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Theoretical Division Annual Report FY 1975

by

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THEORETICAL DIVISION ANNUAL REPORT - FY 1975

Peter A. Carruthers, Division Leader

Compiler: Necia Grant Cooper

ABSTRACT

This report presents an overview of the activities in the Theoretical Division and a summary of research highlights during FY 1975. It is intended to inform a wide audience about the theoretical work of the LASL and therefore contains introductory material which places recent advances in a broader context. The report is organized into two special interest reports: reactor safety research and the Advanced Research Committee, and 11 reports from the T-Division group leaders on the work of their respective groups. Main interests and responsibilities are outlined including the relationship of the group's work to the work of other T-Division groups and other divisions at the Laboratory. The description of research highlights for FY 1975 explains in a fairly simple, straightforward manner the major recent advances and their significance. Each group report is followed by a publication list for FY 1975 and a list of talks given outside the Laboratory.

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Fig. 1. P. A. Carruthers (left) and LASL consultant M. Gell-Mann discuss recent developments in physics.

PREFACE

The Theoretical Division of the Los Alamos Scientific Laboratory (LASL) was formed in 1943 with the single purpose of designing a successful nuclear weapon. Over the years the number of goals of the Division has multiplied enormously. The Division is now an interdisciplinary community of theorists performing pure and applied research in a broad spectrum of disciplines ranging from reactor safety analysis to theoretical biology.

Nuclear weapons design, per se, is no longer the responsibility of T Division. However supporting research necessary to such design, including numerical hydrodynamics, equation of state and opacity research, nuclear data collection and evaluation, and neutron transport theory, remains the single most important effort of the Division.

Newer and growing in importance is the theoretical effort on current and future energy sources. Laser theory and reactor safety analysis are now major programs with both laser fusion and reactor safety studies benefiting greatly from the accumulated experience in weapons physics unique to the LASL. The new Laboratory programs on material properties and energy sources require an increased effort in materials theory and molecular chemistry research. An active program in theoretical chemistry already exists in the laser theory group; expansion and diversification of this effort is planned for the future. In addition, a materials theory effort is in the process of formation.

In recognition of the fact that a healthy program in applied science requires close contact with developments at the frontiers of science, a small but significant effort in basic research has been established in the Division. Originally consisting of low and medium energy nuclear physics research, this effort has been expanded since 1973 to include theoretical biology, elementary particle theory, and applied mathematics. Moreover, vital contacts are maintained with the

academic community through an active visitor and consultant program involving many of the country's best scientists.

The present scientific staff of the Division comprises some 180 staff members. While involved in specialized projects, the scientists participate in a continuous and vigorous interaction across disciplinary and divisional lines. This truly interdisciplinary character makes T Division a unique national resource of pure and applied theoretical research.

The Division is organized by discipline into ten groups, T-1 through T-10. Although the group titles only partially represent the diversity of research interests, the main strengths of the Division are revealed by the following organizational breakdown:

T-DO	Division Office
T-1	Transport Theory, Reactor Theory, and Reactor Safety
T-2	Applied Nuclear Data
T-3	Fluid Dynamics
T-4	Equation of State and Opacity
T-5	Medium Energy Physics Theory
T-6	Laser Theory
T-7	Mathematical Modeling and Analysis
T-8	Particle Physics and Field Theory
T-9	Nuclear and Other Theory
T-10	Theoretical Biology
T-DOT	Other Theory

The individual group reports which follow introduce the work of each group and present the highlights of advances made during FY 1975. Preceding these are two special interest reports: (1) T Division Reactor Safety Research and (2) the Advanced Research Committee.

P. Carmichael

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DIVISION LEADER:	Peter A. Carruthers
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ASSOCIATE DIVISION LEADER:	George I. Bell
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T-1

TRANSPORT THEORY, REACTOR THEORY, AND REACTOR SAFETY

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T-3
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T-4
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T-5

MEDIUM ENERGY PHYSICS THEORY

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T-6

LASER THEORY

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T-8

ELEMENTARY PARTICLES AND FIELD THEORY

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T-9

NUCLEAR PHYSICS AND OTHER THEORY

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T-10

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LOS ALAMOS SCIENTIFIC LABORATORY ORGANIZATION

APRIL 1975

T-DIVISION REACTOR SAFETY RESEARCH

by K. D. Lathrop

In the last three years, two factors have led to a substantial increase in the national reactor safety research effort. First, concern for U.S. energy independence initiated a national assessment of energy options that emphasized the role nuclear reactors would play in future energy generation. Second, the separation of the Nuclear Regulatory Commission (NRC) from the Energy Research and Development Administration (ERDA) provided a focal point for guidance and funding of reactor safety research. Led by the Theoretical Division, the LASL has taken an increasingly active part in national safety research and now has programs concerned with safety problems in Fast Breeder Reactors (FBRs), Light Water Reactors (LWRs), and High Temperature Gas-Cooled Reactors (HTGRs).

There are now 56 LWR plants in the United States with operating licenses, 62 reactor plants under construction, and 101 more on order.* In the first quarter of 1975, the operating plants produced 8.5% of all the electricity sold in the U.S. Even including the more expensive plants required, nuclear reactors offer significant economic advantages over similar coal-fired plants, and the advantage appears to be growing. It seems clear that nuclear energy will become an increasingly important national resource.

In addition to LWRs now being sold, the graphite moderated, helium cooled HTGR is in the licensing process. These reactors are designed to operate at significantly higher temperatures than LWRs, making possible greater plant efficiency. There is now a 300 MWe HTGR demonstration plant at Ft. St. Vrain in Colorado.

* Outside of the U.S. there are 102 plants with operating permits, 85 with construction permits, and 70 more on order.

For the longer term, the Liquid Metal Fast Breeder Reactor (LMFBR) is the current leading candidate to breed fissionable plutonium from ^{238}U as well as to generate electricity. Current predictions are for the construction by ERDA of an LMFBR demonstration plant in the 1980's with commercial power generation by LMFBR's in the 1990's. These reactors are expected to play a major role in extending resources of fissionable material and in power generation until the latter is taken over, it is hoped, by fusion energy generators.

Ideally reactor safety research should:

1. derive a means of cataloging all possible accidents,
2. develop the tools required to predict the consequences of such accidents,
3. estimate the probability of such accidents to quantify, risk in terms of the product of consequence and probability of occurrence,
4. help quantify the meaning of "safe" by developing means to uniformly compare societal risk,
5. and suggest designs to improve plant safety until plants meet or exceed societal safety standards.

Clearly the above tasks are very, very broad and perhaps not totally possible. Initial LASL research is primarily devoted to estimating accident consequences for accidents that are deemed possible and severe although perhaps very unlikely. This research is in line with the present philosophy of designing reactor systems, namely, that the designs must protect against the most severe credible events imaginable as well as against less severe occurrences, including unforeseen ones.

The broadest in scope of the LASL programs is HTGR safety research, which covers all aspects of the reactor system. The effort is directed toward providing the licensing authority with the technical basis for making decisions, and focuses on immediate problems relating to existing reactor designs. At the LASL, the HTGR safety

program is organized as a project that directs research in T, A, and CMB divisions.

The LASL LWR research effort is almost entirely in T Division. There has never been a full-scale test of the Emergency Core Cooling System (ECCS) for LWRs now producing power, so faith in the performance of the ECCS is based in large measure on detailed calculational estimates. There is a continuing desire to verify the performance of the ECCS during loss-of-coolant accident (LOCA) sequences and to obtain a more accurate estimate of the degree of conservatism which constrains LWRs to operate at less-than-possible temperatures and pressures. The LASL Theoretical Division has been commissioned by NRC to produce a computer program to provide a best-estimate model of LWR hydraulic systems performance during LOCAs. The LASL was selected for this program because of the prior achievements of T-3, its theoretical hydrodynamics group.

Again, the LASL's recent entry into FBR safety research was facilitated by the strength of the Theoretical Division's transport theory (T-1), hydrodynamics (T-3), and equation of state and opacity (T-4) groups. In one LASL research task, these groups are jointly developing a computer code to predict the course of hypothetical accidents that might lead to core melting and large-scale motion of material. Because FBRs contain several critical masses of fuel, it is conceivable, although unlikely, that fuel melting could lead to a supercritical arrangement of fuel and an additional energy release. Hence, not only the hydrodynamic motions and the solid, liquid, and gaseous state of the system, but also the neutronic characteristics need to be predicted continuously. The three groups involved have confronted similar problems in weapons research and are ideally suited to meet the challenges of this extremely complicated problem.

Computer programs should be tested against experiments when this is possible, but experiments modeling FBR accidents are difficult to define and expensive to perform. Presently the ERDA is

attempting to select a design for a major LMFBR Safety Research Facility (SAREF), and NRC has asked the LASL to mount a continuing effort to define the required safety research facilities, to define the required experiments, to perform neutronic and design analysis of the proposed experiments and facilities, and to recommend instrumentation. The Theoretical Division is performing the experiment and facility definition portion of this task and A Division (Nuclear Safeguards and Reactor Technology) is responsible for the instrumentation and facility design work.

Within T Division, the largest safety research effort (25 people) is located in Group T-1 and is concentrated on creating the computer programs required. The second largest effort is in Group T-3 (14 people) where the hydrodynamic methods needed to treat multiphase-multicomponent flows and to describe the complex geometries involved are under development. Group T-4 provides equation of state data, T-2 provides nuclear data, and T-7 provides guidance in equation formulation and solution methodology.

I. HIGH TEMPERATURE GAS-COOLED REACTOR SAFETY RESEARCH

Group T-1 is responsible for the accident delineation and systems analysis tasks in the LASL HTGR safety project. Accident delineation is the art of deciding which accidents should be considered and defining the logical progression of accidents from initiating event to conclusion. Systems analysis is the task of developing the tools necessary to permit the estimation of accident consequences. The relationship between accident delineation and systems analysis is symbiotic. For example, no analysis tool can yet predict the progression of an accident, so progressions must be defined. However, analysis can show through sensitivity studies that certain classes of sequences need not be considered because their consequences are benign.

The HTGR is in many respects easier to analyze than a LWR. The

helium coolant is single-phase, and the enormous graphite core has a huge heat capacity so that thermal transients occur more slowly. The primary concern in HTGR accidents is whether or not elevated core temperatures cause the release of fuel fission products into the coolant stream (and eventually, it is assumed, to the surrounding atmosphere after penetration of the primary and secondary containments). To better assess the evolution and consequences of an HTGR accident, Group T-1 is constructing a comprehensive HTGR analysis program (CHAP) which will model the time-temperature history of the entire system, including core, reactor vessel, circulators, steam generators, etc., for a variety of accident sequences and plant designs. The modeling process consists of reducing complex representations to simple ones while retaining all the essential characteristics of the complex model. For example, three-dimensional heat transfer calculations are possible for rather precise geometrical descriptions of an HTGR, but these are prohibitively expensive to perform repetitively during a whole system analysis. Therefore, in the CHAP computer model, the core is represented by calculating the temperatures at axial nodes within selected symmetry elements (channels). This simplified model is tested and calibrated against a more precise model for all variable ranges of interest.

Before CHAP can be used to predict accident consequences, a large amount of data must be supplied. For most among these data are the neutronic response of the HTGR during transient situations (e.g., during the design-basis depressurization where a postulated loss of helium pressure and helium reduces core cooling). Groups T-1 and T-2 are engaged in a major effort to verify almost all of the neutronic analyses performed by the reactor designer. The most difficult of these analyses is the prediction of the net temperature coefficient of reactivity. It is most desirable from a safety standpoint for an increase in core temperature to decrease the neutronic reactivity. In the HTGR, the net coefficient appears to have this property but the coefficient is small and made up of a large number of subtly varying components. For example, as the nuclear fuel is

burned, ^{233}U is produced from ^{232}Th , and the neutronic properties of ^{233}U are such that the numerically calculated net temperature coefficient becomes less negative. However, the experiments performed on representative assemblies have given ambiguous results (the experiment is very hard to do), and numerical calculations depend on a lengthy chain of processes each of which may introduce errors.

Once the CHAP code is developed it will be used both by the LASL and the licensing and technical review divisions of NRC. We will use it to estimate accident consequences for all delineated accidents, to search for unforeseen accident sequences, and to determine system design features that are most critical for plant safety. NRC will use CHAP to confirm vendor design performance as stated in safety analysis reports.

II. LIGHT WATER REACTOR SAFETY RESEARCH

In the LWR design basis loss-of-coolant accident, one of the major coolant pipes ruptures. The high pressure coolant water in the reactor core flashes to steam and emerges through the rupture. Core temperatures rise. To prevent fuel melting and release of fission products, an emergency cooling system is actuated. Does this system work? What is the highest temperature reached by any fuel element in the core?

These and many other related questions will be answered, we hope, by the TRAC (Transient Reactor Analysis Code) computer program, a code now being developed jointly by T-1 and T-3 to describe the complicated thermal-hydraulic behavior of an LWR cooling system. The TRAC code will eventually replace a currently used, one-dimensional system and will more accurately describe both two-phase flow and the actual system geometry.

As in the HTGR project, modeling plays an important part in producing efficient computer simulation of system component behavior.

Existing two- and three-dimensional T-3 hydrodynamics codes provide precise solutions to guide model development for LWR problems. As with the CHAP code for the HTGR, the TRAC code is being designed to allow a choice of numerical models for each reactor component. Thus one user will be able to select all the most detailed models to obtain the best available solution, while another can use simpler models to scope qualitative effects.

Basic fluid dynamics research is also a major part of the LWR safety program. The treatment of two-phase flows recently developed by T-3 for use in the LMFBR program can also be used for LWR two-phase flows. Harlow settled a fundamental controversy in this area by carefully defining the equations to be solved. He succeeded in developing equations which suitably damp numerical instabilities without losing the capability for calculating physically unstable flows. In two-phase calculations, certain rate coefficients are required. Lacking experimental correlations, the form of these must be estimated. Evaporation and condensation processes are especially important, and T-3 is beginning a careful study of the nature of evaporation and condensation.

The development of the TRAC code is part of a carefully scheduled NRC master program which calls for the completion of the advanced systems code by the end of 1977. During its development and after its completion, TRAC will be continually tested for its ability to predict the results of a large number of NRC-conducted experiments.

III. FAST BREEDER REACTOR SAFETY RESEARCH

A. Modeling of Core-Disruptive Accidents

In the LMFBR, if the sodium coolant flow is lost, and if the reactor protective systems fail, the center of the core becomes hot enough to vaporize sodium; this has a positive reactivity effect. A super-prompt critical excursion then begins that is terminated when material expansion has dispersed fuel sufficiently

to cause neutronic shutdown. However, the energy generated is enough to melt surrounding fuel which may then slump and reassemble in a second super-critical configuration. Molten fuel expelled during the first excursion may freeze in the colder regions above the core and then, due to decay heating, melt and fall back into the core. Worse, expelled fuel may be forced into the surrounding sodium and a fuel-coolant thermal interaction may drive fuel back into the core. All these scenarios are highly speculative.

To shed light on what happens in these and other similar accident situations, T-1, T-3, and T-4 are developing a coupled neutronic, hydrodynamic, equation of state computer program called SIMMER (for S_n , Multifield, Multicomponent, Eulerian, Recriticality). The program is being designed to compute, in two spatial dimensions, time-dependent neutron distributions, taking into account the effects of material motion and local temperature on cross sections. Simultaneously, SIMMER will use the fission energy source predicted by the neutronic calculation in computing the hydrodynamic motion of solid, liquid, or vapor phases of fuel, steel, or sodium. Continuous equation of state data are to be provided by interpolation from specially constructed tables. The hydrodynamic methods to be used are a sophisticated development due to T-3 and allow interpenetration of fields, transitions between fields, and representation of rigid structure. (See Fig. 2 and Fig. 3.)

A preliminary version of SIMMER is operating satisfactorily and a first complete version will be used in a detailed testing program beginning January 1, 1976.

SIMMER will be used to design and suggest experiments for a safety test facility and, in turn, part of the function of the facility will be to provide experiments which will help validate SIMMER. The code will also be used to search for generic phenomena in FBR core disruptive accidents and eventually may be able to predict

Fig. 2. Schematic of fast reactor core geometry showing expansion of molten core material - one stage in an accident sequence to be computed by the SIMMER program.

Fig. 3. A KACHINA calculation of a simplified reactor core explosion. The diagram displays the initial configuration. Below it are Marker-Particle configurations at three different times as computed by KACHINA. The cold case material is represented by open squares, the fuel by crosses, and the vapor by dots. The sequence shows the initial explosion of hot fuel.

the interaction of the energy released with the reactor containment systems. Should SIMMER indicate that containments are inadequate (this possibility is believed to be very unlikely), the code would be used to guide FBR redesign.

B. Definition of a Safety Test Facility

Guided by George Bell of T-DO, and with major contributions from Mike Stevenson (T-1), Jay Boudreau (T-1), Ron Palmer (T-DOT), and others in A-Division, P-Division, and the Engineering Dept., a study was initiated for NRC on requirements for new experimental facilities for conducting tests related to the safety of Fast Breeder Reactors. In particular, the desired characteristics for major in-pile facilities were evaluated.

First, a thorough review was conducted to determine the current level of understanding of the initiation, progression, and termination of possible core disruptive accidents. From this review it was apparent that certain classes of in-pile experiments would be valuable for checking and extending the analysis of hypothetical accidents. Facility characteristics which would be required for performing the experiments were examined and it was concluded that four kinds of facilities, denoted by A, B, C, D, deserved further intensive study. Facility A would be used for experiments on fuel pin failure mechanisms and for examining the early stages of sodium, cladding, and fuel motion. The experiments would involve relatively small numbers (<37) of fuel pins. In facility B, extended motions of subassembly amounts of fuel (~ 271 pins) would be observed, while facility C would be used for simulations of whole core disruptive accidents. All of these facilities would need to accommodate short period transients. In facility D, low steady power levels would be imposed on large masses of fuel to study post-accident heat removal problems.

Desired characteristics, such as size, power level, and transient parameters, were delineated for each facility, and the needed experimental data were identified.

Fig. 4. Flash x-radiograph of a bundle of 19 PWR fuel pins showing individual fuel pins and the space within the central fuel pin (dark central rectangle) from which the UO_2 fuel was removed. This picture was made with the PHERMEX² pulsed x-ray machine at LASL and illustrates the capabilities of flash x-radiography for revealing positions of fuel, cladding, and sodium during a transient which might be conducted in an LMFBR Safety Test Facility. A water level, simulating liquid sodium, is also visible near the bottom of the picture. Similar results can be obtained for 61 PWR fuel pins, the amount of fuel present in a full LMFBR subassembly.

Preliminary conceptual design studies were made for class A and B facilities. In particular, a large number of neutronic and transient heat transfer calculations were made for facilities fueled by uranium in a beryllium oxide or graphite matrix and a range of designs satisfying the requirements for facility A was found. The driver fuel was to be in the form of pins (OD $\approx$ 1/2 in.) clad in steel and cooled by liquid sodium.

Possible experimental techniques for observing fuel motion were examined. Flash x-radiography was found to be promising and experiments conducted at LASL'S PHERMEX machine confirmed applicability of this technique. (Fig. 4.)

A preliminary report* was prepared for NRC and has formed a basis for NRC policy. The study is continuing with an expanded level of effort during FY 76.

*G. I. Bell, G. E. Boudreau, T. McLaughlin, R. G. Palmer, V. Starkovich, W. E. Stein, M. G. Stevenson, and G. L. Yarnell, "Study of Fast Reactor Safety Test Facilities," Los Alamos Scientific Laboratory report LA-5978-MS (May 1975).

THE ADVANCED RESEARCH COMMITTEE

by David Sharp

The T-Division Advanced Research Committee was established about a year ago as a kind of "think tank" or consulting group for the major programmatic efforts at the LASL. The Committee is comprised of 20 members from T Division. Individually the members are at the forefront of scientific research in their respective areas and perform consulting functions relating to their individual capacities. Through the Committee, it is hoped that the breadth and depth of their collective knowledge and expertise can be applied to the most difficult, significant, and far-reaching problems facing research and development at the LASL.

The specific objectives of the Committee are:

1. to prepare informed appraisals of on-going Laboratory programs,
2. to provide guidance or solutions for specific problems that arise in individual programs,
3. to stimulate new research in areas of present or potential interest to the LASL,
4. to develop long-range goals for research and development into practical problems of national concern, goals which may not be tied necessarily to existing short-term programmatic goals, and
5. to provide a nucleus of people who can help the Laboratory exploit new ideas quickly or solve particularly difficult problems.

I. COMMITTEE ACTIVITIES: FY 1975

During FY 1975, the Committee met as a group 26 times. During the meetings speakers from throughout the Laboratory presented problematic topics relating to on-going programs. The list of speakers and titles which follows should convey the diversity and practical interest of the material studied at the meetings.

Committee Speakers and Titles for FY 1975

P. Robinson	JUMPER* Project
T. Cotter	JUMPER
S. Rockwood	Physical Chemistry Issues of Laser Isotope Separation
R. L. Morse	Instability in Laser-Driven Implosions
R. Osborn	ESTACA
Jo Ann Howell	Algebraic Manipulation (Macsyma)
B. Nichols	Indexation vs Inflation in Mathematical Economics
W. Beyer	Input-Output Economics and Regional Energy Models
R. G. Shreffler	PACER
L. Klein	Econometrics
C. Anderson	PACER Cavity Stability
L. Asprey	New Experimental Results Pertaining to JUMPER
W. Goad	Molecular Physics
J. Scolman	Weapons Testing at the Nevada Test Site
C. Mader	The Mix Problem
D. Dudziak	Survey of Fission Reactors and Their Characteristics
G. E. Dials	The Societal Cost of Coal
M. Stevenson	Accident Sequences in Liquid Metal
Jay Boudreau	Fast Breeder Reactors
W. Reed	LASL's Reactor Safety Program - An Overview
J. C. Mark	Some Elementary Aspects of Weapons Physics
M. Glantz	Weather and Climate Modifications and the Future of the Sahara

A series of meetings was devoted to each of four of the programs listed, namely, to JUMPER (Fig. 5), Reactor Safety, and Weapons Physics, on the grounds that they are major Laboratory programs of high national priority; and to Econometrics and Regional Planning in which the Laboratory is undertaking a new and substantial commitment.

