor-liquid equilibrium data was further explored with Dr. J. B. Edwards, and the results have been published in his doctoral dissertation.

Current plans include the preparation of several manuscripts for publication and the submission of a research proposal for further study in the areas of thermodynamic consistency.

Project B-164-11 - Ternary Equilibrium (Cont'd)

ABSTRACT

This paper presents a method for using electronic digital computers to determine the thermodynamic consistency of isothermal binary vapor-liquid equilibrium data. Two sets of orthogonal polynomials, $P = P(x)$ and $y = y(x)$, are obtained by fitting the experimental total pressure and vapor composition data as functions of the liquid composition according to the method of least squares. For $P(x)$ and $y(x)$ various polynomials ranging in degree from 2 to the number of experimental data points less one are determined. All the combinations of the degrees of the fitted polynomials are used to compute the excess chemical potentials which are substituted into the Gibbs-Duhem equation. That combination of polynomials, $P = P(x)$ and $y = y(x)$, which minimizes the Gibbs-Duhem equation is then said to characterize the experimental data in the best possible manner with regard to thermodynamic consistency. Criteria are given for determining whether or not data are thermodynamically consistent. The procedure is developed and an example is presented.

Project B-164-12 - Numerical Solution of Partial Differential Equations

Principal Investigator: Mr. A. P. Jensen (and Dr. C. W. Gorton)

The Effect on Velocity Profile of Heat Transfer to a Viscous Fluid in Laminar Flow in a Pipe.

The subject equations:

$$(1) \quad \frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r} \frac{\partial \theta}{\partial r} = \frac{\omega(r)}{a} \frac{\partial \theta}{\partial z} ; \quad r \neq 0$$

and

$$(2) \quad \left(\mu(r) \frac{\partial^2 \omega}{\partial r^2} + \frac{1}{r} \frac{\partial \omega}{\partial r} \right) + \frac{\partial M}{\partial r} \frac{\partial \omega}{\partial r} = \frac{dP}{dz} ; \quad r \neq 0$$

Project B-164-12 - Numerical Solution of Partial Differential
Equations (Cont'd)

where

- θ = fluid temperature,
- r = radial distance from the center of the pipe,
- $\omega(r)$ = axial velocity at radial position r ,
- z = axial distance from entrance to heated section,
- n = viscosity of fluid,
- P = pressure across a section at position z ,

have been reduced to difference form and solutions obtained for (1) for one velocity profile. Investigations to date indicate that stability requirements for (1) are great and place undue hardship on the precision required in the iterative solution of (2). Techniques for minimizing the effect of round-off error have been investigated and applied in obtaining satisfactory solutions of (1).

Efforts to obtain more computable algorithms for (1) and (2) have not produced a worthwhile solution to this system of equations.

Project B-164-13 - Transport Properties of an Ionized Gas

Principal Investigators: Dr. M. R. C. McDowell (Report submitted by Dr. V. D. Crawford, Associate Director of the School of Physics, since Dr. McDowell has returned to England)

Dr. McDowell's work on the transport properties of an ionized gas was supported principally by the U. S. Air Force Office of Scientific Research, under Contract No. AF 18(600)-1524. A considerable amount of computer work resulted from Dr. McDowell's studies and was carried out at the Rich Electronic Computer Center under his direction. This computer work was supported by NSF G-7361.

Project B-164-13 - Transport Properties of an Ionized Gas (Cont'd)

A paper entitled, "Quantal Study of Diffusion and Viscosity Cross Sections for a Screened Coulomb Potential", largely based on the work conducted under the aforementioned contracts, has been published in The Physics of Fluids, Vol.4, pp.1332-1341(1961). This paper was co-authored by Dr. McDowell and Miss G. Peach. Miss Peach was then a doctoral candidate at Royal Holloway College, University of London, England.

The abstract to this paper is quoted in its entirety below. It constitutes a concise resumé of the work.

ABSTRACT

Born's approximation and the Massey-Mohr approximation are used to obtain quantum mechanical values of the diffusion and viscosity cross sections Q_D and Q_η for a screened coulomb potential. The parameters are chosen to represent an ionized gas with $10^8 \leq n_e \leq 10^{18}$, n_e being the electron density, and $5 \times 10^3 \leq T_e \leq 10^7$ °K, T_e being the temperature. The scattering phase shifts are also evaluated and compared with those obtained from direct numerical integration of the scattering equation. Born's approximation to the phase shift is used in a Faxen-Holtmark type analysis to give more accurate values of the cross sections at low T_e and large n_e . The results are used to discuss the behaviour of the electrical conductivity of a fully ionized gas.

The following paper was also published on this work, "Ionization of Lithium by Fast Protons and Electrons". It appeared in The Physical Review, Vol.121, No.5, pp.1383-1387(1961).

Project B-164-14 - Many Particle Systems in Quantum Statistical
Mechanics

Principal Investigator: Dr. V. H. Smith

The work in this investigation is divided under the three following topics. Certain aspects of this work have been or will be presented in the literature and are summarized in the Technical Notes listed at the end. Mr. D. H. Hay and Mr. M. L. Allen participated in the investigation of II, while III was performed by Mr. J. M. Tanner, a doctoral candidate in the School of Physics under Dr. H. A. Bersch.

I. Properties of a Bose System of Particles

The cluster expansion approach discussed by H. A. Bersch and V. H. Smith, in Physical Review, Vol.119, p.886(1960) has been used to determine the complete Hamiltonian for a Bose system of particles with repulsive interactions in the approximation of pair excitations. The cluster expansion is in terms of parameter, formally analogous to the classical fugacity, which indicates in this approximation the depletion of the free particle ground state. The results agree with those obtained using the formalism of second quantization for pair excitation states [Girardeau and Arnowitt, Physical Review, Vol.113, p.755(1959)]. A paper discussing this has been presented at the Louisville meeting of the American Physical Society [V. H. Smith and H. A. Gersch, Bulletin American Physical Society 6, 458, 1961] and the work is summarized in Technical Note No. 1. A numerical investigation of the variational equation obtained from this theory is in progress for several realistic interactions. The problem of higher density effects is also being investigated. A comparison of the trial wave function, often employed in such calculations with a calculation with single pair excitations only is discussed in Technical Note. No. 2.

II. Classical Statistical Mechanics

The question of corrections to the classical Debye-Hückel theory is also under study. In particular, the recently questioned relationship of the theories of Abe and Salpeter has been studied and their first asymptotic correction formulae have been shown to arise from the same terms. This is discussed in Technical Note No. 3. Numerical calculations are in preparation which will help indicate the relative merit of various approximations.

This interest in higher approximation methods led to a consideration of certain integral equations for the pair correlation function for a classical fluid. In particular, consideration was given to the

numerical solution of the integral equation with which a number of names¹ are associated for meaningful values of the parameters. One suggested iterative method for solution of this integral equation begins with the Fourier transform of the Mayer function $-1 + \exp [-\beta V(r)]$, where $\beta = (kT)^{-1}$ and $V(r)$ is the intermolecular potential. An indication of the accuracy of the numerical evaluation of this transform may be obtained by using it to evaluate the third virial coefficient for the system in the gas phase. We have evaluated the transform for a Lennard-Jones 12-6 potential (non-polar) and the third virial coefficient. As we reported at the Tallahassee meeting of the American Physical Society, the latter are in excellent agreement with the direct numerical integration of Bird, Spotz, and Hirschfelder.² They had noticed discrepancies between their results and those obtained earlier by the same method as ours.³ Preliminary calculations have also been made for 9-6 and 28-7 potentials and all results are discussed in Technical Note No. 4. The Fourier transforms have been used to evaluate the ring integral contributions to higher order virial coefficients (Technical Note No. 5). The ring integral contribution to the fourth virial coefficient has been used to show the inherent error in the Gaussian expansion calculations in the literature.⁴ More precise calculation of the fourth virial coefficient is in progress. The Fourier transforms are also being used for their original purpose, the solution of the integral equation. Several other topics are under investigation, including the numerical evaluation of overlap matrices and the use of Padé approximants in the investigation of physical properties for which a limited number of terms of a series are available.

III. Properties of Disordered Lattices

Theoretical and numerical studies of the vibrational frequency spectra of one-dimensional disordered lattices by various investigators have indicated pronounced disorder effects. Dean's numerical calculations⁵ reveal a complex structure of the spectrum at higher frequencies,

¹ See R. Mazo, Ann. Rev. Phys. Chem. 12, 83, 1961.

² Bird, Spotz, and Hirschfelder, J. Chem. Phys., 18, 1395 (1950).

³ Montroll and Mayer, J. Chem. Phys., 9, 626 (1941).

⁴ Boys and Shavitt, Proc. Roy. Soc. A254, 487 (1960).