* JUMPER refers to the Laser Isotope Separation Program.

As a result of the series on JUMPER, the Committee adopted a memorandum (classified) containing a number of recommendations regarding the management of that program. Also stimulated by the JUMPER series, Walter Goad initiated a group effort to explore newly developing opportunities in the design of catalytic and energy transducing systems. This effort continues.

II. PLANNED ACTIVITIES: FY 1976

From the above it is clear that this past year the Committee devoted most of its efforts to informing itself about present Laboratory programs. This year the Committee will continue to meet weekly but will focus its attention on more detailed surveys of a narrower range of topics. Subcommittees will then be formed to do in-depth studies for those areas where specific recommendations are needed.

Fig. 5. A simple "off-the-shelf" CO_2 laser used by the Laser Division to separate, for the first time, valuable isotopes of three elements. These experiments were part of JUMPER, the laser isotope separation program.

INTRODUCTION TO GROUPS T-1, T-2, T-3, and T-4

In the early years of the Laboratory, these four groups provided the essential ingredients for weapons design, working almost exclusively in this area. Today their charter is much broader. They provide the theories, computer codes, and data for a wide range of applications including fission and fusion (plasma and laser) reactor design. Group T-2 (Nuclear Data) provides neutron and high-energy photon cross sections while Group T-4 (Equation of State and Opacity) similarly provides atomic and molecular opacities as well as equation of state libraries. Group T-1 (Transport Theory, Reactor Theory, and Reactor Safety) creates and distributes neutron particle transport codes, and Group T-3 (Fluid Dynamics) does the same for hydrodynamic codes. Moreover each group performs the basic research needed to make its product the best available.

Their most important roles, however, are still support of the LASL weapons program and, in addition, support and direction of reactor safety programs. These efforts involve collaboration and cooperation among the four groups.

A. An Example of Collaboration -- A Problem in Fast Reactor Safety

To introduce the work of each group and illustrate the manner in which each contributes to a program, we will consider a particular problem in fast reactor safety, sketch the physical processes which must be understood in order to solve the problem, and identify research skills, evaluated data, or computing programs which each group contributes toward the solution. Much the same picture could be presented for weapons design, and we will conclude with a few remarks comparing weapons design with reactor safety problems.

A central problem in fast reactor safety is "what happens if the core melts?" Since there may be more than a ton of plutonium in a fast reactor and since the neutron energies are relatively high as in a fission bomb, it is natural to be concerned that a destructive fission explosion might result. Nearly two decades ago, H. A. Bethe and others investigated this problem and proved the impossibility of any explosive energy release which would, per se, threaten the health and safety of the public. However, it was not possible then nor is it possible now to show that an energy release threatening integrity of the reactor containment is impossible. Since any large release of plutonium or fission products to the environment would be disastrous, a large program of analysis and experiments at the LASL, and elsewhere in the USA and other nations, is devoted to assessing the probability and consequences of accidents which might damage and lead to melting of fast reactor cores.

In a liquid metal-cooled fast breeder reactor (LMFBR) there are roughly 10^5 fuel pins cooled by rapidly flowing liquid sodium. A typical pin contains mixed oxide fuel ($\text{PuO}_2 + \text{UO}_2$) within a cladding of stainless steel and has a length ≈ 1 m and a diameter of ≈ 0.5 cm.

An accident is assumed to be initiated by some unintended undercooling and/or excess power generation in the fuel. (Undercooling could be caused by a blockage of sodium flow or by pump failure; excess power could be caused by withdrawal of control rods.) In addition it is assumed, for the purpose of analysis, that the diverse and redundant reactor shutdown systems fail to operate. Given this unlikely sequence of reactor system failures, the probability of which must be eventually evaluated, it is the task of the analysis to calculate the consequences of the accident. To this end, one or more major computer programs must be written and must contain reasonable simulations of the physical effects which are believed to determine the course of the accident.

As the core overheats, liquid sodium will boil and fuel and cladding will melt and perhaps eventually vaporize. The precise order in which

these events occur will depend on details of the postulated accident initiation. As a first step in the accident analysis, it is necessary to predict the motion of the various fluids which are present in the core, given the pressures and temperatures. Group T-3 has been responsible for this predictive capability. Drawing on more than 100 scientists' experience in numerical fluid dynamics, T-3 group members have devised new numerical methods for treating the interactions between multiple phases (vapor, liquid, and solid) and multiple materials (sodium, steel, fuel) in complex geometry. It may be noted that there is no hope of treating the full geometrical complexity, including the 10^5 fuel pins. Idealization to two-dimensional, axially symmetric geometry is currently made in the SIMMER program. A number of other complementary calculations and computer programs, in which fine details are represented for a small portion of the core, are in the planning stage.

In the fluid dynamics calculations, it is necessary to know the pressures exerted by the various materials as functions of their densities and temperatures. These equation of state data are furnished by Group T-4, based on the evaluation of all available experimental information together with basic theoretical studies.

The other major component of the calculation is an ability to follow the behavior of neutrons in the system. In particular, we must determine whether the system is becoming more or less critical as the configuration of materials changes and we must compute the rate of fission energy generation in all the fuel. An approximate, numerical solution of the neutron transport equation is required and furnished by Group T-1, based on more than two decades of experience in neutron transport codes. Neutron cross sections for all materials in the calculation are furnished by Group T-2 from their files of evaluated nuclear data. In the present case, special evaluations of the effects of Doppler broadening of plutonium and uranium resonances may be required.

In Fig. 6, the components of the calculation and contributions of each group are summarized. In the present case, responsibility resides in Group T-1 for assembling all of the components in a single computer program, SIMMER, and for testing, documenting, and using the program. Of course, each group will be engaged in subsidiary calculations and research to establish a solid base for its contribution. For analysis of fast reactor accidents, there is a particularly complex phenomenon which requires further theoretical and experimental study. This is the fragmentation/coalescence of droplets of fuel and cladding within fluids and the transfer of energy and momentum between the various components.

Fig. 6. Responsibilities of Groups T-1 - 4 in a Reactor Safety Calculation.

If we considered a weapons design problem rather than a reactor safety problem, the contributions which Groups T-1, T-2, T-3, and T-4 would be expected to make to the solution would be much the same. However, TD Division would have responsibility for developing the general computer programs and might well employ its own computer codes for treating fluid dynamics and neutron transport. Since temperatures in exploding weapons are far higher than in reactors, the interactions between radiation and matter must be included in weapons calculations. Group T-4 is responsible for supplying weapons designers with cross sections and opacities for such interactions.

GROUP T-1 - TRANSPORT THEORY, REACTOR THEORY, AND REACTOR SAFETY

K. D. Lathrop, Group Leader

I. INTRODUCTION

Group T-1 performs research in two main areas. In the first, the group continues work begun at Los Alamos under Feynman and Serber in 1943 to develop methods for predicting the spatial and angular distributions of neutron particles. This research has always been closely allied with the development of numerical methods and computing machinery, and for many years [until the LASL computing (C) division was formed in 1968] all three functions were performed in Group T-1. In 1974, we added to transport theory research a major program in reactor safety which now involves 25 of the 43 people in the group. The safety effort is primarily devoted to the development of large computer codes for the analysis of accident sequences. This effort is described in a separate section of this report which covers all the safety research of T Division.

Prediction of neutral particle distributions is essential in both fission and fusion devices for weapon or reactor applications. The two major methods (Monte Carlo and S_n -discrete ordinates) for calculating these distributions were invented at LASL. Monte Carlo research is conducted by LASL group TD-6, while T-1 concentrates on deterministic methods. In this area, T-1 is acknowledged as a world leader. Many of the computer programs and numerical methods developed by members of the group are used throughout the free world. The transport theory effort is supported about equally by the ERDA Division of Reactor Research and Development and the Division of Military Applications.

The linear Boltzmann transport equation is a sufficiently accurate model for most fission and fusion applications. Our current

research is therefore devoted to extending the capability of our numerical methods for solving this equation. The following three advances have greatly extended the scope, accuracy, and efficiency of our numerical capabilities: (1) improved difference schemes have made it possible for us to use triangular meshes to better describe complicated assemblies; (2) improved convergence acceleration methods have made possible the more efficient solution of huge systems of equations (10^5 to 10^6 unknowns) resulting from the discretization of the Boltzmann equation; and (3) improved data management techniques have increased the number of independent variables we can treat. In FY 1975 we incorporated these advances in five computer programs which are described below.

Our development of transport computer programs has involved us in a number of subsidiary activities. Locally we maintain a library of 10 of our current codes and provide consulting and code modification services for the LASL applications. We also perform certain shielding and CTR neutronic analyses within the group. Nationally we export our computer programs through the Argonne Code Center and the Oak Ridge Shielding Information Center. For large-scale users we provide consulting and sometimes code modification services. Our interest in code portability has led to our leadership in an ERDA project to develop standards to facilitate computer code exchange. As part of this program we test newly-developed reactor physics programs on our computers. This work keeps us abreast of new methods and makes codes developed elsewhere available at the LASL.

II. RESEARCH HIGHLIGHTS

New computer programs are written when developments in solution techniques warrant replacing older computer programs. During FY 1975 we continued or completed development of the five computer programs listed in the table below.

<u>Code Name</u>	<u>Function</u>	<u>Advances</u>
ONETRAN	Solves the time-independent transport equation in one-dimensional planar, cylindrical, and spherical geometries. Provides consistent initial conditions for TIMEX.	Linear, discontinuous finite element difference scheme, convergence acceleration, data management.
TIMEX	Solves the time-dependent transport equation in the ONETRAN geometries.	Linear discontinuous finite element difference scheme.
TRIDENT	Solves the time-independent transport equation on a triangular grid in either planar or cylindrical two-dimensional geometries.	Linear discontinuous finite element difference scheme plus ray effect remedy, efficient data management.
TWOTIME	Solves the time-dependent transport equation in (x,y) (r, θ) cylindrical or (r,z) cylindrical geometries.	Explicit, efficient time difference algorithms.
THREETRAN	Solves the time-independent, three-space dimensional transport equation.	First general three-dimensional code.

Rather than describe each code, which either has been or will be provided with extensive documentation, we will discuss the general nature of the improvements.

A. Linear, Discontinuous Finite Element Difference Scheme

The linear, discontinuous finite element difference scheme, first derived by William Reed, permits the use of triangular spatial regions, thereby increasing the flexibility of geometric representation. While the usual continuous finite element methodology also makes possible the treatment of arbitrarily shaped zones, it lacks one of the most important properties of previous techniques. Namely the resulting coupling between cells destroys the lower triangular character of

the huge iteration matrices involved. Use of a discontinuous trial function retains this character. The linear discontinuous schemes are more positive (less oscillatory) than previously used schemes and thus interact more favorably with convergence acceleration algorithms. In terms of Padé approximates to exponentials, the discontinuous scheme corresponds to using the second order (1,2) approximate rather than the (1,1) or Crank-Nicholson recipe. These advantages of the scheme induced us to introduce linear discontinuous difference equations for treatment of the spatial variables into the ONETRAN, TIMEX, and TRIDENT codes.

B. Improved Treatment of Angular Variables

In the TRIDENT code we now allow the optional use of a new treatment of the angular variables. We have long used the discrete ordinates approximation which evaluates the distribution function at a set of discrete directions. As a consequence, particle streaming is constrained to these directions. For absorbing media with spatially localized sources, as in reactor shielding applications, this angular approximation can produce anomalous spatial distortions in the solution. During the year, Warren Miller derived a new variant of a remedy for this problem. It has been recognized for several years that the elliptic spherical harmonics equations, which are often used to approximate the Boltzmann equation, are free from the spatial distortions of the hyperbolic discrete ordinates equations. Also known was that, by adding a zero-strength source to the discrete ordinates equations, they could be converted to equations similar to the spherical harmonics equations. Miller derived a version of this source, dependent on the angular distribution being calculated, that has better convergence properties and that is applicable to both cylindrical and rectangular two-dimensional geometries.

C. New Technique for Time Varying Solutions

The TWOTIME code is being developed as part of a fast reactor

accident analysis package. To treat the time variation of the solution, TWOTIME uses an efficient explicit time-differencing algorithm coupled with an exponential predictor method. Since the code attempts to represent six of seven independent variables, storage of the entire distribution function from the previous time step could require potentially prohibitive amounts of storage. But, through a clever application of the rebalancing algorithm for improving the accuracy of the explicit time differencing, Reed avoided the storage problem. The transport equation is solved without including the time-derivative terms while the time-derivative terms are retained in the particle balance equations used to enforce particle conservation in each spatial cell. The resulting storage requirement is thereby reduced to that needed for the angle-integrated distribution function.

D. Data Management

The number of discrete values of spatial and angular variables that our transport codes can handle is limited only by the amount of computer storage available. During the past year we have begun to develop (for ONETRAN, TRIDENT, THREETRAN) data management algorithms that automatically allocate problem data among three levels of storage: fast, faster, and fastest. These techniques make possible the running of much larger problems, or, in the case of THREETRAN, make feasible three-space-dimensional problems. By overlapping input, output, and computation, the penalty for using the slowest storage mode can be reduced. Such data management algorithms require careful planning and testing.

E. Faster Convergence for Iterative Processes

Each of our transport theory computer programs uses iteration to obtain a solution, and some use as many as four nested sequences. Consequently, we are continually interested in more efficient methods of accelerating the convergence of iterative processes. After several years' work we feel we are near success with a technique that

uses an iteration matrix

$$M' = (I - W_\ell W^{-1})M,$$

where M is the iteration matrix of the unaccelerated process, W is the exact solution operator matrix, and W_ℓ is a low-order solution operator matrix which is much cheaper to invert than W . The objective is to have the spectral radius of M' much smaller than that of M . It is plausible that this will be true if W_ℓ is "close" to W , i.e., if $W_\ell W^{-1}$ is nearly I so that the norm of M' is decreased. We have recently found a spatial differencing of the diffusion operator which when used as W_ℓ shows promise of yielding large reductions of computer time. Especially intriguing is the possibility of using the high-order unconverged solution to improve the parameters of the low-order operator matrix as the iteration progresses.

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IV. T-1 OUTSIDE TALKS AND SEMINARS

1. J. S. Gilbert, "Conceptual Laser-Controlled Thermonuclear Reactors," presented at the Department of Mechanical Engineering and the Department of Nuclear Engineering Graduate Seminar, Gainesville, FL, July 1974.
2. K. D. Lathrop, "Numerical Methods in Reactor Physics," presented at West Point, NY, December 1974.
3. R. D. O'Dell, "Reactor Theory Applications to Criticality Safety," and "The Method of Discrete-Ordinates for Solving the One-Dimensional Transport Equation," presented at the Nuclear Criticality Safety Short-Course, University of New Mexico, May 1975.
4. T. J. Seed, " S_N Methods in Neutron Transport Calculations," five invited one-hour lectures presented at the Department of Nuclear Engineering, University of Washington, Seattle, WA, May 1975.

5. L. L. Smith (LASL), D. R. Ferguson and J. E. Calahan (ANL), "Time-Dependent Reactor Physics in the FFTF Unprotected Loss-of-Flow Accident," presented at the American Nuclear Society Topical Meeting on Advanced Reactors; Physics, Design, and Economics, Atlanta, GA, September 1974.
6. B. R. Wienke, "Impulse Approximations," presented to the Physics Department, University of California, Fullerton, CA, January 1975.
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GROUP T-2 - APPLIED NUCLEAR DATA

Phillip G. Young, Group Leader

I. INTRODUCTION

The primary responsibility of Group T-2 is to provide accurate nuclear data for use in weapons, reactor, and shielding applications. Implicit in this charter is the development of improved methods for obtaining, handling, and using nuclear data. In addition, because of our expertise with data bases, we have recently become involved in developing a nonnuclear data base of energy- and environment-related information for the LASL regional energy assessment program.

In the most general sense, a data base consists of those data or parameters that are required for the analytical description or modeling of some process. For the modeling of nuclear weapons explosions, reactor physics processes, and radiation transport in matter, T-2 prepares nuclear data bases which include, for example, nuclear interaction cross sections and yields, fission reaction data, and nuclear decay and branching information for elements found in and around nuclear weapons, fission and fusion reactors, and accelerator shield walls.

The commonality of weapons and nonweapons nuclear data requirements makes possible the development of general-purpose nuclear data files. Therefore, in addition to the Division of Military Applications, we are funded by the Division of Controlled Thermonuclear Research, the Division of Reactor Research and Development, and the Division of Physical Research of ERDA, and by the Defense Nuclear Agency and the Nuclear Regulatory Agency. We coordinate our nuclear data activities with those of other laboratories and with the national nuclear data effort (ENDF/B). Our broad support base and our interaction with the national system greatly reduces duplication of effort

and provides the LASL users with access to a more extensive data base and computer code system than would otherwise be available.

Group T-2 is presently comprised of 14 full-time staff members, four full-time graded personnel, and several part-time and casual members. Approximately one-third of our total effort goes into each of the following activities: evaluation, processing, and validation of nuclear data.

In our evaluation work, we analyze available experimental and theoretical information to obtain basic differential cross-section data for nuclear interactions over a continuum of incident and exit reaction energies and angles. The derivations often involve resolution of discrepant experimental results together with application of theoretical nuclear models to fit, interpolate, and extrapolate from the measurements. The evaluated data sets are formatted for computer use and are entered into data libraries.

Since the evaluated libraries are generally too long and detailed for many applications, T-2 processes the data into forms suitable for direct use. For example, many nuclear design codes require data in multigroup form, i.e., cross sections are averaged or grouped into relatively large energy bins using a weighting function appropriate for the specific application. (Fig. 7 and Fig. 8.)

Finally, we test the processed data sets by using them to calculate well-measured integral experiments. These experiments, which are usually sensitive to several quantities in the data file, are chosen to be computationally simple and to test aspects of the data important for particular applications. If the data sets perform well, they are validated for use in nuclear design; if not, they are restudied. Defective and missing nuclear data required for particular applications then can be assessed.

In the course of our activities, we interact with and supply nuclear data to many laboratory groups, including most groups in T,

Fig. 7. Pointwise and multigrouped cross sections for the $^{nat}\text{Fe}(n,\gamma)$ reaction. The smooth curve represents the evaluated (n,γ) cross section from the ENDF/B data file, and the histogram indicates the same data after multigrouping into the TD-Division 30-group set.

Fig. 8. Photon production cross sections for natural iron after processing into the TD-Division 30-neutron by 12-photon multi-group set. Neutron and photon energies decrease with increasing group number, and the maximum neutron and photon energies in the array are 17 and 20 MeV, respectively. The vertical scale is logarithmic and varies from a minimum of 0.1 mb to a maximum of 1.5 b.

P, and TD divisions. The most important laboratory users are the weapons design programs in Groups TD-2 and TD-4, weapons physics in TD-1, weapons output in TD-3, Monte Carlo in TD-6, and the transport theory, reactor theory, and reactor safety projects in Group T-1. We also work closely with Group T-9 in certain nuclear theory calculations and with Groups P-3 and P-9 in supporting and utilizing their nuclear data measurement programs. In addition, through our involvement with ENDF/B system, our results are made available to outside users in both the U. S. and Europe.

Recent highlights of our activities in the three areas of evaluation, processing, and validation of nuclear data are outlined in the sections that follow. In addition, we discuss our role in a personnel exchange with a French laboratory and our involvement in developing a data base for the regional energy assessment program at the LASL.

II. RESEARCH HIGHLIGHTS

A. Nuclear Data Evaluation

1. Model code development

During FY 1975, we developed a completely new multipurpose reaction theory code, called GNASH, for calculating neutron, gamma ray, and charged-particle energy spectra and level-excitation cross sections from almost any combination of neutron-induced reactions in the 0-50 MeV region.³⁰ This covers energy regions of importance to fission reactors (a few MeV), fusion reactors (14 MeV and below), weapons (14 MeV and below), and shielding design (all energies). The code combines simple statistical, optical, and giant dipole resonance models to obtain estimates of particle and gamma-ray widths, and includes a pre-equilibrium model to account for semi-direct processes.

We have continued our extensive use of the R-matrix fitting code EDA (Energy-Dependent Analysis) in several studies of light

element systems. Most of our effort has centered on analyses of the ${}^7\text{Li}$ and ${}^{11}\text{B}$ systems because of the need for very accurate cross sections for the $n + {}^6\text{Li} \rightarrow \alpha + t$ and $n + {}^{10}\text{B} \rightarrow \alpha + {}^7\text{Li}$ reactions.^{12,28} Owing to their large cross sections and the easy detectability of their charged particle products, these reactions are used as standards against which many other nuclear reactions are measured. (Fig. 9.)

Using EDA, we have also extended the energy range of an earlier analysis of the mass 5 system, making use of a simple model to account for the ${}^5\text{He}$ - ${}^5\text{Li}$ charge difference. The purpose of this analysis was to obtain more accurate modeling of the $d + t \rightarrow n + {}^4\text{He}$ fusion reaction (an important energy-producing reaction for weapons and fusion reactors) so that more accurate predictions could be made of the unmeasured cross section at very low energies. The analysis was performed by fitting R-matrix parameters to all available low-energy measurements in the mass 5 system. The analysis²⁹ yields significantly better data at low energies than frequently-used extrapolations based on a very simple physical model. The improved results are due primarily to the accurate description of resonance contributions by the R-matrix analysis. We have used the new data to calculate reaction rates, and these were found to differ significantly from reaction rates commonly used in the past. The new results permit more accurate determination of fusion heating in weapons and thermonuclear reactor design calculations.

2. Basic cross-section evaluations

We have re-evaluated neutron-induced cross sections of ${}^6\text{Li}$ for neutron energies in the range 1 to 20 MeV. Particular attention was paid to improving older, inadequate representations of energy and angular distributions of secondary neutrons. The results make possible more accurate neutronics calculations for fusion reactor and weapons applications in which ${}^6\text{Li}$ is an important material.

Neutron-induced reactions with ${}^{15}\text{N}$ generally have high-thresholds ($E_n \sim 8$ MeV). The enrichment of commonly-used nitride-based

Fig. 9. R-matrix analysis of the mass 7 system. The solid curves were calculated with parameters from an R-matrix analysis; the various point symbols indicate experimental measurements. The $n + {}^6\text{Li}$ total and $n + {}^6\text{Li} \rightarrow \alpha + t$ integrated cross sections were calculated using some of the experimental data.

(^{14}N) reactor fuels with ^{15}N therefore offers the possibility of reducing undesirable neutron absorption and helium production. We have obtained evaluated neutron-induced cross sections for ^{15}N up to 20 MeV, primarily from an R-matrix analysis below 6 MeV with the code EDA and from statistical theory calculations at higher energies with the GNASH code.

The proper definition of errors in basic nuclear data is of considerable importance since uncertainties can result in costly overdesign of nuclear systems. For example, because of safety requirements, an overestimate in the uncertainty in the neutron total cross section of a shielding material might necessitate design of a substantially thicker (and more expensive) shield wall for a high-energy accelerator than is really required. During FY 1975, a detailed evaluation of errors was carried out for ^{27}Al neutron cross sections, and a less thorough study of uncertainties was performed for some 28 other reactions of interest in the Tokamak Fusion Test Reactor design. These results are being used in a joint T-1, T-2 project to assess neutron cross-section data requirements for the national CTR program.^{22,23}

Development of the fission-product yield and radioactive decay data base for ENDF/B continued.¹¹ A chain library, which details the various radioactive decay modes a disintegrating nucleus can follow, was prepared for estimating neutron absorption buildup in the fission of ^{233}U , ^{235}U , ^{238}U , ^{239}Pu , and ^{232}Th . These data are important for the calculation of fission reactor performance.

An evaluation was completed this fiscal year of the spectrum and intensity of gamma rays as functions of time following neutron-induced fission of ^{235}U and ^{239}Pu . The data span the time region from the prompt gamma-ray burst at approximately the time of fission out to 60 s after fission and are required for accurate estimates of, for example, radiation levels following a nuclear detonation.

B. Nuclear Data Processing

1. Processing code development

Group T-2 has sole responsibility under combined DMA/RRD funding for development of a modern ENDF/B processing code system. This code system is designed to transform basic cross-section data from the ENDF/B data repository into forms suitable for direct use in nuclear design codes. The MINX and ETOPL codes, which have been under development for several years, are part of this system. MINX processes evaluated ENDF/B data into more compact multigroup forms. The ETOPL code, when linked with MINX, provides pointwise cross sections for input into design codes that require continuous energy representations, for example, the MCN code developed in group TD-6.

A number of new features and improvements were added to MINX this year. These include increased generality in weighting function capabilities, expansion of output capability to include the CCCC Version III interface format, improved routines for calculating elastic and inelastic transfer matrices, and incorporation of a significantly improved quadrature scheme for calculating statistical averages.

Development of a second generation version of the MINX code, called NJOY, was continued during FY 1975 and is nearly complete. NJOY is a highly modular code that not only performs the functions of MINX, but also includes the capabilities of LAPHAN (multigroup photon production cross sections and $n \rightarrow \gamma$ transfer matrices), GAMLEG (photon interaction cross sections), ETOPL (preparation of libraries for continuous energy Monte Carlo codes), FLANGE (multigroup thermal neutron scattering cross sections and transfer matrices), and PUFF (multigroup covariance matrix processing). NJOY is a more compact code than its MINX predecessor and incorporates more efficient techniques for manipulating large blocks of data. These improvements result in substantially shorter running times.

Development of the CINDER code⁹ for processing ENDF/B fission product data continued in FY 1975. A new code, PHONEX,²⁵ was developed for calculating photoneutron spectra for arbitrary incident energy distributions of gamma rays. Using both CINDER and PHONEX, calculations were made of photoneutron spectra induced by gamma rays coming from the decay of fission products.^{26,27}

A new code, NASPRO, was developed to process Monte Carlo histories obtained from intranuclear-cascade calculations into a medium-energy cross-section library.

A number of existing processing codes were made operational at the LASL, largely in support of high temperature gas-cooled reactor (HTGR) neutronic calculations in Group T-1. These codes include MC², FLANGE, GLEN, JMBLFAT, TOR, HEXSCAT, and GASKET. Several code modifications were necessary to generate the required HTGR-related data, particularly for the MC² and GLEN codes.

2. Data supply

During FY 1975, T-2 processed a large number of data sets into both multigroup and Doppler-broadened pointwise form, mainly utilizing ENDF/B Versions III and IV evaluations. A wide assortment of evaluated data sets for isotopes and elements found in weapons, reactors, and shields were processed for the LASL users. In addition, several external distributions of processed data were made, including a 50-group MINX-generated library which was sent to outside laboratories (and to T-1) for testing of MINX and Version IV of ENDF/B. Several problems in MINX were consequently discovered and removed.

3. Energy release from fission products

A knowledge of the behavior of radioactive debris from nuclear explosions is required for planning of troop movement, civilian population evacuation, etc., under battlefield conditions. We have calculated the beta and gamma-ray energy release from gaseous and solid fission products as a function of time following ²³⁵U and ²³⁹Pu

fission bursts.¹⁰ The CINDEF and RIBD codes along with the ENDF/B-IV fission product data base were used for the calculations. The results indicate that at times near 1 day after the burst, about 50% of the gamma-ray energy release results from decay of gaseous fission products. Since gases released in radioactive fallout have a different spatial distribution than solid fission products, these results are important for proper assessment of tactical battlefield situations.

C. Nuclear Data Validation

1. Testing of ENDF/B data

Every new version of the ENDF/B data library is tested by computing various integral quantities for a set of benchmark critical experiments and comparing the results with observed values.²⁰ We have participated in testing Version IV of ENDF/B by calculating eigenvalues and central spectral indices for several critical assemblies. The data testing results from all participating laboratories were compiled by the Data Testing Subcommittee of the Cross-Section Evaluation Working Group (CSEWG) and were presented at a recent CSEWG meeting.

2. Data adjustment techniques

Large libraries of basic differential nuclear data must be adjusted periodically to agree with improved measurements of both differential and integral quantities. Data adjustment techniques have been investigated for both uncorrelated and correlated basic nuclear data libraries. We have recently demonstrated that the problem of inverting very large matrices of order $N \times N$, where N is the number of basic data points in the library, can be greatly reduced by expressing the adjustments to the basic differential data in terms of adjustments to the normally sparser integral data. The required adjustment technique was coded as an option into the ALVIN sensitivity and adjustment code,¹⁴ and a sample adjustment was performed on a small data library to illustrate the technique.

III. SPECIAL PROJECTS

A. French-American Personnel Exchange

Group T-2 is participating in a DMA-sponsored personnel exchange between Los Alamos Scientific Laboratory and the French Laboratory Bruyeres-le-Chatel, located near Paris. The two laboratories share many of the same requirements for unclassified nuclear data. The exchange is designed to promote collaboration and exchange of information relating to the measurement, calculation, evaluation, and processing of nuclear data.

The initial LASL representative to Bruyeres-le-Chatel was an evaluator from T-2. His French counterpart is spending 2 months in T-2 during the summer of 1975. During the LASL visit to Bruyeres-le-Chatel, the calculation and evaluation of cross sections for threshold reactions were studied, and detailed analyses were made of ^{93}Nb and $^{169}\text{Tm}(n,2n)$ cross sections.^{31,32}

B. Regional Energy Assessment Program

The LASL regional studies program (REAP) has been established to assess the present and future impact of developing the energy resources of the Rocky Mountain States (Arizona, Colorado, Idaho, Montana, New Mexico, Nevada, Utah, and Wyoming). Because of our experience with data bases, T-2 has been assigned the task of collecting and evaluating a wide variety of data relevant to the program.

A study has been completed, in conjunction with the LASL groups T-7 and Q-DOT, in which the present energy situation is delineated through a collection of data concerning the activities during 1974 of the major energy related industries. The resulting data base serves as a source of information concerning supply and demand, pricing, employment patterns, and sources of waste in the energy system. (Fig. 10.)

Fig. 10. Energy flow diagram for the eight states in the Rocky Mountain Region, 1974. Energy production, consumption and loss, and the amount available for export are illustrated.

Impacts of energy development on the ecology and economy of the region have been studied by the LASL groups H-8 and T-7, respectively. In support of these efforts, T-2 has been involved in accumulating air and water quality data and state economic input-output tables.

REAP has focused considerable attention on the proposal by two major natural gas companies to develop the strippable coal reserves of northwestern New Mexico for coal gasification. The LASL group C-5 has been applying linear programming techniques to evaluate the multifaceted local impact of these projects. As input to their model, T-2 has collected data from scattered sources concerning demography, water quality and quantity, crops and livestock, and the coal gasification process itself.

Group T-2 has worked on gaining access to and evaluating the usefulness of several existing energy-related data bases. The group also made progress toward forming a resource library on energy-related programs in the Rocky Mountain region.

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GROUP T-3 - FLUID DYNAMICS

C. W. Hirt, Group Leader

I. INTRODUCTION

The activities of Group T-3 cover a wide range of fundamental and applied research in fluid dynamics.

Our principal area of expertise is the development of new numerical solution techniques for time-dependent, fluid dynamics problems in several space dimensions. When necessary we derive new or alternative mathematical formulations for relevant physical processes and often develop simplified models for complex flow phenomena based on the results of our detailed numerical calculations. The group contains 28 members of which 20 are supported on reimbursable contracts from a variety of government agencies, including ERDA, BRL, DNA, NRC, NOS, ONR, AFWL, and NSF.

Our accomplishments during FY 1975 have been in three principal directions. First, we have developed new numerical techniques for analyzing multiphase fluid flows associated with reactor safety problems, for treating chemically reacting flows occurring in chemical lasers, and for handling many specialized two- and three-dimensional fluid flow problems arising in such diverse applications as the dynamics of floating bodies, the prediction of blast loads on structures, the theory of centrifuge operation, and the dynamics of colliding nuclei. In several instances these new methods have already been recognized as setting the standards for future research directions in their respective fields. Second, we have pioneered the application of numerical fluid dynamics to a variety of problem areas in astrophysics, biophysics, industrial processes, and the ocean sciences. These efforts are bringing recognition to the LASL and in several instances are producing reimbursable accounts. Third,

we have expanded our efforts to increase the acceptance and outside use of the numerical techniques developed by our group. Highlights of our accomplishments during FY 1975 in each of the above-mentioned directions are sketched in more detail in Secs. II and III of this report.

In addition to our research and educational activities, we are often asked to consult on fluid dynamics problems arising in other groups and divisions at the LASL. A selection of the type of help given to other divisions this fiscal year is contained in Sec. IV.

II. RESEARCH HIGHLIGHTS

A. New Numerical Methodology

1. Multiphase and multicomponent fluid dynamics

We have undertaken, in collaboration with Groups T-1, T-4, T-7, and C-5, programs in the safety analysis of light water and liquid metal-cooled reactors. These programs are funded by the Light Water Reactor and Fast Breeder Reactor sections of NRC. Our task has been the development of numerical, mathematical, and physical models for multiphase and multicomponent fluid dynamics. The primary objective of this work is the study of fundamental flow processes likely to occur in reactor accidents. For this purpose we have written several new computer codes^{1,3,4,11,12,14,16} that solve the equations of motion for interpenetrating materials. We have developed for incorporation into these codes improved models for various microphysical phenomena. These codes were recognized at the Spring American Nuclear Society meeting as likely to be the best available for reactor safety analysis for at least the next five years. The NRC has been so pleased that it significantly increased our funding in mid-year as well as for the next fiscal year. The NRC has also recommended that Aerojet Nuclear Company and Pacific Northwest Laboratories adopt our codes as the basis for their LWR analyses.

Because important multiphase fluid dynamics problems arise in

industrial processes, meteorology, biology, oceanography, and practically every other field of science and engineering, we anticipate extensive use of these new computational tools for many other purposes.

2. Reactive fluid dynamics

Our program in the theoretical modeling of continuous-wave chemical lasers for the Air Force Weapons Laboratory is in its fourth year. The RICE computer code, developed for the calculation of the nonlinear fluid dynamics, species transport, and chemical reactions occurring in these lasers, has been modified recently to include a coupled laser-energy output package.^{17,22} This unique numerical program has been used as a design aid and is still the most advanced theoretical tool available for analyzing data from experimental chemical lasers. It has recently been acquired by the Army to support its chemical laser program.

The RICE code²² also serves as a good illustration of how general techniques developed for one purpose can be used to generate new projects. For example, the existence of RICE led us this year into the investigation of the interior ballistics of liquid propellant guns, a program funded by the Navy. Furthermore, the presentation of these calculations at an NSF-sponsored workshop has now generated interest in applying RICE to internal combustion engines. RICE and its derivatives appear to be the only numerical tools currently available that can tackle the problems associated with optimizing engine design for efficiency and cleanliness.

3. Three-dimensional calculations

The three-dimensional magnetohydrodynamics (MHD) computations started last year for the CTR program have continued on a larger scale this year. Our group involvement extended through January when the project was taken over and expanded by Group CTR-6.

Development of the three-dimensional MHD code relied heavily on our previous methodological developments.²⁰ In particular, the Arbitrary-Lagrangian-Eulerian (ALE) zoning and implicit (ICE)

Fig. 11. Calculation of three-dimensional flow in a curved tube using the BAAL code, from which the MHD code was developed. Shown are perspective view plots of: (a) the computational grid; (b) velocity vectors (top) and pressure contours (bottom) in the horizontal plane of the curve; (c) velocity and pressure distributions in a plane perpendicular to the plane of the bend; and (d) the transport and dispersal of particulate matter injected into the flow.

features give this code unique capabilities for studying plasma stability in realistic fusion reactor geometries. The ALE and ICE features permit efficient three-dimensional calculations to be made without loss of accuracy by continually optimizing the size and location of mesh zones and by permitting larger time steps than possible with more standard codes (Fig. 11).

Another three-dimensional code written this year (SOLA-3D) has been used to study wind forces on various shaped buildings. This code is a highly simplified version of the MAC (Marker and Cell) technique that utilizes a variable, rectangular zone mesh. A detailed series of comparisons with experimentally obtained pressure loading data in wind tunnel tests has demonstrated the utility and accuracy of fully three-dimensional calculations. This NSF-sponsored work has been directed towards the analysis of tornado-generated winds on buildings and other structures.^{9,23} We believe that benchmark calculations of this sort establish a firm basis on which further three-dimensional modeling will be performed. The SOLA-3D code completes a four-year development of relatively simple three-dimensional problems. We are now documenting the code and will make it available through the Argonne Code Center.

4. Slip and rezone techniques

The YAQUI code, developed by Group T-3 several years ago, is still one of the only codes having an optional mixture of Lagrangian and Eulerian zoning. This combination enables one to attain optimal zoning for accuracy and economy. During FY 1975 we extended YAQUI to include new types of interface slip and interface rezoning for the calculation of highly distorting multimaterial fluid problems. Preliminary calculations have already proved that these techniques allow a significantly greater degree of material interface distortion than that tolerated in ordinary Lagrangian codes (Fig. 12).

B. New Applications and Extensions of Numerical Methodology

Group T-3 has greatly expanded the scope of its work by extending

Fig. 12. Lagrangian calculation with slip of piston driven flow past an obstacle. The uppermost figure shows the initial conditions (not drawn to same scale as lower figures). Material piles up at the front of the obstacle and slides past below. Downward bulge of interface is caused by faster moving shock in obstacle.

and applying its numerical techniques to many new problem areas. Representative highlights are described below.

1. Viscous nozzle code

Our nozzle flow code, originally developed and used for the design of the Intense Neutron Source facility, has been extended to treat fully viscous flows. This extension made possible the analysis of a nozzle of particular interest to the Air Force for a chemical laser system. The code was also used in a preliminary analysis of a chemical vapor deposition furnace for CMB-3 and, in this capacity, was instrumental in bringing to the LASL a large reimbursable project to further study such furnaces.

2. Centrifuge theory

Our numerical and analytical studies of high-speed centrifuges continued at an intense pace this year. On the basis of our theoretical predictions, modifications made to experimental centrifuges have significantly increased their efficiency over standard designs. Because of this, enormous dollar savings should be realized when the nation's isotope separation facilities are improved and expanded.

3. Nuclear hydrodynamics code

A new variation of the Particle-in-Cell (PIC) technique, developed many years ago by Group T-3 for general compressible fluid flow calculations, was written to solve the relativistic equations of motion for head-on collisions of heavy atomic nuclei.^{2,13} Early results show considerable promise for guiding the development of equations of state for nuclear matter, and have already influenced the choice of energy ranges to be measured in an experimental program under way at Berkeley. A fully three-dimensional version of this code that permits collisions with finite impact parameters was written and is being prooftested.

4. Astrophysics

For general astrophysical fluid dynamics applications, the group

has developed a special implicit, spherical geometry code that is much more efficient than comparable codes elsewhere. At present, the basic code is based on a three-fluid model in which one fluid component may undergo nuclear burn to produce a second component, with a third component that remains inert. In addition to full nonlinear hydrodynamics, the code permits radiation diffusion with variable opacities, has a model for turbulent diffusion, and has an equation of state that accounts for dissociation, ionization, and electron degeneracy. Computational results for a collapsing proto-star model attracted considerable attention at a recent AAS meeting.

5. Biological fluid dynamics

Biological flow problems received increased attention this year. Among new developments are the capabilities for treating constricted elastic tubes [(e.g., arteries with stenoses (Fig. 13)], and bifurcating (branching) blood vessels of air passages.^{7,19} The bifurcation studies are performed with the BAAL code, a fully three-dimensional computing tool designed to study secondary flows, wall stresses, and the deposition of entrained pollutants on the channel walls.²⁰ This work was presented to persons at ERDA, NSF, and NIH and received very favorable response. As a result we are anticipating ERDA support for a continuation of work on air flow structure and particulate deposition occurring in the upper respiratory tract.

III. EDUCATIONAL ACTIVITIES

To introduce our numerical methods to more investigators, we have assembled a series of relatively simple, well-documented codes for inclusion in the Argonne Code Center.¹⁵ The first two members of this series, already sent to Argonne, are SOLA and SOLA-SURF. These codes calculate time-dependent incompressible fluid flows in two space dimensions. One application of the SOLA-SURF code has been the investigations of the dynamics of floating bodies, a project funded by the Office of Naval Research. The next contributions, which are now being documented, are SOLA-3D (a three-dimensional

Fig. 13. Flow through a constricted artery. Velocity, pressure, and shear stress plots are shown at two stages of pulsatile flow through a constricted section of artery. Normalizing velocities are listed below each velocity plot and contour intervals below each contour plot. Flow is from bottom to top, with the left boundary an axis of symmetry and the right boundary a no-slip wall. In the velocity plots, notice the boundary layer development, the flow acceleration through the constriction, and the separated region with flow reversal downstream from the constriction. The upstream side of the constriction is a region of strong pressure gradient and high wall shear, while a low-pressure region exists at the point of minimum radius.

version of SOLA) and SOLA-ICE (an implicit version for two-dimensional compressible flows). A two-field code, SOLA-TIF and a code for two-phase flow, SOLA-DF, are under development.^{3,4,14}

IV. INTERDIVISIONAL CONSULTING ACTIVITIES

Group T-3 routinely supplies consulting services and codes to other groups and other divisions. Selected examples of help given in FY 1975 include:

1. for Q-26, estimates of pressure loading on a cryogenic vessel caused by a spark-gap induced shock.
2. for CMB-3, preliminary calculations of flow in a chemical vapor deposition furnace. Calculations were included in a proposal to the Air Force that has been funded for FY 1976.
3. for Q-23, development of a two-dimensional viscous flow code for the study of molten rock flowing in heated pipes in certain subterrene designs.
4. consulting and codes for the study of volcanic eruptions (J-10) and for the investigation of circulation patterns in solar energy storage tanks (Q-25).
5. with TD-3, an outline of some specific problem areas experienced by weapon's codes. As a result, we have developed a new sliding interface capability that looks promising as a general interface treatment.

V. T-3 PUBLICATIONS

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3. T. D. Butler, "Multiphase Flow Methods for Reactor Safety Analysis," Trans. Am. Nucl. Soc. 21, 217 (1975).
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15. C. W. Hirt, B. D. Nichols, and N. C. Romero, "SOLA - A Numerical Solution Algorithm for Transient Fluid Flows," Los Alamos Scientific Laboratory report LA-5852 (1975).
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17. R. C. Mjolsness, "A Model for the CW Power Output of the HF Chemical Laser," Los Alamos Scientific Laboratory report LA-5683-MS (1974).
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VI. T-3 OUTSIDE TALKS AND SEMINARS

1. T. D. Butler, O. A. Farmer, R. C. Mjolsness, and W. C. Rivard, "Numerical Studies of CW Chemical Lasers with the RICE Program," presented at the Tri-Service Chemical Laser Symposium, Albuquerque, NM, February 1975.
2. L. D. Cloutman and H. M. Ruppel, "A General Numerical Fluid Dynamics Algorithm for Astrophysical Application," Bulletin of The American Astro. Soc. 1, No. 2, Part 1, 255 (1975).
3. R. A. Gentry, "Basic Elements of Computational Fluid Dynamics," a series of six invited lectures at the School of Engineering, University of Arizona, Tucson, AZ, April 30-May 3, 1975.
4. C. W. Hirt, "Numerical Methods of Fluid Flow Calculations," a series of five invited lectures at the Department of Nuclear Engineering at the Massachusetts Institute of Technology, Cambridge, MA, January 1975.
5. C. W. Hirt and N. C. Romero, "Advanced Code Development for Light Water Reactor Safety Analysis," The First Semiannual Code Development Workshop, Aerojet Nuclear Corp., Idaho Falls, ID, March 1975.
6. C. W. Hirt and B. D. Nichols, "Numerical Methods for Marine Science and Technology," a series of three lectures at the Scripps Institution of Oceanography, La Jolla, CA, June 1975.
7. P. J. O'Rourke and T. D. Butler, "Numerical Simulation of the Interior Ballistics of Liquid Propellant Guns," Liquid Propellant Gun Technology Review Meeting, White Oak, MD, June 1975.