⁵ P. Dean, Proceedings of the Royal Society, A254, 507 (1960).

where the complexity arises from the presence of numerous "spikes" in the distribution function. Dean identifies a few of these as resulting from certain local-order phenomena. Langer's investigations⁶ of a lattice with a low concentration of light impurities exhibit analytical support for the presence of such "spikes" in the spectra.

The efforts of this investigator have been to study such systems by Green's function techniques with an intent to

- (1) add further analytical verification of these "spikes";
- (2) gain additional insight into the origin of these irregularities.

A small number of the "spikes" in Dean's work have been correlated with certain types of impurity ordering. If the present efforts are successful, extension of this work to three-dimensional systems appears feasible. At this stage it will probably be advantageous, if not absolutely necessary, to incorporate rather extensive numerical calculations to extract meaningful results.

Technical Notes

1. "Cluster Expansions and the Theory of Many-Boson Systems", V. H. Smith and H. A. Gersch
2. "Theory of Many-Boson Systems: Pair Approximation and the Jastrow Trial Pair Function", H. A. Gersch and V. H. Smith
3. "Corrections to the Debye-Hückel Theory", V. H. Smith
4. "Virial Coefficients for the Lennard-Jones Potential", V. H. Smith and D. H. Hay
5. "Ring Contributions to Higher Virial Coefficients", V. H. Smith and D. H. Hay
6. "An Algorithm for the Division of Power Series", V. H. Smith and M. L. Allen (will appear in the Nov. 1962 issue of the Communications of the ACM)
7. "Generating Functions for Direct and Inverse Sums of Powers of Roots of Polynomial Equations", V. H. Smith and M. L. Allen

⁶J. S. Langer, Journal of Math. Phys., 2, 584 (1961)

Project B-164-15 - A Study of Properties Relating to Uniform
Approximations

Principal Investigator: Dr. W. J. Kammerer

The study consisted of two separate investigations concerning best approximations in the uniform norm.

A study of best uniform approximations which lie above (or below) the function to be approximated was undertaken. Various results were obtained and a paper entitled, "Best One-Sided Approximations in the Uniform Norm" was submitted for possible publication in SIAM (Society for Industrial and Applied Mathematics). As yet no word of their decision has been received.

The question of convergence of the best L_p approximation, to a best uniform approximation (as $p \rightarrow \infty$) was studied. We were able to show convergence when the domain of definition was a finite point set. However, convergence for the general case (when the domain of definition is a compact Hausdorff space) remains an unsolved problem.

Project B-164-16 - A Study of Ill-Conditioned Matrices

Principal Investigator: Mr. F. E. Schlaepfer

Properties of an ill-conditioned matrix A were studied and methods for determining its inverse applicable on electronic computers were devised.

A best possible upper bound for the P- condition as a function of the order, the determinant and the Euclidean norm was derived.

All the inversion methods studies reduce the problem of inverting an ill-conditioned matrix to the problem of inverting a well-conditioned matrix.

In the first method the condition of the matrix is improved during the execution of the Gaussian algorithm. Column vectors of A are replaced by linear combinations of other column vectors. (Reconditioning). More accurate inverses as well as more accurate values for the determinant than by an ordinary Gaussian process could be obtained. The efficiency of the method was theoretically investigated.

Project B-164-16 - A Study of Ill-Conditioned Matrices (Cont'd)

The second procedure already demands a first approximation Z of the inverse A^{-1} . The error matrix $E = A \cdot Z - I$ ($I =$ identity matrix) is computed and a better approximation $Z_1 = Z (I + E)^{-1}$ is evaluated.

For symmetric ill-conditioned matrices the second procedure could be simplified and connected with the Choleskey-inversion method. The necessary number of multiplications was reduced to less than half without loss of accuracy.

The three methods were tested numerically on finite segments of Hilbert matrices up to order 9. All the results of the methods mentioned compared favorably with the results of common inversion procedures.

A publication is in preparation.

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16. Smith, V. H., "Corrections to the Debye-Hückel Theory", to be submitted for publication to Physical Review.
17. Smith, V. H., and Hay, D. H., "Virial Coefficients for the Lennard-Jones Potential", to be submitted for publication to Journal of Chemical Physics.
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20. Smith, V. H., and Allen, M. L., "Generating Functions for Direct and Inverse Sums of Powers of Roots of Polynomial Equations", to be submitted to Mathematics of Computation.
21. Techo, R., "An Accurate Method for Testing the Thermodynamic Consistency of Isothermal Binary Vapor-Liquid Equilibrium Data", currently being reviewed for publication in Journal of Chemical Science.