8. W. C. Rivard and M. D. Torrey, "KACHINA - A Two-Field Code for Application to the Safety Analysis of Light Water Reactors," The First Semiannual Code Development Workshop, Aerojet Nuclear Corp., Idaho Falls, ID, March 1975.

GROUP T-4 - EQUATION OF STATE AND OPACITY

J. F. Barnes, Group Leader

I. INTRODUCTION

Group T-4 is charged with the responsibility of maintaining and improving the computer-based equation of state (EOS) and opacity data base used by most of the weapons-related codes employed in Laboratory programs. Data management and relatively routine production of new data in response to user requests with our SESAME (EOS), LEO (light element opacity), HEO (heavy element opacity), ABSCO (air opacity), and MOOP (Molecular opacity) codes constitutes roughly a third of the group's activity. The remainder of our effort is spent in a strong program of basic research into bulk properties of matter, atomic physics, interaction of radiation with matter, and related topics in detonation physics, hydrodynamics, astrophysics, and geophysics. Both the intrinsic interest in these topics and the resulting continual improvement in the data base motivate our research program.

In the EOS data library, the material pressure and internal energy for a large number of materials are tabulated as functions of density and temperature over a very wide range of variables. The opacity library, as presently constructed, consists of a tabulation of mean absorption coefficients as a function of the same independent variables. A new data bank of monochromatic absorption coefficients for a number of elements is being constructed and this, together with a new computer program to calculate mean opacities of mixtures, will greatly improve the quality of the opacity data as presently used. Members of the group who work primarily on the libraries interact closely with personnel of the Theoretical Design Division, Dynamic Testing Division, Field Testing Division, and the various groups engaged in reactor safety research, as well as with others.

In the following section, we present some highlights of the year's activity under three main headings: A. Equation of State and Opacity Libraries, B. Equation of State and Opacity Research, and C. Related Research. Section III briefly outlines some special projects done at the request of other LASL groups or groups outside the LASL.

II. RESEARCH HIGHLIGHTS

A. Equation of State and Opacity Libraries

1. SESAME

Our SESAME code is used to generate and manage the data in our EOS library. SESAME utilizes the Thomas-Fermi-Dirac statistical model of the atom with various corrections in the lower temperature and mixed-phase regimes. The equation of state thus generated for a given substance is corrected to agree with all existing experimental data.

In the past year we have made several improvements in the code, primarily in its data management capabilities, and we have added 11 new materials to the data bank.

SESAME was modified early this year to operate on libraries stored either on the HYDRA disk or photostore. During the third quarter, the SESAME code and a copy of all SESAME tables were placed on a photostore file, T4LIB, where they presently reside. This is the file into which new equations of state are first placed. From here "consumer approved" equations of state are transferred to a HYDRA disk file, T4EOS, with universal read access for the use of the entire LASL community.

Microfiche has come into full use within SESAME in the first half of this year. System routines have automated the procedure for processing microfiche output, and fiche is now used for all computer output for which long-term storage is desired. With a systematic

reduction of all past computer listings to microfiche we will drastically reduce storage space requirements and enhance retrieval.

We have expanded our package of output routines, basing the system on a compact tabulation of an n -dimensional vector function of two variables (x,y) on a convex region of the x - y plane. Special loci, such as phase or table boundaries, are tabulated in auxiliary tables. The working location of a table-set is Large Core Memory (LCM), but, before and during function evaluation, portions of the appropriate table are read into Small Core Memory (SCM). The function is determined by its table together with an associated interpolation function, for which there are several options that can be selected at compilation. Also included in the output package are a contour plotter, a table printer, and an adiabat integrator, as well as translators from SESAME and MAPLE to a working table format. (MAPLE is a relatively coarse-grid subset of the SESAME data used by codes in which high-temperature phenomena are of importance.) The translation can be either verbatim (pressure and energy as functions of temperature and compression) or inverted (pressure as a function of volume and energy), and with or without derivatives.

2. Plutonium equation of state

An understanding of properties of plutonium is essential to the weapons program, and the construction of a SESAME table that accurately predicts weapons phenomena is one of our chief endeavors. We made further progress during the year on an EOS for unalloyed plutonium that is compatible with experimental data on the shock Hugoniot, heat capacity, thermal expansion, vapor pressure, sound speed, phase diagram and release adiabats. An interactive code was written to generate a complete set of pressure and energy isotherms by combining the experimental data with elementary theoretical models. Using this code it is feasible to vary the many unknowns in the problem and to observe the effects of such variation almost immediately.

3. New opacity library

We have progressed in the establishment of the new opacity

library to the final stages of checking detailed absorption coefficients and equation of state data. The first 20 elements chosen (all with $Z < 30$), are the ones for which NSF funding has been obtained. Between 20 and 25 additional elements will be added during the next few years. A program to predict opacities for mixtures of the basic elements will be available to all users. Besides the usual EOS and radiative and total Rosseland opacities, it will also make available the number of free electrons, degeneracy parameters, electron conduction, Planck opacities, and a number of types of group-mean opacities with groups to be specified by the user. The main advantages of the library are its speed, flexibility, reproducibility of data, and the possibility of greatly improving the basic data.

B. Equation of State and Opacity Research

1. EOS of solids from band structure calculations

Equations of state have long been constructed using various treatments of Thomas-Fermi statistical theory. Since this is a rather unsophisticated model of a solid, we are doing calculations that are more firmly based on physical principles. These band structure calculations may prove too expensive for routine use, however they provide checkpoints for establishing confidence limits on our tabular data. We can also use them to obtain information on, e.g., lattice vibration, polymorphic transitions, and melting -- information that could never follow from the simpler theory.

Within the group, we use basically two different techniques for performing self-consistent band structure calculations that are then applied to equations of state for solids. Both use a local density approximation to exchange.

a. scattered-wave method

For a number of years, a scattered-wave method has been used for solids with one atom per unit cell. We have recently obtained a program from IBM that performs these calculations for the CsCl

structure, with two different atoms per unit cell. The program has been adapted to the LASL computers and generalized to include the NaCl structure. Within the past year we have completed the zero-temperature equations of state for LiH and MgO and have made substantial progress on NaCl and H₂O. In the case of H₂O (actually ice VII), a special approximation is necessary which essentially neglects the directional effect of the covalent bond between oxygen and hydrogen atoms. This approximation reduces the accuracy of the results at low pressures and creates uncertainties at higher pressures as well.

b. augmented plane-wave method

The second band structure code that is maintained in the group uses the Augmented Plane-Wave (APW) technique. This code has recently been extended to do relativistic calculations and hence is applicable to plutonium and uranium.

In this past year we have completed (with H. H. Hill, CMB-5) an extensive study of melting in f-electron metals such as plutonium. The ability to predict the melting point of plutonium under compression is important since the effects of material strength below this point should be added to the fluid EOS in calculating material response to applied stress.

Using the APW program, we have determined the hybridization of valence electrons (i.e., the admixture of states, most of which are normally unoccupied in the free atom). The result of the calculations supports the notion of B. T. Matthias et al., that the melting point in the early actinides (thorium through americium) is anomalously low because of the participation of f-electrons in the bonding. The poor bonding characteristics of f-electrons results from the unfavorable geometric properties in the cubic structure of the actinide metals.

The APW program has also been used this year to calculate points on the zero-temperature EOS for plutonium, in anticipated support of work mentioned in Sec. A.2. above. This is a tedious process because

the limited numerical precision negates use of the virial theorem; pressure must therefore be calculated from derivatives on a fine grid of energy dependence on volume.

2. Self-consistent phonon calculations for hydrogen

The study of hydrogen has long been performed for weapons applications, and in recent years this element has also been of interest because it may possess a metastable super-conducting metallic state. A method for the accurate calculation of the low-temperature EOS is the self-consistent phonon approximation. We have applied this technique with a short-range correlation function to determine the zero-degree isotherm for the face-centered cubic phase of para-hydrogen and ortho-deuterium. Other lattice dynamical properties of these solids were calculated as a function of pressure, including sound velocities, phonon density of states, ground state energies, and bulk moduli.

3. Calculations of shock-loaded beryllium

Beryllium is frequently used in weapon systems, and an understanding of its behavior under shock loading must be obtained. Previous calculations of the response of polycrystalline beryllium to plate impact, using the normal technique of hydrodynamic calculations with an elastic-perfectly plastic treatment, have not successfully matched results of experiment. In particular, the observed damped rise of the elastic precursor and the velocity of the rarefaction waves are not reproduced by this usual treatment.

We have developed a new model³³ based on the observation that single crystal beryllium, due to its inherent anisotropy, exhibits different yield strengths depending on the direction of stress with respect to the crystal axes. We considered individual cells in the Lagrangian hydrodynamics calculations as representing grains of beryllium arranged so that the shock propagates along different directions. Different yield strengths are assigned to the cells. The sample is "textured" by varying the relative number of cells oriented

in certain directions -- technologically this is accomplished by rolling the sample.

The resulting calculations are in far better agreement with experiment and exhibit qualitatively the consequences of texturing.

4. Atomic physics in support of controlled thermonuclear research

We have completed the initial calculations for radiative power loss from Tokamak-like plasmas and for interpretation of observed position and intensity of K_{α} emission (K_{α} -diagnostics) for such plasmas; these calculations were described in some detail in the most recent semi-annual T-Division progress report. We are now making improvements on the cross sections. A computer program, RCG, has been modified to make possible the accurate calculation of dielectronic recombination coefficients and of the detailed relative intensities of spectrum lines resulting from such recombinations. These calculations were performed for iron ions and have improved the predictions necessary for interpretation of the Princeton ST Tokamak K_{α} -diagnostics. (See Fig. 14.)

We have developed an approximate method of calculating dielectronic recombination rates (accurate to about a factor of two) that requires only calculation of radial wave functions, and not detailed spectrum calculations.

We have written a program to calculate the excitation cross section for the 2s and 2p transition of lithium-like Ne VIII. The results (without exchange) agree with literature values to within 2-3%. Work is now under way to rewrite the program to provide the capability of handling any transition between any configuration of open shells (but temporarily limited to two f-electrons).

Collaboration on collision cross-section calculations has been initiated with J. Peek of Sandia Laboratories (Albuquerque) and with W. D. Robb (who will join our group) of the Joint Institute for

PRINCETON TOKAMAK REACTOR

Fig. 14. Approximate power loss spectrum ($\text{W cm}^{-3}\text{keV}^{-1}$) as a function of $u = h\nu/kT$ for a plasma with electron density $N_e = 10^{14} \text{ cm}^{-3}$ at temperature $kT = 1 \text{ keV}$ and seeded with 1% iron as impurity. The group of strong emission lines at $u \approx 0.1$ is due to the $2p \rightarrow 2s$ transitions of iron. These calculations are used to interpret the Princeton ST Tokamak K_α - diagnostics. A schematic of a Tokamak fusion reactor appears above.

Laboratory Astrophysics (Boulder). This work will greatly enhance our capabilities to predict equation of state and absorption, emission, and scattering properties of materials not in local thermodynamic equilibrium.

Radiative recombination coefficients have been calculated non-hydrogenically for C, O, Fe, and Au ions. These coefficients will be used in conjunction with other ionization and recombination coefficients by various Tokamak groups in heavy-ion transport calculations.

5. Progress on the air opacity program

We added atomic line broadening to the ABSCO air opacity code. Contributions to the collision width due to Stark (electron and ion perturbers), Van der Waals, and resonance broadening mechanisms are included. The contribution of molecular perturbers to the Van der Waals broadening is neglected. The semi-empirical treatment of Griem is used for the Stark broadening of absorption lines of ions. The Gaunt factor, g , is interpolated between limiting forms for $\epsilon \approx 0$ ($g \approx 0.2$) and $kT \ll \epsilon$ ($g \approx g_{\text{Coulomb}}$) where ϵ = initial energy of the perturbing electron. The new half-widths for N I and N II calculated at several temperatures in the 10^4 to 2.3×10^4 °K range at electron densities $\sim 10^{16} \text{ cm}^{-3}$ are in reasonable agreement with measured values quoted in Griem's books of 1964 and 1974.

C. Related Research

1. High explosive detonation wave research

Detonation wave research as well as the study of the properties of high explosive (HE) detonation products is carried out in Group T-4 (Fig. 15). We are also directing efforts of the High Explosive Working Group (HEWG), an informal inter-divisional (T, TD, M) group that is attempting to improve HE treatment in hydrodynamics codes.

Through the HEWG we have evaluated the accuracy of cylinder test calculations by TD Division's two-dimensional Lagrangian MAGEE

Fig. 15. Picture plots of the pressure, temperature, density, and energy of a detonation wave proceeding perpendicular to an aluminum plate (i.e., the wave is traveling from left to right along the x axis). In each plot, the region on the left is HE; the center region is aluminum; and the region on the right is air. These plots were calculated using Eulerian reactive hydrodynamic code 2DE developed in Group T-4.

code. The cylinder test is an experimental procedure that measures HE performance in short-time applications. In our study, we compared MAGEE calculations with a more accurate calculation of the steady flow near the detonation front by the method of characteristics. We have found that refining the computational mesh in MAGEE produces a surprising artifact: a large pressure hump on the axis that comes from a spurious conical wave originating at the detonation front's edge. Nevertheless, MAGEE calculates the late wall displacement and velocity to within about 2% of the characteristics solution. It is still an open question whether the hump is a feature of all Lagrangian codes in this geometry.

Also through the HEWG, we are testing the build-up model of the detonation process (in which the energy release increases with length of run) in the MAGEE code and we are calculating the equations of state for the build-up description.

To calculate sharp shock burn, the one-dimensional COMBO code requires an analytical EOS with 132 constants for the detonation products. We have produced the constants for a beta-law form of the EOS by adapting an old TD-Division code (VAGABOND) that generates the constants from a Becker-Kistiakowsky-Wilson EOS. Through these efforts with MAGEE and COMBO we now have the capability of furnishing the necessary constants for the explosive equations of state required by users of these codes.

In other HE work we have studied the HE/metal magnification ratio.¹² Pressure profiles in detonating HE have long been inferred by observing the decay of shock pressure with distance in a witness plate driven by the HE, where both the HE and the witness plate have a slab geometry. The measured shock-pressure vs distance profile in the witness plate is an approximate, magnified image of the pressure-distance profile in the HE at the instant the detonation front reaches the interface. The magnification ratio increases with distance of run. We have used the results of several different types of one-dimensional calculations to show that the imaging is reasonably

accurate and to find the variation of the magnification ratio with distance of run for different configurations of explosive and witness-plate materials.

2. Astrophysical research

a. microwave radio astronomy

In astrophysical research, we have completed an analysis of the radio observations in the 3-mm wavelength range of comet Kohoutek. Most of this work was reported in the last semi-annual report.

We have also completed the calculation of the cross sections of microwave rotational transitions of numerous molecules of astrophysical interest. Roughly 6 000 transitions are included.

b. black holes

We have studied the process of pair creation by vacuum polarization near a black hole. The energy spectrum of the particles produced and the time variation of this spectrum have been calculated as well as the time variation of the total energy converted into ultra-relativistic particles. We have then investigated the efficiency of this process for extracting energy from the black hole, and have calculated an upper limit to the electric charge of a Kerr-Newman black hole -- it is approximately a factor of 10^6 less than what has previously been thought to be the upper limit. If the observed x-ray sources contain such charged black holes, this process could be contributing to the energy output.

In an attempt to interpret some of the Vela satellite data on gamma-ray bursts, we have investigated the properties of accretion disks around black holes. It appears that an instability of the innermost region of the accreted plasma could lead to enhanced mass flow into the hole and the sudden deposition of heat, thus raising the plasma temperature on a time scale of 10^{-3} s.

3. Research in support of the reactor safety program

a. nonequilibrium equations of state

Among the SESAME EOS tables we produced this year are those to be accessed by the preliminary version of the SIMMER, a code being constructed by Groups T-1 and T-3 for safety studies of the Liquid Metal Fast Breeder Reactor. The required EOS tables are for sodium, uranium dioxide (fuel), and iron (steel) (Fig. 16). In the course of this work, it became apparent that, in addition to our usual form of the EOS that assumes liquid-vapor equilibrium in the coexistence region, the nonequilibrium description is needed as well. This is because condensation and evaporation rates are important to reactor safety considerations. Since the Van der Waals loops normally are generated by our formulation, it was a relatively straightforward procedure to furnish this information for sodium and iron. The uranium dioxide EOS, however, requires a better treatment of dissociation before the Van der Waals loops are well defined. This work is in progress.

b. calculation of shear viscosity

We have developed a method of constructing values of the shear viscosity over a large range of temperature and density; SIMMER calculations require not only equilibrium and nonequilibrium equations of state, but also nonequilibrium material transport properties. Experimental measurements of transport coefficients have been restricted for most materials to portions of the saturation curve. Our theoretical method is based on the auto-correlation function approach of nonequilibrium statistical mechanics, and the EOS is utilized in the calculation of the infinite-frequency elastic shear modulus.

We have applied the results to determine the viscosity of fluid sodium, but we have found that, in order to complete the work, we must correct a known deficiency in the specific internal energy at large volume as given by our tabular EOS.²

Fig. 16. Equation of state of sodium currently used in the LASL reactor safety calculations. η is the ratio of density to normal density of the solid, i.e., $\eta = \rho/\rho_0$.

III. SPECIAL PROJECTS FOR OUTSIDE GROUPS

As we pointed out in the introduction, a large portion of the group's effort is in response to the needs of other organizations. Most of our work on the libraries is carried out for that reason. We briefly mention here some of the other projects done for outside groups.

We gave high priority to several extensive calculations for TD Division to investigate the effects of impurities on opacity. Large opacity tables were calculated for TD Division for ${}^6\text{Li}$, Be, B, C, and O, and smaller tables for LiB, ${}^6\text{LiH}$, white granite, and high explosive. For J-Division we prepared opacity tables for Be, Al, Fe, air, and astrophysical mixtures as well as group-mean opacities and emissivities for dry and humid air. We calculated emissivities, opacities, and the EOS of SiO_2 for laser implosion studies in T Division and L Division. We collaborated with L Division on a study to measure opacities in laser-heated microcavities. Frequency-dependent photoelectric cross sections of Mo and Pt have been calculated for TD Division, and oscillator strengths in C III, C IV, O II, and O III for CTR Division. We prepared Dirac-Hartree-Fock charge densities for $Z = 5, 10, 15, \dots, 100$ for J Division.

We prepared air opacities and equations of state for Lawrence Livermore Laboratory. Radiative power loss and theoretical results have been obtained for Princeton and Oak Ridge Tokamak groups for K_α -diagnostics.

We calculated astrophysical opacities for S. Starrfield (Arizona State University) and astrophysical group-mean opacities for E. E. Salpeter (Cornell University). We obtained Dirac-Hartree-Fock charge densities in the nucleus of Te for P. H. Barrett (University of California), and similar charge densities for many atoms and ions of 5d transition elements were sent to F. E. Wagner (Technical University, Munich). Hartree-Fock ion wave functions were made available to G. Tranfield (University of Warwick, Coventry), and Dirac-Hartree-Fock

wave functions and potentials were obtained for Ar and Ne and sent to M. Fink and P. Moore (University of Texas). Extensive tables of opacities for Ba, Sn, Dy, Ag, Pt, Mo, and Eu have been calculated for System Applications, Incorporated.

IV. T-4 PUBLICATIONS

1. W. D. Barfield and W. F. Huebner, "On the Calculation of Scattering Cross Sections from Absorption Cross Sections," J. Quant. Spectr. Rad. Transfer (in press).
2. J. F. Barnes, "An Equation of State for Sodium Over an Extended Temperature and Density Range," in Thermodynamics of Nuclear Materials 1974, Vol. I, pp. 327-339, (1975).
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19. D. Buhl, W. F. Huebner, and L. E. Snyder, "Detection of Molecular Microwave Transitions in the 3-mm Wavelength Range in Comet Kohoutek (1973f)," IAU Colloquium No. 25: The Study of Comets (in press).
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33. R. E. Swanson, "One-Dimensional Calculations of Shock-Loaded Polycrystalline Beryllium," Los Alamos Scientific Laboratory report LA-5943-MS (1975).

V. T-4 OUTSIDE TALKS AND SEMINARS

1. J. F. Barnes, "An Equation of State for Sodium Over an Extended Temperature and Density Range," presented at the International Atomic Energy Agency Symposium on Thermodynamics of Nuclear Materials, Vienna, Austria (October 1974).
2. J. F. Barnes, J. D. Jacobson, J. D. Kershner, and G. T. Rood, "Los Alamos Equation of State Library," presented at EIVR-Material Properties and Code Development, Lawrence Livermore Laboratory (December 1974).
3. R. D. Cowan, "Approximate Relativistic Corrections to Hartree-Fock Wavefunctions," presented at Spectroscopy Seminar, National Bureau of Standards (July 1974).
4. R. D. Cowan, "Effect of Continuum Configuration Interaction on the Position of sp^6 in Neutral Chlorine and Other Halogens," presented at Sixth Annual Meeting of the European Group for Atomic Spectroscopy, W. Berlin, Germany (July 1974).
5. R. D. Cowan, "Approximate Relativistic Corrections to Hartree-Fock Wavefunctions," presented at Fourth International Conference on Atomic Physics, Heidelberg, Germany (July 1974).
6. R. D. Cowan, "Relativistic Effects in Hartree-Fock Calculations for Neutral Rare-Earth Atoms," presented at International Symposium on the Electronic Structure of the Actinides, Argonne National Laboratory (October 1974).
7. R. D. Cowan, "Atomic Radial Wavefunctions," and "Identification of Lines in the Spectra of the Solar Corona and Solar Flares," presented at Spectroscopy Seminars, Purdue University (October 1974).

8. R. D. Cowan, "Theoretical Calculation of Atomic Spin-Orbit Parameters," presented at Annual Meeting of the Optical Society of America, Houston, TX (October 1974).
9. R. D. Cowan, "Calculation of Dielectronic Recombination Rates and K_{α} -Diagnostics in the ST Tokamak," presented at Workshop on Atomic Data for CTR, NBS Washington, DC (March 1975); also at Princeton University (March 1975).
10. W. F. Huebner, "Panel Discussion on the Nucleus," presented at IAU Colloquium No. 25: The Study of Comets, NASA: Goddard Space Flight Center, Maryland (October 1974).
11. D. Buhl, W. F. Huebner, and L. E. Snyder, "Detection of Molecular Microwave Transitions in the 3-mm Wavelength Range in Comet Kohoutek (1973f)," presented at IAU Colloquium No. 25: The Study of Comets, NASA/GSFC (October 1974).
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13. E. A. Kmetko, "Alloying Behavior and Physical Properties of Pu in Terms of Band Structure," invited presentation at the International Symposium on the Electronic Structure of the Actinides, Argonne National Laboratory (October 1974).
14. C. L. Mader, "Numerical Reactive Hydrodynamics," invited colloquium on Applied Mathematics and Science, Ballistic Research Laboratory, Aberdeen Proving Grounds, MD (September 1974).
15. C. L. Mader, "A Continuous Eulerian Technique for Multicomponent, Reactive, Compressible Flow Calculations," presented at EIVR Meeting, Lawrence Livermore Laboratory (December 1974).
16. C. L. Mader, "Recent Advances in Detonation Physics," seminar at Swedish Detonics and Combustion Section of the Combustion Institute, Stockholm, Sweden (June 1975).
17. C. L. Mader, "Theory of Shock Initiation of Explosives," seminar at Hercules, Inc., Magna, UT (May 1975).
18. C. L. Mader, "A Proposal for Theoretical Studies of Propellant Initiation of Detonation," High Energy Propellant Safety Program, Los Alamos Scientific Laboratory (May 1975).
19. N. H. Magee, Jr., A. L. Merts, and W. F. Huebner, "Improved Opacity Calculations," presented at Gainesville, FL (December 1974).
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23. R. E. Swanson and C. L. Mader, "One-Dimensional Elastic-Plastic Calculations Involving Strain Hardening and Strain Rate Effects for Aluminum," presented at American Physical Society Meeting, Anaheim, CA (January 1975).

GROUP T-5 - MEDIUM ENERGY PHYSICS THEORY

W. R. Gibbs, Group Leader

I. INTRODUCTION

Group T-5 was formed as a theoretical center for medium-energy physics in connection with the opening of LAMPF (the meson physics facility at the LASL), where a very active experimental program in medium-energy physics is carried out (Fig. 17). From the start, Group T-5 has been involved in collaborative efforts with LAMPF personnel, suggesting and designing experiments, interpreting data, and extracting final results. In addition, Group T-5 is providing theoretical guidance for a large number of experimental groups in Europe and thereby gaining an international reputation.

Medium energy physics was defined as a separate field with the advent of medium energy accelerators, the so-called "meson factories." The high-intensity meson beams (mostly pions and muons), produced at these accelerators by high-intensity proton beams with energies between 500 to 1 000 MeV, are a new tool for probing nuclear matter and have made accessible for study many important phenomena in both nuclear and particle physics. The current research interests of Group T-5 include: (1) the interactions of incident pions with nuclei (since the exchange of pions and other mesons is responsible for the strong "forces" which bind nucleons together, these studies enable us to probe the structure of nuclei and learn more about the dynamics of composite systems of nucleons), (2) the pion-plus-two nucleon system, (3) nucleon-nucleon scattering, (4) the three-nucleon system, and (5) weak interaction effects in nuclear and particle physics.

Before presenting details of our accomplishments for FY 1975, we will briefly survey the progress made in each of the above-mentioned areas.

Fig. 17. LAMPF, the Los Alamos Meson Physics Facility. The LASL now has a very strong program in medium energy physics including the experimental effort at LAMPF and the theoretical effort by T-5, and members of T-8 and the T-Division Office.

The study of pion-nucleus interactions has occupied the attention of several members of Group T-5, and it is in this area that advances have been most striking. In particular, three major puzzles were solved through very careful application of existing models. These concern (1) neutron removal from ^{12}C by π^+ as compared with π^- , (2) single pion charge exchange on light nuclei (^7Li , ^{10}B , ^{13}C), and (3) pion elastic scattering on ^4He . Equally important are recent advances in: (1) the treatment in potential theory of a pion interacting with a nucleon which is moving about in the interior of a nucleus and (2) understanding the knockout of nucleons by the quasi-elastic scattering of pions from nuclei.

The gross features of pion-nucleus interactions, important in many practical applications such as shielding and biomedical uses, are studied by exposing targets to pion fluxes and observing the nuclides produced by their de-excitation gamma spectra. We have shown that the yields observed in these experiments can be explained by a relatively simple model provided the angular distribution of the p-wave pion-nucleon interaction is taken into account in the formation process.

It is well known that pion-nucleus scattering lengths are not simply equal to the sum of the pion-nucleon scattering lengths. We have obtained a semi-empirical expression giving the pion-nucleus scattering lengths as a function of neutron and proton number. This equation allows qualitative predictions of low-energy pion-nucleus elastic scattering and charge exchange reactions.

Our research on the pion-plus-two-nucleon system deserves to be considered separately. From this system we are learning about nucleon-nucleon properties as well as pion-nucleon properties. Presently under way is a careful analysis of the angular distribution of the $\pi^+ + d \rightarrow p + p$ reaction at pion energies of about 50 MeV. This study promises to give us a good measure (perhaps even the best) of the deuteron D-state probability. Our analysis of the total cross section of this

same reaction around the energy of the pion-nucleon $\bar{3}$ -3 resonance has furnished information about the short-range behavior of the $\bar{3}$ -wave pion-nucleon wave function. Another reaction under study is radiative capture of negative stopped pions. From the shape of the neutron-neutron spectrum, we will be able to infer low-energy neutron-neutron scattering parameters to a remarkable accuracy, while a comparison with the absolute rate of capture will help to eliminate some of the more extreme proposals for the short-range neutron-neutron wave function. In addition to these studies on the interactions among the constituents, we are using the pion-deuteron elastic scattering data as a partial testing ground for pion-nucleus scattering theories. Considerable progress has been made in all of these areas during the past year.

The study of nucleon-nucleon scattering is another major facet of our research. In one project we are using nucleon-nucleon bremsstrahlung data to study the short-range nucleon-nucleon wave function. The interpretation of such experiments is very involved because the measured photon spectrum contains contributions other than the radiation of the charged nucleons themselves. Recent work has shown that these corrections can be very large in certain kinematical regions. Also under study is pion production in nucleon-nucleon collisions, an important inelastic channel of fundamental interest. We have studied it theoretically and compared the theoretical predictions with four sets of data taken this past year.

The three-nucleon system provides a laboratory for learning to deal with the mathematical difficulties inherent in models of three interacting particles. It also offers another opportunity to learn about the short-range nucleon-nucleon interaction. In order to obtain the desired information, one must correlate theoretical predictions and experimental results for many different reactions involving the three-nucleon system. In conjunction with an upcoming experiment at MIT's Bates electron facility, we have studied the photodisintegration of ^3He using separable-potential Faddeev equations.

To learn about the three-neutron system, we are now analyzing the reaction $\pi^- + {}^3\text{H} \rightarrow \gamma + 3n$.

If we replace one nucleon with a strange particle (usually a Λ^0 or Σ^0), we obtain a hypernuclei such as ${}^3_\Lambda\text{H}$. This three-body system contains a particle with different interactions and further, since the particle is nonidentical, the effects of the Pauli principle are entirely different. We have investigated the binding energy of the hypertriton to determine the sensitivity of the predicted binding energy to the potentials assumed. This study has taught us more about the $\Lambda^0(\Sigma^0)$ -nucleon interaction.

Our work in weak interactions has focused on two areas. First, several studies were made concerning the interpretation of parity violating effects in strangeness conserving nonleptonic processes. Experiments in this area are conducted at the LASL. Second, some effects of a possible charged lepton-hadron neutral current interaction have been investigated with particular emphasis on the possibility of studying such effects at LAMPF and similar facilities.

Finally, a comprehensive review of tests of time-reversal invariance in nuclear electromagnetic transitions has been made in order to summarize the present status from a unified point of view and to guide future work in this area.

This completes an overview of our work during FY 1975. In Sec. II we list the experimental groups with whom we have worked most closely. In Sec. III we present a more detailed account of our recent advances.

II. INTERACTIONS AND AFFILIATIONS WITH EXPERIMENTAL GROUPS

Most of our theoretical work is motivated by and in support of experimental efforts. Below is a partial listing of those experimental groups with whom we have discussed the design of experiments or the interpretation of preliminary data:

1. Radio-chemical measurement of pion charge exchange ("Tel-Aviv group," Alster et al.¹),
2. Radio-chemistry group at Los Alamos (Dropesky et al.²),
3. Pion production by protons on Hydrogen ("Team 17," Glass et al.³),
4. The $\pi^+ + d \rightarrow p + p$ reaction (Preedom et al.⁴),
5. Pion production by protons on Hydrogen and Deuterium ("Rice group," Hudomalj-Gabitzsch et al.⁵),
6. Parity violation experiments (D. Nagle et al., LAMPF),
7. Measurement of T_{20} for recoiling deuterons from pion scattering at 180° to determine D-state (Gruebler proposal at SIN),
8. $\pi^- + d \rightarrow n + n + \gamma$, and $\mu^- + d \rightarrow n + n + \nu$ spectrum to determine n-n scattering length (C. Joseph University of Lausanne and W. Breunlich, Vienna),
9. Low-energy pion-nucleon scattering (experiment no. 96 at LAMPF),
10. Complete set of experiments on the pion (three-nucleon system), (J. Spencer, LAMPF),
11. $p + p \rightarrow d + \pi^+$ compared to $n + p \rightarrow d + \pi^0$ ("Team 17," Glass et al.³),
12. Pion photo-capture on the triton (H. Baer, K. Crowe, LAMPF experiment no. 50),
13. The $^3\text{He}(\gamma, n)2p$ reaction (H. Jeremie, Montreal, and J. Matthews, MIT - this is a Bates experiment), and
14. Interpretation of γ -de-excitation of nuclei following bombardment by pions (R. Segal and H. Jackson, ANL, and H. Funston, William and Mary).

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2. G. W. Butler, B. J. Dropesky, A. E. Norris, C. J. Orth, R. A. Williams, LASL; G. Friedlander, G. D. Harp, J. Hudis, BNL;

- N. P. Jacob, Jr., S. S. Markowitz, LBL; S. Kaufmann, ANL; and M. A. Yates, CMU; "Activation Studies of Pion-Induced Reactions on C, H, O, F, Al, and Cu." Abstract submitted to the VI International Conference on High Energy Physics and Nuclear Structure, Santa Fe and Los Alamos, NM (June 1975).
3. G. Glass, M. E. Evans, Mahavir Jain, R. A. Kenefick, and L. C. Northcliffe, TAMU; C. G. Cassapakis, UNM; C. W. Bjork and P. J. Riley, UTEX; B. C. Bonner, and J. E. Simmons, LASL; "Neutron Production at 0° from the Reaction $pp \rightarrow np\pi^+$ of Medium Energies." Abstract submitted at the VI International Conference on High Energy Physics and Nuclear Structure, Santa Fe and Los Alamos, NM (June 1975).
 4. B. M. Freedom, C. W. Darden, R. D. Edge, and J. Marks, U. of SC; M. J. Saltmarsh, E. E. Gross, C. A. Ludeman, and K. Gabethuler, ORNL; M. Blecher, K. Gotow, and P. Y. Bertin, VPI and State U.; J. Alster, R. L. Burman, J. P. Perroud, and R. P. Redwine, LASL; "An Experimental Study of the $\pi^+ + d \rightarrow p + p$ Reactions at Pion Energies of 40, 50, and 60 MeV." Abstract submitted at the VI International Conference on High Energy Physics and Nuclear Structure, Santa Fe and Los Alamos, NM (June 1975).
 5. E. V. Hungerford, J. C. Allred, M. Warneke, L. Y. Lee, and B. W. Mayes, U. of Houston; J. Witten, J. Hudomalj-Gabitzsch, N. Gabitzsch, T. M. Williams, J. Clement, G. S. Mutchler, and G. C. Phillips, Rice U.; "Pion Production through the Reaction $d(p, d\pi^+)n$ at 600 MeV." Abstract submitted at the VI International Conference on High Energy Physics and Nuclear Structure, Santa Fe and Los Alamos, NM (June 1975).

III. RESEARCH HIGHLIGHTS

A. Studies of Nuclei with a Pi-Meson Probe

1. Momentum-dependence of the off-energy-shell T-matrix

In nonrelativistic potential theory, the off-energy-shell T-matrix plays a central role in two-body bremsstrahlung and in scattering off a composite target if three-body forces can be neglected and the impulse approximation is valid. Attempts to apply the same kind of analysis in the relativistic region have led to a number of published ad hoc prescriptions for the total-three-momentum ($\vec{Q}$) dependence of the off-energy-shell matrix elements, which give significant numerical differences for back angle pion scattering.

Using the Bakamjian-Thomas formulation of a Lorentz invariant theory for two directly interacting particles, we succeeded in deriving this $\vec{Q}$ dependence, i.e., an equation which specifies the

matrix elements in terms of others for which the total momentum is zero. We also showed that attempts, by others, to solve this problem by "Lorentz transforming the off-energy-shell matrix elements" are ill-conceived. Such transformations make sense only in manifestly Lorentz invariant theories where one deals with off-mass-shell amplitudes, completely different objects. We also considered the nonuniqueness of our result by examining formulations other than that of Bakamjian and Thomas. From the work of Foldy and Krajcik it appears that there is considerable arbitrariness in the Q -dependence, but only by introducing three-body forces in addition to those which may be required by the nature of the two-body forces.

2. The A -dependence of pion-nucleus scattering lengths

Pion-nucleus scattering lengths are not simply equal to the sum of pion-nucleon scattering lengths. To determine this difference, we analyzed s -wave π^- -nucleus scattering lengths, separating the isoscalar (charge-independent) from the isovector (charge-dependent) contributions as a function of the neutron (N) and proton (Z) number. We have used the natural parametric form for the scattering amplitude:

$$a[\pi^-(N,Z)] = a_0 A + a_1(N-Z) + b_0 A + b_1(N-Z)$$

where $A = N+Z$, a_0 and a_1 are the free π -nucleon scattering lengths, and b_0 and b_1 represent the effects of scattering from nucleons which are not free. Our fit to the nuclei ^4He , ^{10}B , ^{12}C , ^{14}N , ^{16}O , ^7Li , ^9Be , and ^{19}F yields values for b_0 and b_1 with errors comparable to the uncertainties in the basic scattering lengths a_0 and a_1 . Most interesting is the result that b_1 has an A -dependence indicating a contribution from double scattering -- in other words, multiple scattering is responsible for at least part of the difference between pion-nucleus scattering lengths and the sum of free pion-nucleon scattering lengths.

Our results also suggest that charge-exchange scattering to the isobaric analog state vanishes in the vicinity of $A = 17$ for low-energy pions.

3. Resolution of the "neutron knock-out" puzzle

In this case "neutron-knockout" refers to neutron removal from a $T = 0$ nucleus by pion beams on the $(3,3)$ resonance. The π^+ to π^- ratio for this reaction is calculated to be 1:3 when one assumes a simple single interaction (i.e., the pion interacts only with the neutron removed and the neutron suffers no further interaction while leaving the nucleus). Some years ago experimental results seemed to indicate that this ratio is 1:1 for ^{12}C , ^{14}N , and ^{16}O . Many attempts have been made to explain this discrepancy over the years.

This past year Dropesky's group remeasured the reaction on ^{12}C as a function of energy with quite different results -- the ratio found is not 1 and, in fact, has considerable energy dependence. In view of these new findings, we calculated the effect of nucleon charge-exchange interactions in the final state and found that the resulting ratio complete with its energy-dependence is in good agreement with Dropesky's results.¹⁹ This approach was then applied to other nuclei. Equally good agreement with recently measured values tends to confirm the presence of nucleon-charge-exchange final state interactions (Fig. 18).

4. Pion charge-exchange on light nuclei

The charge-exchange reaction has recently been measured at LAMPF by the Tel-Aviv group to have a cross section of the order of 1 mb -- in disagreement with the 3 mb value obtained by Chivers et al. Theoretical cross sections have been of the order of 0.2 mb. The Tel Aviv group also measured single charge-exchange on ^7Li and ^{10}B . The ^{13}C is a pure isobaric analog transition; the ^7Li has one analog and one nonanalog; and the ^{10}B is a nonanalog transition.

Using a multiple scattering technique based on the assumption of fixed nucleons and separable off-shell T-matrices, we have

Fig. 18. Ratios of neutron knockout cross sections as a function of incident pion energy, T_π , for three light nuclei. Experimental points were measured with activation techniques by N. P. Jacobs and S. S. Markowitz. The curves were calculated by T-5 using the nucleon charge exchange model.

calculated cross sections for these three reactions. For the pure nonanalog transition ^{10}B we find excellent agreement. The reaction is rather complicated being made up of monopole and quadrupole, spin-flip and nonspin-flip, and proceeding through two final states (Fig. 19). For the ^7Li case we are too low as in the ^{13}C case where we get a cross section of the order of 0.5 mb.

We have argued that the production of low-energy protons in the thick targets used in the experiments will cause an artificial augmentation of the observed cross section in the case of the ^{13}C and ^7Li . This is due to the very large (p,n) analog cross section. The ^{10}B would be unaffected by this process because it is a nonanalog reaction.

Our estimates of this process range from 0.2-0.6 mb and might therefore explain the entire discrepancy. The experimental group has made their own estimate and believes the correction to be about 0.1 mb in the case of ^{13}C and 0.2 for ^7Li . These estimates are difficult to make in any reliable fashion and the final resolution of the problem will await definitive measurements (perhaps with the use of the π^0 spectrometer).

5. Elastic scattering of pions from light nuclei

We have recently compared theory with experiment for elastic scattering of pions on D, ^3He , ^4He , ^{12}C , and ^{16}O , including Coulomb effects in an approximate fashion. The most interesting case is ^4He .

For several years it has been noted that pion- ^4He scattering shows a minimum at about 75° which is stationary from 60 MeV to 260 MeV. Any diffraction theory will predict a minimum that moves toward smaller angles as energy increases. Glauber theory, optical models, and our multiple scattering model in its primitive form give a minimum at much too large an angle.

Fig. 19. Single pion charge exchange cross section as a function of incident pion energy, T_π , for the non-analog transition in ^{10}B . Experimental points were measured by Y. Shamaï et al. The solid curve was calculated in the multiple scattering formalism assuming fixed nucleons and separable off-shell T-matrices.

Several authors have pointed out the need for angle transformations, i.e., the evaluation of the basic pion-nucleon amplitude at different energies and momenta depending on the final pion scattering angle. For nuclei as heavy as ^{12}C , absorption effects will cloud the effects of angle transformation corrections; however, the ^4He reaction is approximated well enough by a single interaction to make visible these corrections to the pion-nucleon scattering amplitude.

We have included this correction in our multiple scattering theory referred to in Sec. 4 above. Results place the theory in almost perfect agreement with experiments from 51 to 110 MeV. (At higher energies, a required relativistic correction introduces higher partial waves into the interaction, making the calculation much more difficult.)

These momentum and energy corrections clearly explain the seemingly strange behavior of the minimum, a fact that could not be demonstrated before a reliable multiple scattering theory existed for its inclusion.

6. Observation of residual nuclei after pion bombardment

A number of experiments have been performed in which a target is exposed to a pion beam and the resulting gamma spectrum observed. From these spectra the relative abundance of nuclides can be deduced and in many cases absolute cross sections obtained. The dominant nuclides observed whose mass number differs greatly from that of the target are those differing by an integral number of α -particles -- a striking observation. To model the effects of pion bombardment on nuclei, we have written an evaporation code which permits evaporation of neutrons, protons, and α 's and includes true Q-values and angular momentum. Assuming the excitation mechanism is predominantly a pion striking one nucleon which then deposits its energy in the nucleus, the code gives reasonable agreement with the data. Because of the forward-backward peaking of the pion-

nucleon angular distribution, the calculated excitation energy of the nucleus has a peak at low energies and another peak at high energies. This sort of behavior is apparently required by the data. It is interesting to note that this distribution is far from the one that would be assumed if the nucleus were given a statistical equilibrium distribution about a given temperature.

This calculation is much simpler than the internuclear cascade calculations usually done for these reactions and has the added virtue of having the input physics more visible.

Thus the gross features of a portion of the pion-nucleus interaction may be visualized in a simple manner.

7. Observation of the recoil proton in quasielastic pion scattering

We have calculated the cross section for knockout of a nucleon by quasielastic scattering of pions from ^{12}C , ^{27}Al , ^{63}Cu , and ^{208}Pb . We find that the effective number of protons rises very slowly with Z ($\sim Z^{2/5}$) in agreement with naive expectations.²²

It is difficult to determine from the pion spectrum alone whether or not a true quasielastic event has taken place. Therefore we suggest that a first attempt to observe quasielastic pion scattering using counters may best be undertaken with a (π, p) experiment as opposed to a (π, π') experiment.

B. The Pion Plus Two Nucleon Systems

1. Pion absorption on the deuteron

Recent data by Freedom, et al., on the $\pi^+ + d \rightarrow p + p$ reaction at 40, 50, and 60 MeV show a somewhat flatter angular distribution than might have been supposed from earlier experiments (although the angular distribution coefficient is within the earlier error bars).

We have calculated these angular distributions using a rescattering model developed previously. Modifications were made to include off-shell effects in the s-wave, fermi-motion, and the angle transformation; these altered the angular distributions only slightly. However, the calculations show appreciable sensitivity to the D-state percentage of the assumed deuteron wave function. The data can be fit easily by using a D-state of about 4% (7% is several standard deviations away). Once we are convinced that the theory is sufficiently reliable, this may be the most accurate measure to date of the deuteron D-state.

2. Restrictions of phase shift equivalent transformations

It has been pointed out (most recently by Sauer) that a large class of unitary transformations can be applied to the nucleon-nucleon wave function leaving the phase shifts invariant but altering the short-range part drastically. Sauer shows that the extraction of the Coulomb-corrected proton-proton scattering length is very sensitive to these transformations. We have looked for a way to reduce the number of such transforms with a view to reducing the ambiguity in the Coulomb-corrected p-p scattering length.

To this end we have investigated the $\pi^- + d \rightarrow n + n + \gamma$ reaction. The absolute rate is not sufficiently sensitive to restrict the transforms very greatly except in the following sense. If either the deuteron wave function alone or the n-n wave function alone is transformed, then the change in the absolute rate is noticeable. If, however, the same transformation is made on both wave functions there is very little change in the rate.

Thus a careful measurement of the rate can restrict the short-range character of the $T = 0$ nucleon-nucleon interaction to be (nearly) the same as that of the $T = 1$ interaction.

C. Nucleon-Nucleon Scattering

1. Neutron-proton bremsstrahlung

We are studying neutron-proton bremsstrahlung including the effects of meson exchange currents. We have found that the one-pion-exchange (OPE) current alone accounts for 80% of the theoretically predicted differential cross section $d\sigma/d\Omega_n d\Omega_p d\theta_\gamma$ for some kinematical regions. Strong interaction distortion of the initial and final nucleon-nucleon states is found to be important for both the shape and size of the exchange current contribution.

Assuming that the charge density is unmodified and using charge conservation and an analyticity assumption, we have obtained the electromagnetic Hamiltonian corresponding to all meson exchanges and nonlocal interactions in the zero photon momentum limit. The cross section with this approximate electromagnetic Hamiltonian is considerably smaller than that calculated with the OPE current alone. Since the zero photon momentum limit cannot account for this difference, other meson exchanges are probably responsible for the large cancellations that occur. We plan to study these and other possible corrections to the OPE approximation.

2. Pion production by protons on protons

In a recent experiment by Glass, et al., the neutron spectrum was observed after proton bombardment of a hydrogen target. This spectrum shows clear evidence of the (3,3) resonance.

We were able to fit the peak to within 20% using a rescattering model in which the pion is produced off-shell from one nucleon and put back on-shell by scattering from a second nucleon. The introduction of absorption into the initial channel (with the aid of one parameter, the absorption radius) yielded an exact fit to the peak magnitude. However, there remained a shoulder on the lower energy side of the (3,3) peak which deviated from our calculated curve. At this neutron energy, the final n-p pair can be at

zero relative energy. Therefore, we thought the strong n-p interaction at low energies was the source of the deviation.

By calculating the effect of a simple on-shell n-p rescattering with adjustable strength, we reproduced the features of the experimental curve; however, the angular dependence of the neutron spectrum is yet to be understood.

Results of this work were presented at the Santa Fe Conference.²⁶

D. The Three-Nucleon Problem

1. Radiative pion capture in tritium

We have begun an examination of the reaction $\pi^- + {}^3\text{H} \rightarrow \gamma + 3n$ where the pion is in a bound atomic orbital. Experiment No. 50 at LAMPF measures the γ spectrum from this reaction.

This is the simplest reaction that permits one to investigate the trineutron system at low energy. Because $\pi^- {}^3\text{H}$ is a "one-electron" system, one avoids atomic problems associated with capture in ${}^3\text{He}$ or higher Z-elements.

We have formulated the problem in a separable-potential Faddeev model. Preliminary results have been obtained in the first rescattering approximation (i.e., we allow two of the nucleons to interact in the final state). We are now studying the singularity structure of the amplitudes in order to solve the integral equations defining the complete Faddeev solutions. The solutions will then be compared with the results of Experiment No. 50.

2. Binding energy of the hypertriton ${}^3_{\Lambda}\text{H}$

We have previously investigated the n-p- Λ system (hypertriton) as a means of testing low-energy properties of theoretical hyperon-nucleon (Y-N) potentials.⁷ The binding energy of ${}^3_{\Lambda}\text{H}$ was calculated in a Faddeev, separable-potential model for two proposed Y-N potentials

and found to be sensitive to the Λ -N scattering length and effective range parameters. Our conclusions were based on an effective interaction approximation, i.e., the N-N isospin triplet, Λ -p, and Λ -N isospin triplet and singlet interactions were replaced by simple s-wave potentials determined from scattering lengths and effective ranges and implicit Λ - Σ coupling was neglected. We have now shown that our previous conclusions are unaltered by including explicit Λ - Σ coupling, short-range repulsion, and a tensor component in the triplet N-N interaction.

3. The three-body photodisintegration of ${}^3\text{He}$

We have calculated the reactions ${}^3\text{He}(\gamma, n)2p$ and ${}^3\text{He}(\gamma, p)np$ in a consistent Hamiltonian formalism where both the initial bound state and final 3N scattering state are solutions of the same separable-potential Faddeev problem. We have restricted our calculations to s-wave, rank-one triplet and singlet potentials whose parameters are determined by the low-energy N-N data. We treated the photodisintegration operator in the long wavelength, electric dipole approximation. Our results for the total cross section: (1) confirm the enhancement of the $T = 3/2$ component and suppression of the $T = 1/2$ component previously reported by Barbour and Phillips, (2) indicate that the normalization of Barbour and Phillips is 15-20% too high due to an inconsistent approximation in the ground state wave function, and (3) give reasonable agreement with the data. We have also approximated Coulomb effects in the final state p-p interaction and find that they improve the fit to the neutron spectra markedly in the region of the peak corresponding to the strong (p-p) final state scattering.

Thus, there seems to be no problem in our understanding of these reactions.

E. Studies in Weak Interactions

1. Parity violating effects in strangeness conserving non-leptonic processes

During the past several years, parity nonconserving effects were observed in numerous nonleptonic nuclear transitions. The order of magnitude of these effects suggests that they may be manifestations of a first-order strangeness conserving nonleptonic weak interaction whose existence is predicted by current theories of the weak interactions. An exception, which stimulated considerable interest, is the photon circular polarization P_γ in the radiative capture of unpolarized thermal neutrons by protons: $n + p \rightarrow d + \gamma$. Calculations of P_γ based on current weak interaction models give values which are about two orders of magnitude smaller than the observed one. This circumstance led to studies of possible additional contributions (e.g., exchange-current effects) and also to an inquiry into the possibility that fundamentally new effects were present, such as parity violation in the electromagnetic interactions of hadrons.

The present status of the field has been discussed in an invited talk at the Sixth International Conference on High Energy Physics and Nuclear Structure this summer.¹³ The only way to reconcile theory and experiment appears to be, as originally observed by McKellar, the introduction of a new interaction, which should have the effect of increasing the isotensor parity-violating couplings by roughly two orders of magnitude. It has been suggested¹³ that the origin of this interaction might perhaps be an isotensor axial vector hadronic current coupled to the photon. An experiment which can give decisive information on the question of the presence of a large isotensor interaction is the study of parity violation in proton-proton scattering, presently under way at the Laboratory.

Below we describe briefly the investigations that have been made in this area.

- a. Exchange-current contributions from $\Delta S = 0$ weak radiative mesonic transitions to parity violating nuclear processes

We investigated a set of exchange-current diagrams corresponding to parity violating transitions of the type $M \rightarrow \pi\gamma$ where M is a vector or axial vector meson. Their contribution to the photon circular polarization P_γ in the $n + p \rightarrow d + \gamma$ reaction has been evaluated and found to be smaller by an order of magnitude or more than the contribution arising from admixtures of opposite parity $n - p$ states, and thus far too small to explain the observed circular polarization.¹²

- b. Parity violating asymmetry in $n + p \rightarrow d + \gamma$ and the isospin structure of the $\Delta S = 0$ nonleptonic weak interactions

Another parity violating effect of interest in the $n + p \rightarrow d + \gamma$ reaction is the asymmetry α in the photon angular distribution with respect to an initial neutron polarization. Since α is sensitive to the isovector term in the nonleptonic weak Hamiltonian and the strength of this term is in some models larger by an order of magnitude compared to the Cabibbo value, a measurement of α could serve as a means of distinguishing various models of the weak interactions.

We have calculated α (the contribution from admixtures of opposite parity states in the initial $n - p$ and the deuteron states, as well as the exchange-current contributions) using a two-nucleon strong interaction given by the Reid soft-core potential and several of its phase equivalents. In preliminary results¹⁴ we obtain $|\alpha| \approx 5 \times 10^{-9}$ for the Cabibbo theory and $|\alpha| \approx 5 \times 10^{-8}$ for theories in which the isovector weak coupling is larger by an order of magnitude. In the presence of an isotensor axial current of a strength required to explain the circular polarization,¹³ $|\alpha|$ could be as large as 5×10^{-6} – 10^{-5} . A proposal to measure α has been approved and will be started this year at Grenoble.

2. Neutral current interactions and the decays of the neutral pion

One of the outstanding developments in particle physics in

recent years is, on the experimental side, the discovery of neutral currents in neutrino-hadron interactions, and on the theoretical side, the construction of renormalizable unified theories of the weak, electromagnetic, and strong interactions, most of which predict the existence of such currents.

An important question concerning neutral current interactions is whether such interactions also occur between charged leptons and hadrons, as predicted by some of the gauge theories and if the answer is yes, whether they are parity conserving or parity violating. The existence of high-flux pion beams in meson factories makes it especially interesting to investigate what one can learn about this question from studies of the various decay modes of the neutral pion.

We performed a detailed analysis of π^0 decays in the presence of a general neutral current interaction. Parity conserving effects are in most cases completely masked by the electromagnetic and strong interactions. If CP invariance holds, the simplest decay mode in which parity violating interference is possible between the weak and the electromagnetic amplitudes is the radiative decay $\pi^0 \rightarrow e^+ e^- \gamma$. We calculated the circular polarization of the photon P_γ and the longitudinal polarization of the photon P_L as functions of the Dalitz variables. These observables turn out to depend only on the hadronic vector -- leptonic axial vector neutral current coupling. In Weinberg's model we found $P_L \approx P_\gamma \approx 10^6 - 10^{-7}$ (Ref. 15). However, present experimental limits on neutral current coupling allow (and some models suggest) magnitudes which are larger by at least one order of magnitude. We suggested that the feasibility of performing this experiment at LAMPF and other meson factories be studied.

F. Review Article on Tests of Time-Reversal Invariance in Nuclear Electromagnetic Transitions

The discovery of CP-violation in the decays of K_L^0 led to considerable, but so far unsuccessful efforts to find CP violating and

time-reversal invariance violating effects in various other processes.

Among the most accurate experiments for testing time-reversal invariance are studies of angular distributions and correlations in nuclear γ -transitions. Experiments of this kind are being conducted at this Laboratory (W. A. Steyert and collaborators in the Q-26 group) among others.

To guide future work in this area, we have made in collaboration with F. Boehm (Caltech), W. A. Steyert (Q-26), and W. Weyhman (Univ. of Minnesota) a comprehensive review in which the following topics are discussed: (1) information on CP and T-violation from particle physics data; (2) the electric dipole moment of the neutron and its implications for T-odd observables in nuclear physics; (3) the phenomenology of time-reversal invariance tests in nuclear electromagnetic transitions, with emphasis on some as yet unexplored experimental possibilities; (4) the problem of final state interactions in correlation tests; (5) a detailed account of the existing experiments in nuclear γ -transitions (coincidence experiments, Mossbauer tests, etc.) and their bearing on models of CP-violations. Some aspects of this review have been presented in invited talks by F. Boehm and P. Herczeg at the Gordon Research Conference on Nuclear Chemistry, New London, June 1975. The full review is now being prepared for publication in Physics Reports.

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GROUP T-6 - LASER THEORY

Dale B. Henderson, Group Leader

I. INTRODUCTION

The Laser Theory Group provides the theoretical component of the laser project at the LASL. The development of economically practical systems for laser-induced fusion and laser isotope separation is the major goal of this project.

In a laser-induced fusion system, high-energy, short-pulse lasers are focused from one or more directions on a tiny pellet containing deuterium-tritium fuel and layers of other materials. The highly concentrated laser energy heats the outer region of the pellet, causing it to ablate and blow off. In much the same way that a rocket works, the blow off creates a pressure in the opposite direction, causing the inner region of the pellet to implode. The densities and temperatures of the imploded pellet core are sufficient to induce thermonuclear burn.

Work on spherical implosion systems originated during the early days of Los Alamos when Seth Neddermeyer, John Von Neumann, and Edward Teller explored the applicability to fission weapons of high-explosive-driven spherical implosion systems. Present work on the laser fusion project includes research on the physics of laser-induced pellet implosions and development of short-pulse, high-energy lasers, both of which call for progress in challenging areas of fundamental and applied research.

The idea of laser isotope separation is to focus monochromatic laser light on a mixture of isotopes of an element, causing one isotope to undergo a different physical or chemical process than the others in such a way that it can be separated from the rest. Success

in this area will have very wide application including the efficient separation of the various uranium isotopes and the separation of isotopes used in medical research. Techniques are also being developed to stimulate chemical reactions through selective excitation of molecules by lasers. Such laser-stimulated chemistry could have profound impact on the chemical industry. Work on laser isotope separation includes development of the required lasers [which must have certain wavelengths (colors) for this purpose] and research on the chemical and physical processes which occur in the material to be irradiated and separated.

The theoretical effort in T-6 has two primary objectives: (1) to provide direct support for the experimental program in the Laser Division; and (2) to develop and evaluate new approaches to laser fusion and laser isotope separation. Members of T-4 and T-DOT also participate in this effort.

In Sec. II we will outline the status, experimental and theoretical, of the laser fusion project and present some details of our recent theoretical work in this area. In Sec. III, "Laser Development", we will discuss our work on new laser systems for fusion and isotope separation, laser optics, and molecular physics related to both laser development and isotope separation processes.

II. LASER FUSION

Confidence in laser-induced fusion as a promising means of energy generation is based on computer simulation studies. Fusion energies 50 - 100 times larger than laser input energies are predicted provided the input energies are of the order of $10^5 - 10^6$ joules. The required energies and shapes of the laser pulses as well as the course of implosion and thermonuclear burn have been estimated by conventional numerical thermal conduction, hydrodynamics and burn calculations. The requirements for lower levels of thermonuclear burn down to the lowest detectable levels have also been estimated through numerical simulations.

These studies describe the following course of implosion and burn. The initial part of the laser pulse ablates the outer surface of the target creating a low density atmosphere around the pellet. Subsequent parts of the laser pulse incident on this low density plasma are absorbed by collisional damping of the electromagnetic wave (inverse bremsstrahlung) or by collective plasma phenomena. The absorbed energy appears first in the kinetic energy of the electrons and is then transported to the dense interior by diffusive electron thermal conduction or by longer range electron transport if the electrons are so energetic that their ranges are of the order of the target dimensions. At the surface of the dense, relatively cold core of the target, an ablation process occurs. The steep thermal gradient at the ablation front causes compression and shock heating of the interior while the heated outer regions ablate and blow off. Core compression creates high enough densities for fusion reactions to proceed efficiently. When the fuel reaches low thermonuclear temperatures, i.e., 5 to 10 keV, the fusion reaction rate for $d + t \rightarrow \alpha + n$ is sufficiently high that the α particles, most of which are recaptured in the fuel, cause the fuel temperature and, with it, the reaction rate to rise rapidly. This ignition process is required and responsible for the prediction of high yield ratios of 50 to 100 (or more) needed for economic energy production. Preheat of the core by very hot electrons will reduce the efficiency of this process. (See Fig. 20 and Fig. 21.)

The lasers required for high thermonuclear yields [i.e., lasers capable of producing several ten's of kilojoules of energy in pulses of about 1 ns (10^{-9} s) duration] are beyond the current state of laser technology and still in the planning stage. Nonetheless thermonuclear burn well above detection threshold is predicted theoretically from laser energies of a few tens of Joules in pulses of a few tenths of a nanosecond. These smaller pulses are available and have been used successfully at the LASL and elsewhere to obtain detectable nuclear yields. However, the details of the experimental results are not always in good agreement with theoretical predictions. The measured yields are smaller, sometimes much smaller, than predicted and some scalings do not agree. There are possible sources of discrepancy in both the theory and the experiments.

Fig. 20. Schematic diagram of energy flow and compression in a laser fusion event.

Fig. 21. A shaped laser pulse (left) and a plot of density and temperature as a function of distance in an irradiated fusion target (right). Light energy absorbed at or below the critical density, ρ_c , is conducted to the ablation surface where high pressures are developed which compress the pellet far above the initial solid density (dashed profile). Shaped pulses can give higher compressions and are especially useful with solid pellets.

At the present time laser-target experiments are done with two kinds of lasers: (1) neodymium-doped glass lasers which produce 1.06 μm light from the Nd^{3+} ion and (2) CO_2 lasers which produce 10.6 μm light from a vibrational transition of the CO_2 molecule. The work with CO_2 lasers is newer and more interesting because these lasers are more efficient. Since the CO_2 laser produces longer wavelength light, absorption takes place at lower plasma densities ($n_e < 10^{19} \text{cm}^{-3}$) where collisional frequencies are lower and collective effects more important. Consequently greater theoretical understanding of collective effects is needed to interpret the results of CO_2 -target experiments.

In general, experimental limitations make comparison with theory very difficult, especially where details of the implosion dynamics are concerned. Measurements requiring time and/or spatial resolution are such that it is often impossible to be sure that experimental conditions are those assumed in the calculations. The most useful implosion diagnostics available are neutron output (a measure of thermonuclear burn), α particle output (from which we infer ion temperatures), and time-integrated x-ray photography and spectroscopy (a summary of the temperature history of the implosion process). A streak camera has been designed to attain time-resolved x-ray spectra but it is not yet operational.

On the theoretical side, many questions remain concerning the physics of laser energy absorption in the low-density plasma and subsequent heat flow and hydrodynamic behavior, especially the possible effects of plasma instabilities and small-scale hydrodynamic behavior. For example, classical theory predicts a much larger electron heat conduction to the target interior than is observed experimentally (this may be one reason for the lower experimental yields) and recent theoretical work indicates that plasma instabilities may be responsible.

The theoretical effort is therefore directed at improving understanding of the basic processes involved, developing more sophisticated computational tools for simulating these processes, and applying these advances in theoretical understanding and computational techniques to improve target design. Details of these three efforts are presented below.

A. Target Design

A large effort in T-6 is devoted to calculating the performance of various laser targets and devising new targets for improved performance.

All fusion targets contain a spherical pellet which houses the thermonuclear fuel. The simplest pellets in current use are called microballoons and typically have the composition shown in Fig. 22. The thinwall glass shell is available from standard commercial processes. The DT gas is introduced into the interior by a diffusion process. These pellets are suitable for irradiation by laser energies of ten to a few hundred joules. As laser energies increase, the appropriate mass of the pellet increases in approximately direct proportion. Simple and advanced target designs are shown in Fig. 23.

Fig. 22. Composition of a simple microballoon target.

Fig. 23. A simple microballoon target on a human hair (top) and a ball and disc target (bottom).

1. Advantages of structured microballoon targets

Both simple and structured microballoon targets have been studied to understand implosion phenomenology, stability, burn, and scaling laws for various laser parameters. We have shown that structured targets with high Z, dense outer shells have many advantages over simple targets. First, by shielding hot electrons from the interior, high Z, high-density shells prevent preheat and help to regulate the timing of a given implosion. Also they serve as tampers, i.e., they inhibit the disassembly of compressed fuel thereby improving the thermonuclear yield.

2. Matching current targets and laser pulses

To match current targets and laser pulses optimally, it is necessary to know how compression and performance trends vary with respect to shell mass, aspect ratio (the ratio of shell thickness to radius), and initial density. We have conducted an extensive numerical simulation study to answer these questions using bare DT shells, non-fuel shells, and DT-filled microballoon targets with ramp, Gaussian, and square laser pulses. Scaling laws were determined for the best pulse energy and time scale.

3. Radiative preheat from microballoon targets

An important result of microballoon target studies is that radiative preheat is at least as important as hot electron preheat. The radiative preheat results from recombination and line radiation near the ablation front and is responsible for a fivefold reduction in tamper density and a twofold reduction in $\langle pR \rangle_{\text{tot}}$ when compared with purely ablative implosions. Detailed comparisons of our code calculations with present experiments, e.g., those of KMS Fusion, Inc., support our conclusions.

4. Satellite line radiation as a diagnostic tool

In another study with help from T-4, we considered in detail the possibility of using satellite line radiation from present glass microballoon experiments as a diagnostic tool to determine electron temperature.

5. Studies of hydrodynamic instabilities

A large effort has been made to understand hydrodynamic instabilities which are expected to arise in some large aspect ratio shell targets of interest. To examine the effects of the resulting turbulence on implosion dynamics, we have implemented a model turbulent mixing calculation via a turbulent mixing operator. Further, we have extended the theory of stability calculations to include the effects of thermally generated magnetic fields.

B. Code Developments

1. Hydro-heat flow codes for modeling implosions

We have continued work on the PAL (Particle Lagrangian) fluid algorithm for modeling laser-driven pellet implosions. A particular PAL code, IRIS, a fully two-dimensional (r,z) hydro-heat flow code, is being developed for the study of exotic laser fusion targets. Much like the well-known PIC methods originally developed by Harlow and coworkers, the PAL scheme involves a finite number of particles whose velocities and locations are computed on an Eulerian staggered mesh. But, unlike the conventional PIC method, all quantities rather than just mass and position are carried by the particles, e.g., electron- and ion- entropy, momentum, mass and species number. At the present time IRIS can handle coupled hydro-heat flow problems with both electron and ion thermal conduction present. A sophisticated Monte Carlo laser deposition package which includes diffraction and refraction effects is being implemented. The code has been used to calculate the course of implosion for advanced laser fusion targets such as ball and disk targets.

IRIS is built up from substructures called "phases," with each phase independent of all other phases in terms of both computational assignment and memory allocation for variable storage. The initialization package allows one to define arbitrary geometrical shapes of

revolution and to build almost any desired structure from these shapes. Each region can have any desired number of particles with any desired material properties. Furthermore, particle loading can be varied to anticipate expansions or contractions of the fluid.

In another area of code development, we with members of ID-3 have modified a current two-dimension Lagrangian code to allow for electron conduction and ray tracing of the laser light.

2. Code for calculating x-ray pin-hole pictures

To facilitate comparison of numerical predictions with experimental data, a code has been written to calculate x-ray pinhole pictures for spherical laser fusion targets. The code is a postprocessor for data output from any one-dimensional spherically symmetric Lagrangian hydrodynamics code. Calculated densities and electron temperatures are used to obtain values for frequency-dependent emission and opacity coefficients from tables produced by the Equation of State and Opacity Group (T-4).

C. Research on the Plasma Physics of Laser-Driven Implosions

1. Effects of plasma instabilities on laser energy absorption and large-scale hydrodynamics

The process of inverse bremsstrahlung (binary collisions) is insufficient to explain the observed absorption of laser energy. Efforts have therefore been made to understand how collective plasma phenomena may be enhancing absorption. The collective effects involve instability and resonance phenomena near the critical density (i.e., the deepest point of electromagnetic wave propagation, where the plasma and incident laser frequencies are equal).

In plasma simulation codes, these effects, involving complicated changes in density and velocity profiles due to pondermotive forces and turbulence, are observed to occur in the vicinity of the critical density. These occur over scale lengths much shorter than the

hydrodynamics codes can resolve, yet their effects on energy absorption and electron transport may influence the large-scale hydrodynamics of the plasma. This detailed plasma behavior must be understood well enough to cast in a form amenable for use in an Eulerian or Lagrangian hydrodynamics code.

From a one-dimensional hybrid code in which electrons are treated as a fluid and ions as particles, we have reproduced the gross profile modification observed in full two-dimensional particle codes. This hybrid code includes ponderomotive force effects arising from the two-dimensional laser and plasma wave electric fields, but can only describe instability, and hence absorption, involving waves propagating in one direction. This year we have completed a tedious two-dimensional theoretical calculation in which we completely describe the stability properties of the plasma in the vicinity of the critical density for a given density profile. The electric field eigenfunctions observed in full, two-dimensional PIC plasma simulations completely match those predicted from this theoretical calculation.

2. The effects of plasma instabilities on electron thermal conduction

Laser-target experiments at the LASL and other laboratories indicate that thermal conduction by electrons through the low-density plasma to the ablation front is much lower than predicted by classical theory. We have successfully modeled most features of these experiments (e.g., the bremsstrahlung spectrum and the appearance of a fast ion component) by introducing a stringent flux limiter for the electron heat conduction. To understand how such a flux limitation could arise, we have undertaken microscopic plasma simulation studies which involve electrostatic current-driven instabilities and self-generated magnetic fields. The current instabilities arise from a velocity space distribution in which hot electrons are superimposed on a drifting Maxwellian distribution of cold electrons. Depending on the drift velocity and density

of hot electrons, the resulting drift velocities of the cold return-current electrons imply either stability, ion-acoustic instability or Buneman two-stream instability. The resulting ion turbulence appears capable of limiting the hot electron flux. (See Fig. 24.)

3. Studies of magnetic field effects

Direct experimental evidence for microscopic magnetic fields in laser-target interactions has been reported in the literature. Because the observed fields occur in the nearly collisionless, underdense plasma, the value of the usual fluid description of their generation is open to question. Consequently, simulation studies of the generation of magnetic fields in collisionless plasmas have been carried out along with studies of turbulent magnetic field generation by both Weibel instability and turbulent ion waves. This work complements our efforts on electrostatic current stabilities described above.

III. LASER DEVELOPMENT

The lasers used in fusion research are adequate in many respects for low-energy experimentation but fall short of the requirements for producing significant thermonuclear energy yields. While the present pulse lengths of $\lesssim 50$ ps are sufficiently short, the beam quality, i.e., the size and uniformity of the focal spots, is often poor and unpredictable due to various linear and nonlinear optical effects. Moreover, total pulse energies presently available are orders of magnitude too low.

Although present laser systems can be scaled up to achieve larger energies, their relative inefficiency makes this impractical. Instead, we are seeking to optimize the efficiency of pumping and energy extraction through a better understanding of the molecular and atomic physics, and therefore the kinetics, of laser systems.

Fig. 24. Reduced thermal conduction from plasma instabilities. Two curves for J_i , the blow-off ion current, are shown above. The upper curve is representative of the hot electron transport model. The lower curve for J_i is typical of results obtained using the reduced thermal conduction model described in the text and closely resembles experimental measurements. Two-stream instability, as indicated above, may be responsible for reduced thermal conduction.

In the long run, these efforts to model laser systems from the molecular level on up may lead to the identification of new laser systems that are intrinsically more efficient. To date, the most efficient fusion laser system suitable for target work is the CO_2 system with an efficiency of a few percent and a possible optimized efficiency of about 10%. On the other hand, the HF system ($\text{H}_2 + \text{F}_2 \rightarrow 2\text{HF}$), recently identified as a possible fusion laser, has a potential efficiency close to 20% and a lower capital cost per joule because much of the energy is provided by chemical burning instead of expensive high-voltage, short-pulse power supplies. However, the HF system does not yet produce a short enough pulse for fusion work.

The search for new laser systems is also motivated by laser wavelength requirements. In fusion work, there are recurring concerns that the 10.6- μm light from CO_2 may be less effective in some respects than the 2.7- to 3.0- μm light from HF. Wavelength requirements are much more stringent for laser chemistry and isotope separation work since lasers must excite a particular atomic or molecular transition without exciting others nearby. The pulse length requirements, however, are not as severe, and the need for high efficiencies is not nearly as great as for fusion.

Theoretical work in optics, fundamental atomic and molecular physics, and more general system studies is essential to meet these laser development needs. Much of the necessary information cannot be obtained empirically because of the ambiguities and complexities of the experimental situations.

The following paragraphs describe in detail some of the recent theoretical contributions to laser development.

A. New Laser Systems

Considerable theoretical research on new laser systems is directed toward achieving shorter pulses from the HF laser mentioned above. During the last fiscal year, we developed insight into the mechanisms for the production and loss of vibrationally excited HF in electron-beam-initiated $\text{H}_2\text{-F}_2$ mixtures. Extraction of the energy on a nano-second time scale requires that the chemistry proceed more rapidly than the electron beam initiation process. This places considerable emphasis on understanding the details of formation of the population inversion.

In the present computer model of the electron-beam-initiated HF laser, the predicted rate of production of vibrationally excited HF, using presently accepted rate constants, is too slow to account for the observed pulse rise time. Included in this model are the $\text{H}_2\text{-F}_2$ chemistry, the time-dependent photon kinetics and collisional dynamics for each rotational level in the HF molecule, and all important V-V and V-T collision processes for each molecule. Aside from the total optical flux and energy output, the principle quantities directly observed experimentally are the individual time histories of the multitude of laser transitions. Although one can never hope to reproduce completely the experimental patterns in detail, one can aspire to an eventual understanding of the trends as a function of the input parameters, e.g., rate constants, deactivation rates, etc.

A possible cause for the discrepancy between the theoretical and measured pulse rise time is the absence in the theoretical model of the effects due to super-thermal F-atoms. Super-thermal F-atoms react with H_2 more rapidly than thermal F-atoms and, hence, effectively increase the rate of production of vibrationally excited HF. Consequently, much effort has been devoted to obtaining quantitative rates for the production of super-thermal F-atoms for the electron-beam initiation laser.

As a first step in determining this production rate, we have calculated the potential energy curves for the ground and excited states of F_2^+ , F_2 , and F_2^- . Only the ground state of F_2 is well characterized experimentally; the calculated dissociation energy is within 15% of the experimental value. The calculated potential energy curves are now being used to determine the kinetic energy distribution of the fluorine atoms obtained from excitation of a given excited state. Estimates of the electron impact excitation cross sections are being made using first-order scattering theory.

In order to develop an accurate model of the HF laser, it is also necessary to know the rates at which the various vibrational and rotational states of HF are relaxed by collisions with the atoms and molecules present. Accordingly, a series of calculations of the rates of these processes has been undertaken. The rate constants calculated in this study will then be used in the modeling codes to determine and understand such phenomena as the rotational state distribution, the conversion of vibrational energy into rotational energy, the absence of lasing from high vibrational levels, etc.

B. Optics

Excellent beam quality is essential for the optimization of a high power glass laser system. Hot spots, i.e., small regions of high intensity, are excessively amplified as a result of the nonlinear index of refraction of an amplifier, leading to beam breakup and damage to the laser glass. Frequently the origin of hot spots can be traced to diffraction phenomena arising from aperture truncation of the propagating beam. One solution which has achieved some success without degrading the performance of the amplifier is to truncate the beam gently, by the use of soft or apodized apertures, prior to passing the beam through amplifiers. Unfortunately, no simple aperture has yet been developed which works adequately for the $2\text{--}3\text{ J/cm}^2$ energy fluxes encountered at the high energy end of a glass amplifier chain.

We have now completed theoretical studies of a simple annular lens soft aperture constructed of laser glass or quartz which does not damage at the pulse energies encountered in a high power amplifier system. This lens is so constructed that the central portion of the beam is transmitted unaffected, while the outer portion is refracted out of the beam. To characterize further the effect of this lens on laser beams, a series of calculations has been done with a laser pulse propagation code (see below). The agreement with the results of geometrical optics theory is satisfactory.

The laser pulse propagation code LAPU, including a new Fresnel integral subroutine, has been used to study the optical quality of the laser pulse along the chain of four amplifiers of the LASL "Kilojoule" CO₂ laser amplifier system. Since the code propagates through the four stage amplifier a temporally finite pulse which varies in intensity over the pulse length, the addition of the Fresnel subroutine produced a time resolved calculation of the focal spot intensity vs. radius distribution.

The Fresnel integral subroutine was used to calculate focal spots for two different output pulses of CO₂ laser amplifier system. The first calculation was done on a pulse which had been severely apertured at several places along its passage through the four stage system. It was found that the output pulse had an appreciable divergence (several milliradians). This effect appears to have occurred because the abnormally severe aperturing of the pulse led to strongly diverging waves in the shadow region behind the aperture edge. These diverging waves were amplified enormously by successive laser amplifier stages while the central region of the pulse received less overall gain due to its higher intensity and consequent effects of gain saturation. The Fresnel integral subroutine was then applied to an output pulse representative of the current plan for the system. The resultant 207-J output pulse produced a peak intensity of 9.5×10^{14} w/cm² near the focus of a mirror of 213.36-cm focal length.

C. Molecular Physics

To understand the complex chemical phenomena occurring in chemical lasers and in laser isotope separation requires detailed knowledge of the structure, spectra and dynamics of the atoms and molecules involved. Research in molecular physics during the last year included extensive revision of the molecular structure codes, development of a new approximation for the electronic wave functions of molecules, investigation of new methods for calculating the elastic and inelastic cross sections for scattering electrons off atoms and molecules, calculation of the potential energy curves for the ground and excited states of the fluorine molecule (see the section on New Laser Systems) and the transition matrix elements coupling the states, the initiation of a program to investigate and analyze the vibrational-rotational spectra of molecules, and a study of associative recombination in helium systems.

Analyzing earlier studies of the electronic states of O_3 and HF and the calculations of Prof. H. F. Schafer, III, (University of California, Berkeley), a new type of configuration interaction (CI) wave function has been proposed, the polarization CI (POL-CI) wave function. The POL-CI wave function accounts for the space and spin polarization effects neglected in most orbital methods and includes molecular near-degeneracy effects. In an extensive series of calculations on the ground and excited states of NH, it was found that the POL-CI calculations satisfactorily reproduced the results of far more extensive calculations. In addition, the POL-CI wave function can be readily extended to describe higher states of the same symmetry as lower states.

A theoretical interpretation has been developed for associative ionization (Hornbeck-Molnar process) in the rare gases, and cross sections for this reaction in helium have been calculated for the first time. A semiclassical model was derived to treat the multistate curve-crossing problem which arises in the diabatic

representation of the electronic states. The required structure parameters were obtained from ab initio calculations on the Rydberg states of He_2 . Energy dependent cross sections, needed for modeling of helium discharges, were obtained for associative ionization and excitation transfer. The results are in good agreement with recent experiments in the cases where comparison is possible.

We are developing the theory and related computational techniques for the description of elastic and inelastic scattering of electrons from atoms and molecules. A new variational technique for solving the Schrodinger equation in the continuum region has been developed based on the R-matrix formalism of nuclear physics. The central idea is to divide space into two regions. In the internal region, we solve the full $(N+1)$ electron problem including exchange using matrix variational techniques. In the external region, we assume that exchange, but not long-range electrostatic forces, is negligible and solve the Schrodinger equation numerically including all important open and closed channels. The R-matrix method has been applied to the elastic scattering of electrons from H_2 in the static exchange approximation. The agreement with other, less general, methods is good. The theory has now been extended to treat general elastic and/or inelastic electron-molecule collisions including polarization and short-range electron correlation. The major difficulty has been the development of a coupled channel code to account for the effects of long-range polarization potentials outside the R-matrix box.

During the past year, an active theoretical program has been initiated to support experimental research on the infrared spectra of molecules. Much of the theoretical work to date has been concerned with CH_4 and SF_6 . Methane is a prototype spherical top molecule because its infrared spectrum, obtained on conventional spectrometers, is familiar and well resolved. A detailed analysis of portions of the spectrum with a laser spectrometer is in progress. Preliminary results of force-field calculations for methane are in

good agreement with the observed fine-structure splittings. The laser spectrum of SF_6 is also well resolved and not significantly complicated by hot bands at low temperatures; hence, this molecule is particularly suitable for testing the theory for octahedral molecules. Definite assignments have been made for many lines in the ν_3 band of SF_6 based on the statistical weights of Cantrell and Galbraith and application of the formulas for the positions from Moret-Bailly.

D. Solid State Physics

The rate of relaxation of a molecule in a host solid is crucial in assessing the practicality of laser isotope separation processes in the solid phase. For diatomic molecules the vibrational frequencies are many times the highest lattice frequencies and, hence, vibrational relaxation is a multiphonon process. Such processes, which arise from anharmonicities are slow. We have recently done a number of studies on the molecules isolated in solid matrices.

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GROUP T-7 - MATHEMATICAL MODELING AND ANALYSIS

Burton Wendroff, Group Leader

I. INTRODUCTION

Changing times for the economy and the energy crisis prognosis have generated major new trends in public policies; these are reflected, in turn, in shifted priorities for the natural sciences in general, and applied mathematics in particular.

Research programs of Group T-7, the mathematical modeling and analysis group, are focusing on this challenge: the analysis of energy systems and economic resources allocation models which require a specific mathematical sophistication in both their computational and analytic complexities. This focus is related to many of the LASL's major programs and is intended to benefit them directly through our educational and consulting functions, an intrinsic component of our responsibilities.

The group's research progress in 1975 should first be globally surveyed with respect to these specific goals. We have been involved in four major research areas: numerical methods and computer arithmetic; mathematics of energy systems; economics and energy resources modeling; and discrete mathematics.

In the past year, we have devoted a large part of our activities to the specific numerical analysis problems originating in energy related models; in particular, the construction of stable, efficient and accurate algorithms for the solution of systems of partial differential equations describing mass and heat flow in such complex systems as nuclear reactors.

In this work we have initiated new directions in finite element methods and operator splitting techniques. The finite element method could be characterized, in general, as enabling the computer to generate its own set of equations, whose solution then approximates the given physical problem. Higher order accurate finite element methods are desirable for multicomponent, multidimensional flows. We have tested the improved computational efficiency of higher order finite element methods on a wide array of typical nonlinear model equations, for example, the "quench problem" in reactor safety which corresponds to the propagation of a sharp cooling front in a fuel rod. Operator splitting techniques, which reduce a complex problem to a combination of simpler ones, have been effective in permitting the use of large time steps in the solution of huge systems of hydrodynamical-heat flow equations. We have also deepened the analysis of some alternating direction methods for classes of nonlinear time-dependent problems.

Differential equations characterizing such energy-related systems seem to be far more sensitive to perturbation of data and error propagation than the usual wave or diffusion equations. As a corollary, an increased and promising effort in sensitivity analysis has been initiated, considering the effect on the computational results of inaccuracies in the input data. Special emphasis has been directed toward problems of significance arithmetic in a computer; significance arithmetic utilizes an unnormalized representation that exhibits the error in a quantity, and arithmetic operations properly reflect the interaction of such errors. A successful program has been continued on the development of algorithms for efficient performance of arithmetic operations, and evaluation of functions generally, to be used in computer programs.

A second major facet of our activities focuses on the inherent mathematical difficulties induced by energy-related models; in particular, problems of nonlinearities (e.g., shock waves), and relevant global stability questions.

Our research in two-phase flow fits within expanded reactor safety programs (in particular, the Light Water Reactor Safety Research Program, sponsored by the Nuclear Regulatory Commission). This brings us in close contact with the T-1 and T-3 efforts. For two-phase flows, we have shown that extending the analysis of simple nonlinear wave propagation schemes shall require new techniques, and we have been able to unravel the related model equations which are well-posed from those that are ill-posed.

The laser-induced fusion and laser isotope separation programs generate an endless field of mathematical queries. We have carried out a new theory, which has been verified experimentally by the Laser Division, for the nonlinear optics of self-focusing problems in very high-powered lasers. In these lasers, being developed for the fusion program, self-focusing difficulties provide the principal limitation to achievable intensity. Our theory shows that with proper spatial filtering the intensity can be raised to about 2.5 times that without filtering.

Tunable lasers as energy sources are producing infrared spectra of a quality undreamt of a few years ago. We have emphasized powerful group theoretical techniques that can form a basis for a comprehensive theory of the infrared spectra of polyatomic molecules. Its usefulness is considerable as a back-up of laser isotope separation programs. As a consequence, we were able to calculate some intensity ratios which were crucial in the interpretation of the experimental infrared spectra of SF_6 taken by the laser isotope group (L-Division). A related program in group theoretical methods has been furthered in the theory of irreducible tensor operators.

Nuclear reactor systems require more sophisticated transport codes; we have investigated the stability and convergence difficulties of the synthetic method of neutron transport theory in various geometries. Necessary and sufficient conditions for convergence have been outlined, with specific applications to a code written by T-1.

The nuclear fusion program is encountering difficulties in micro-instability analysis of high temperature plasmas. Such microinstabilities must be studied within complex nonlinear systems of equations of statistical mechanics. Mathematically, the multiplicity and stability analysis of their solutions is inextricably tied to the continuous spectra properties of the relevant operators. We have worked out the first abstract theory of bifurcation of multiple solutions from a continuous spectrum for a class of nonlinear problems originating in statistical mechanics. Implications for experiments are nontrivial since the asymptotic behavior of such systems is tied to a delicate balance between hydrodynamic modes and nonlinear contributions of the continuous spectrum.

A third facet of our activities has concerned the actual modeling and analysis of economic and energy resources allocation planning policies. The LASL is the lead laboratory in ERDA's regional assessment program for the eight Rocky Mountain States. Our contribution has dealt with an important tool with respect to information flow, namely, input-output national and regional economic matrices and related problems of coefficient aggregation and sensitivity analysis in inverting such matrices. Specifically, the mathematical aspects of economic-ecologic input-output models have been deepened. A practical application of an economic-ecologic input-output model has been carried out by T-7 for the San Juan River Basin.

On the broader level of research on the management and improvement of public policy performance, a whole new effort has been initiated; we have carried out an extensive review of problems raised by the stability effects of price indexation in a multiple market economy. There are major differences of opinion as to what results can be attributed to price indexing as a means of fighting inflation. To further our preliminary calculations, extensive methods of "global analysis" of dynamical systems will be needed. T-7 will continue work on the stability of indexing schemes.

Finally, we have pursued work on discrete mathematics, such as graph theory (metric graphs, random trees), with application to theoretical biology, and partially ordered sets, combinatorics, and number theory. Some of these questions, such as the "knapsack problem," arise in many contexts, including that of laser energy levels.

We intend to expand our program of mathematical and numerical analysis of systems, emphasizing stability and error propagation studies. Such a goal cannot be successful without an aggressive interactive program in applied mathematics. We have pursued in-depth consulting, advisory and service work, which puts us in contact with every technical division of the Laboratory, such as the C (computer), Q (energy), L (laser), J (field testing), M (dynamic testing), and P (physics) divisions. A course of ten 1-h lectures on the "Elements of Graph Theory" was presented to interested Laboratory personnel. An active visitor program in applied mathematics has been initiated, where visitors from universities can relate their theoretical work to the programmatic efforts at the LASL. This program has been spread between short-term and long-term visitors with the initiation of full-year stays, such as that of Professor R. D. Richtmyer (from the University of Colorado, on a shared basis with C Division and CTR Division). We intend to continue our program of full-year visitors.

We now turn to a brief technical review of the research topics investigated by T-7 in the fiscal year 1975.

II. RESEARCH HIGHLIGHTS

A. Numerical Methods and Computer Arithmetic

1. Higher order finite element methods^{22,24,25} have been evaluated and shown that improved computational efficiency results from the use of a refinement of a spatial mesh in the following

tested cases: a) in a neighborhood of a front due to a moving localized source in the heat equation; b) around a shock wave solution of

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = Q,$$

where Q is an artificial viscosity; and c) for traveling wave solutions of the nonlinear parabolic equation ("quench problem" in nuclear reactor safety):

$$u_t = u_{xx} - f(u), \quad u(-\infty) = 0, \quad u(+\infty) = u_\infty;$$

$$f(u) = \begin{cases} 0 & u_{\text{crit}} < u < u_\infty \\ au, & u < u_{\text{crit}} \end{cases}.$$

2. The effectiveness of Galerkin's method^{23,26} using piecewise-linear functions has been tested for the computational handling of boundary conditions in the numerical solution of a one-dimensional problem in gas dynamics (compressible isentropic flow).

3. The convergence rate of some alternating direction methods has been analyzed for the approximate solution of, respectively, a nonlinear parabolic and a nonlinear second-order hyperbolic partial differential equation.^{3,4} The D'jakonov iteration scheme has been investigated for nonlinear parabolic problems.

4. We have initiated new directions in operator splitting methods which permit the use of large time steps in the approximate solution of the parabolic portion of a huge system of hydrodynamic heat-flow equations.

5. The notion of "operator modification" has been created in order to develop nonlinear explicit, unconditionally stable numerical schemes of very high order accuracy in discretization schemes for nonlinear parabolic and hyperbolic equations.

6. Algorithms and complexity of arithmetical operations in computer programs have been surveyed; a method has been developed for evaluating the redundancy of various algorithms and constructing more efficient algorithms.¹¹

7. Research has been done on the roots of $x^m \pm 1$ in the p-adic field $\mathbb{Q}_p$ (an aspect of the work on algorithms concerns p-adic fields).¹²

8. Research in significance arithmetic has been continued;¹⁰ a symmetric function approach was used to prove formulas in significance arithmetic.

9. Error sensitivity analysis has been emphasized with respect to the effect on the computational results of inaccuracies in the input data. Specific application was made to Burgers' equation.

10. A generalized geometrical optics design code ("Climb") has been developed.⁵ We investigated codes for mirror systems and constructed a code to optimize the design of an electrical probe to detect defects in nuclear core cladding (joint work with M Division).

11. Intranuclear cascades at very high energies have prompted us to develop improved Monte Carlo calculations.

B. Mathematics of Energy Systems

1. Wave propagation in two-phase, two-component flow (e.g., mixtures of gas and water) spurred an in-depth survey of simple one-dimensional mathematical models (respectively, homogeneous; mechanical equilibrium isentropic; and mechanical equilibrium-thermal equilibrium models); the analytic derivation of the corresponding shock waves, rarefaction waves, and flow in a shock tube was completed.

2. We analyzed the "synthetic method" as used in neutron transport codes; convergence properties in various geometries (including the finite slab surrounded by vacuum) and optimal choice of the related diffusion constant have been clarified.

3. In very high power laser systems using optically dense host materials, self-focusing difficulties provide the principal limitation to achievable intensity. A theory of small-scale self-focusing has been proposed, verified experimentally, and extended to finite beams with initial convergence or divergence, to media of nonlinear gain, and to disc amplifier systems. We also investigated beam aberration due to nonlinearity of the refractive index.¹⁹⁻²¹ A new

numerical scheme has been devised for the laser "Husky-Pup" optical alpha experiment, in conjunction with J Division.

4. Concerning MHD equilibrium, nothing is known beyond the cylindrical geometry about the configuration of magnetic fields which admit an equilibrium. We have approached this problem by studying equilibria which nearly satisfy a cylinder condition. As to radioflash (EMP) problems, we contributed to the new JOWOG handbook on radioflash.

5. In the field of infrared spectra of polyatomic molecules (tunable laser sources), we developed group theoretical techniques for the polyatomic molecule model with strong emphasis on Eckart vectors and Eckart frames.⁷ We applied it to the practical computation of intensity ratios thereby unravelling experimental infrared spectra of SF_6 taken by the laser isotope group.

6. Group theoretical work has focused on the theory of irreducible tensor operators: the canonical resolution of the multiplicity problem for the $U(3)$ Wigner operators has been completed. Also considered were the structural properties of the canonical $U(3)$ Racah functions and the $U(3):U(2)$ projective functions,^{8,9} a generalization of Gauss' hypergeometric function, and hypergeometric series well-posed in $SU(n)$.⁶

7. Generalized spectral resolution (in the sense of distributions) has been studied for the linear transport operator; with the help of more refined estimates on the resolvent, we proved the existence of such a distributional spectral resolution (continuous spectrum plus point spectrum in a bounded geometry). This is a first step in devising methods for the problem of spectral concentration for general non-self-adjoint operators of statistical mechanics.

8. We considered the bifurcation of solutions from a point in the essential ("continuous") spectrum, for an abstract class of nonlinear operators; the latter is a canonical form for many operators of nonequilibrium statistical mechanics, with one-dimensional space evolution. We found that the corresponding nontrivial bifurcated solution can be interpreted as a continuous, steady profile, traveling shock wave.^{13,14} Implications for collision-dominated plasmas

are important. Mathematical peculiarities include a sequence of embedded bifurcation problems and analysis of a global functional-differential operator.

C. Economics and Energy Resources Modeling

1. Economic-ecologic input-output models analyze the flow of goods within the economic sector and the flows to and from the ecologic sector of a region. We have completed a new discussion of the static Leontief matrix economic model and its relation with Victor's model. We have shown that ecologic residual can be treated as economic by-products. A constant interaction has been maintained with the Q (energy) Division.

2. Practical application of a simplified Victor's economic-ecologic input-output matrix has been made to the San Juan Basin.

3. Concerning error estimates for Leontief input-output matrices, we have given error estimates for the inverse of such a matrix, whose entries are subject to statistical errors.

4. The influence of price indexation on the stability of multiple market equilibrium is an open problem. An extensive review of this problem has been carried out; widely diverse views are held regarding the net consequences of indexing schemes, and a minimum of analysis has been previously performed. Our first results show that indexing a subgroup of prices in an initially globally stable economic system may destabilize the latter.

D. Discrete Mathematics

1. "Knapsack problem": this is the problem of finding accurate approximations to the number of integral solutions to a specific inequality which occurs in many contexts, including that of laser energy levels.

2. Random trees: in biology, one is interested in estimating the number of free sites on molecules which are conceived as being the result of random combinations of smaller molecules. We have

investigated a model for this process, namely the random "growth" of combinatorial trees with restricted degrees.

3. Partially ordered sets: given a labeled partially ordered set on n elements, it is of interest to know how many of the $n!$ permutations are consistent with the order relations of the latter set. For a special class of such "posets," we developed an efficient algorithm for evaluating this number.

4. Number theory: we have considered various problems in periodic continued fraction expansions; and on large binary words made of k -tuples of some prime numbers.

5. "The Constants of Mathematics": this is the first draft of a volume for the "Encyclopedia of Applicable Mathematics" (general editor: Prof. Gian-Carlo Rota). Contents: binomial coefficients; Stirling Bernoulli, Euler, Gnocchi, and other numbers; partitions and partitions-indexed sequences; primes and other number theoretic sequences; graphical and logical sequences.¹⁸

6. Mathematical biology: a new metric for biological sequences has been introduced and analyzed.¹ Typical biological sequences are amino-acid sequences (proteins) or nucleotide sequences (nucleic acids).

7. Mathematical biology -- additive evolutionary trees: development and application of the mathematics of metric graph theory to the study of protein molecules has been completed.

III. T-7 PUBLICATIONS

1. W. A. Beyer and C. DeLisi, "The Asymptotic Form of Partition Functions of Linear Chain Molecules: An Application of Renewal Theory," to be published in J. Math. Anal. Appl.
2. W. A. Beyer, J. Mycielski, and G.-C. Rota, editors, Sets, Numbers, and Universes, Selected Works of S. M. Ulam (MIT Press, Cambridge, Mass., 1974).
3. J. E. Dendy and G. Fairweather, "Alternating-direction Galerkin Methods for Parabolic and Hyperbolic Problems on Rectangular Polygons," SIAM J. Numer. Anal. 12, 144-163 (1974).
4. J. E. Dendy, "An Analysis of Some Galerkin Schemes for the Solution of Nonlinear Time-dependent Problems," to be published in SIAM J. Numer. Anal.

5. M. Klein and B. Brixner, "Climb: A New LASL Lens Design Code," to be published in International Lens Design Conf. Proc., Applied Optics or J.O.S.A.
6. J. D. Louck, W. J. Holman, and L. C. Biedenharn, "On Hypergeometric Series Well-Posed in $SU(n)$," to be published in SIAM J. Math. Anal.
7. J. D. Louck and H. W. Galbraith, "Eckart Vectors, Eckart Frames, and Polyatomic Molecules," to be published in Rev. Modern Phys.
8. J. D. Louck, M. Lohe, and L. C. Biedenharn, "Structural Properties of the Canonical $U(3)$ Racah Functions and the $U(3):U(2)$ Projective Functions," to be published in J. Math. Phys.
9. J. D. Louck, L. C. Biedenharn, and M. Lohe, "The Canonical Resolution of the Multiplicity Problem for $U(3)$," to be published in Proc. of the Conf. on Group Theoretical Methods in Physics, University of Nijmegen (1975).
10. N. Metropolis and G.-C. Rota, "Significance Arithmetic: On the Algebra of Binary Strings," in Studies in Numerical Analysis-Papers, presented to Cornelius Lanczos, B.K.P. Scaife, editor (Academic Press, London, 1974).
11. N. Metropolis, F. Faltin, B. Ross, and G.-C. Rota, "The Real Numbers as a Wreath Product," Advances in Mathematics 16, 278-304 (1975).
12. C. J. Everett and N. Metropolis, "On the Roots of $x^m \pm 1$ in the p -adic Field O_p ," accepted by Notices of the American Mathematical Society.
13. B. Nicolaenko and J. K. Thurber, "Weak Shock and Bifurcating Solutions of the Nonlinear Boltzmann Equation," J. de Mecanique 14, no. 2, 1-34 (1975).
14. B. Nicolaenko, "Shock Wave Solutions of Kinetic Equations as a Nonlinear Bifurcation Problem from a Point in a Continuous Spectrum," to be published in Proc. Conf. on Classical and Relativistic Kinetic Theories, C.N.R.S., Paris (1975).
15. S. V. Parter, "Solutions of a Differential Equation Arising in Chemical Reactor Processes," SIAM J. Appl. Math. 26, 687-716 (1974).
16. R. D. Richtmyer, "Continued Fraction Expansion of Algebraic Numbers," Advances in Mathematics 16 (197).
17. R. D. Richtmyer and S. A. Orszag, "Lectures on Hydrodynamical Stability Theory," Los Alamos Scientific Laboratory report (to be published).
18. P. R. Stein, The Constants of Mathematics, a volume in the Encyclopedia of Applicable Mathematics, G.-C. Rota, editor, to be published.
19. B. R. Suydam, "Self-Focusing of Very Powerful Laser Beams II," I.E.E.E. J. Quantum Electronics QE-10, No. 11, 837-843 (1974).

20. B. R. Suydam, "Effect of Refractive Index Nonlinearity on the Optical Quality of High-Power Laser Beams," I.E.E.E. J. Quantum Electronics QE-11, No. 6, 225-230 (1975).
21. B. R. Suydam and James C. Elliott, "Self-Focusing Phenomena in Air-Glass Laser Structures," to be published in I.E.E.E. J. Quantum Electronics.
22. B. Swartz and B. Wendroff, "The Relative Efficiency of Finite Difference and Finite Element Methods. I: Hyperbolic Problems and Splines," SIAM J. Numer. Anal. 11, 979-993 (1974).
23. B. Swartz and B. Wendroff, "The Relation Between the Galerkin and Collocation Methods Using Smooth Splines," SIAM J. Numer. Anal. 11, 994-996 (1974).
24. B. Swartz, "The Construction and Comparison of Finite Difference Analogs of Some Finite Element Schemes," in Mathematical Aspects of Finite Elements in Partial Differential Equations, C. deBoor, editor, (Academic Press, New York, 1974) pp. 279-312.
25. B. Swartz, "Comparing Certain Classes of Difference and Finite Element Methods for a Hyperbolic Problem," in Advances in Computer Methods for Partial Differential Equations, R. Vichnevetsky, editor, Proc. AICA Symp. (June 1975) pp. 17-19.
26. B. Wendroff and V. Thomée, "Convergence Estimates for Galerkin Methods for Variable Coefficient Initial Value Problems," SIAM J. Numer. Anal. 11, 1059-1068 (1974).

IV. T-7 OUTSIDE TALKS AND SEMINARS

1. M. Klein and B. Brixner, "Climb: A New LASL Lens Design Code," invited paper at the International Lens Design Conference, Haverford, PA (June 1975).
2. J. D. Louck, "The Canonical Resolution of the Multiplicity Problem for $U(3)$," invited paper (with L. C. Biedenharn and M. Lohe) presented by J. D. Louck at the Conference on Group Theoretical Methods in Physics, U. of Nijmegen (June 1975).
3. B. Nicolaenko, "Bifurcation Problems for Nonlinear Boltzmann Operators," a series of invited lectures at the Université Pierre et Marie Curie (ex-Paris-VI), Paris, France (April-May 1975).
4. B. Nicolaenko, "A Class of Abstract Nonlinear Bifurcation Problems from a Point in the Essential Spectrum," invited seminar talks at the University Pierre et Marie Curie (ex-Paris-VI) (May 1975); University Paris-XI, Orsay, France (May 1975); University Lyon-I (June 1975); Ecole Polytechnique, Paris, France (June 1975).
5. B. Nicolaenko, "A General Class of Nonlinear Bifurcation Problems from a Point in the Continuous Spectrum: Application to Shock Waves," invited seminar at the U. of Utah (January 1975).

6. P. R. Stein, "Plane Trees, Molecules, and Generalized Catalan Numbers," invited seminar at the U. of Strasbourg, France (February 1975).
7. B. Swartz, "Comparing Certain Classes of Difference and Finite Element Methods for a Hyperbolic Problem," invited paper presented at an AICA Symp. on Advances in Computer Methods in Partial Differential Equations (June 1975).
8. B. Swartz, "The Relative Efficiency of Some Finite Element and Finite Difference Methods for the Heat Equation," invited seminar at Stanford U (May 1975).
9. B. Swartz, "Comparing the Efficiency of Certain Difference Schemes for the Heat Equation," invited seminar at the U. S. Naval Ordnance Laboratory, White Oak, MD (June 1975).
10. B. Wendroff, "Numerical Methods for Conservation Laws," invited talk at the annual meeting of the American Mathematical Society, Washington, DC (January 1975).
11. G. M. Wing, "Thoughts -- Some Old and Some New -- on the W.K.B. Approximation for Wave Propagation," invited seminar at Texas Tech. U., Lubbock, TX (December 1974).

GROUP T-8 - ELEMENTARY PARTICLES AND FIELD THEORY

G. B. West, Group Leader

I. INTRODUCTION

The search for elementary building blocks, the prime focus of elementary particle physics, dates back to ancient Greece and to Democritus who introduced the concept of an indivisible entity or atom. During the last hundred years, knowledge of the atom became increasingly more sophisticated, but elementarity itself remained a surprisingly elusive concept. From Rutherford's classic scattering experiments, the prototype for present accelerator experiments, we learned of the existence of the atomic nucleus -- a dense ball of positive matter only 10^{-13} cm in extent. As accelerator energies increased and incident particles probed deeper into nuclear matter, we found that not only does the nucleus have structure but so too do its constituents. In the 1950's and 1960's, the neutron and proton were joined by a hundred or more so-called "elementary" particles and the concept of elementarity, of a unity in nature, seemed less and less plausible.

Inevitably it was suggested that these particles were not the elementary building blocks but were simply manifestations of even more elementary objects called, by Gell-Mann, quarks. A remarkably simple hypothesis -- the existence of three such quarks endowed with specific quantum numbers (spin, isospin, and strangeness) was sufficient to predict the spectroscopy of the observed families of strongly interacting particles or hadrons. In the last few years, new experimental results (e.g., the discovery at SLAC of very narrow resonances, the ψ 's) have led to an enlarged version of the quark model, but still this framework seems to explain, at least qualitatively, the entire phenomenology of hadronic particles. Perhaps quarks are, in fact, the fundamental elements of nature. (See Fig. 25.)

Fig. 25. A drawing of a bubble chamber photograph taken at Brookhaven National Laboratory by N. Samios et al. Their analysis suggests that this may be the first observed event for neutrino production of a charmed hadron. Charm is a new quantum number which has been postulated for weak interactions of quarks. The BNL broad-band neutrino beam entered from the left of the picture and struck a nucleus at the observed vertex. Track 1 and 4 are consistent with being formed by either a π^- or μ^- . Track 2 is a π^+ that decays to a μ^+ . Track 3 is consistent with either π^+ or μ^+ . Track 5 is identified as π^+ by its elastic scattering off of a proton. Tracks 6 and 7 are a proton and a π^- which come from the characteristic V-vertex of a Λ (strangeness $S=1$). Detailed analysis strongly suggests that none of the tracks could be a misidentified kaon. Thus, either the $\Delta S = \Delta Q$ rule is violated, or a charmed baryon of mass $2.43 \pm .01$ GeV was created by the weak interaction which subsequently decayed into Λ and pions (and/or a muon). Theoretical studies have suggested that such decay modes involving $S \neq 0$ final states should be dominant for charmed hadrons.

A very crucial problem, however, remains mysterious in this model -- the empirical absence of quarks. Clearly this is a classical paradox analogous to the old Bohr atom where the quantization condition predicted the observed atomic spectroscopy but failed to explain why electrons in atoms resist radiation damping. An answer to the quark paradox may be found within conventional quantum field theory, the present conceptual framework of particle physics. On the other hand, a resolution may entail a profound change in our physical understanding just as the solution of the Bohr atom paradox introduced the uncertainty principle and the theory of quantum mechanics. In any case the field of elementary particle physics is at a critical and exciting stage.

It should be emphasized that the theoretical foundations of particle physics are still rather shaky and investigators are now seeking answers to a diverse set of fundamental questions. What is the algebraic structure of the fundamental quantum field theory? What are the appropriate techniques for calculating dynamical predictions from the field equations? Do the field equations predict the observed particles as bound states of the quarks? Can the strong, weak, and electromagnetic interactions be unified in a model consistent with empirical observations? What is the relationship of successful phenomenological models to fundamental theory? Recent progress in these areas has been tremendously stimulated by new experimental discoveries such as the ψ 's. Indeed all theoretical speculations have been strongly tied to and guided by the hundreds of experiments performed at various accelerators around the world. In this one aspect our present speculations concerning elementarity differ quite crucially from our spiritual forefathers, the ancient Greeks, who spurned direct confrontation with experiment.

It is within this context that the Group T-8 (Elementary Particles and Field Theory) was formed in the Theoretical Division at the LASL. Of course in the early days of the Laboratory, there was a very active interest in this area, but more recent theoretical

research has centered mostly on nuclear physics. A renewed interest in "elementary" particle physics developed with the advent of LAMPF and now work in this area includes considerable interaction of T-8 with members of MP Division, T-5 (Medium Energy Physics), T-9 (Nuclear Theory), and the T-Division Office.

Although the Group is still rather small and has only been in existence for little over a year, we have gained a national reputation. Our main areas of interest have been the analytical and algebraic structure of wave equations and field theory, their possible solutions, multiparticle production in hadronic collisions, the nature of the newly discovered particles, and interpretations of deep inelastic experiments in terms of the quark model. Before presenting any details of this work, it might be useful to explain and summarize some of the accomplishments.

We have been examining the consistency of high-spin wave equations and interacting field theories. Until now, such formulations for particles with spin greater than 1 have led to fundamental inconsistencies such as the violation of causality. We have shown that this disease can be cured for the spin $\frac{3}{2}$ case, and have applied some of these ideas of high-spin wave equations to explain the relative decay widths of the vector mesons (ρ , ω , ϕ , and the new ψ 's) into electron-positron pairs.

In other work on the structure of field theory, we have been trying to determine whether the complete physical content of a theory can be derived purely from currents (i.e., from dynamical observables rather than quantum fields) which carry the relevant quantum numbers (such as charge, strangeness, etc.) and which obey commutation relations required by the algebraic group structure of the theory. We have formulated nonrelativistic field theory in the language of currents and have devised approximation schemes for their solutions.

Along somewhat related lines, we have been investigating the possibility that the algebra of octonions may explain the new quantum number, color, recently introduced ad hoc into the conventional quark model. This new algebra may give rise to a master group of all the fundamental particles including the leptons (i.e., electrons, neutrinos, etc., which do not partake in the strong interactions), the conventional hadrons, and the newly discovered particles (the " ψ 's").

It has been suggested that the ψ 's are bound states of a new quark which carries a new quantum number (called "charm") and that these "charmed" quarks give rise to a new spectroscopy. Are the ψ 's really hadrons and are they, in fact, bound states of quarks? By examining the production of ψ 's in scattering experiments, we have been trying to devise a conclusive test for these speculations.

We have also been examining realistic nonrelativistic analogs of the quark model for deep inelastic electron scattering, a model which has led to a deeper understanding of the observed scaling phenomena. Perhaps even more interesting is our result that elementary particle techniques when applied to nuclear and liquid physics yield new scaling laws that are beautifully confirmed by existing data.

The possibility that conventional field theory holds the key to quark confinement has spurred a flurry of interest in many-body solutions to the field equations. We have been examining particular solutions, the so-called abnormal states, and their implications for ultra-dense matter as might exist in neutron stars.

Perhaps the most active area of interest within the group has been multiparticle production in high energy collisions. In most ultra-high-energy experiments, a large number of hadrons are produced (high multiplicity) and they seem to cluster together in phase space. A description in terms of the fundamental fields (the quarks) may be not only exceedingly difficult, but not very useful in the

same sense that describing the flow of a river in terms of the properties of the hydrogen and oxygen atoms is not very useful. Instead, a large effort has been made to explain these phenomena in terms of hydrodynamic and thermodynamic analogs. We have shown how to cast field theory into equations reminiscent of traditional transport theory and also demonstrated that such equations often exhibit collective mode-like solutions (plasmons), a possible origin for the clustering effects that have been observed in experiments. In a phenomenological approach, we have been analyzing the experimental data, and have shown that clusters of particles really are there. By examining explicit properties of the solutions to the transport equations, we have shown that pion production by a simple source provides a field theoretic realization of Landau's original model and that these kinds of theories are consistent in the sense that they are renormalizable (i.e., yield finite answers).

A popular view of large transverse momentum particle production experiments has been the quark parton model. We have studied an alternative description in which single clusters of particles are produced and then decay. In general, our results indicate that this is a satisfactory alternative interpretation. Such models are clearly important in judging the unique successes of the quark picture.

This then completes the review of the main interests of the Group; further details are contained in Sec. II. There are a number of other interests in T-8 including the theory of liquids and astrophysics.

One important aspect of our involvement is the rather strong interaction we have with other laboratories and with the academic community. Indeed this is reflected in our very active visitors program which has enabled some of the most prominent physicists in the field to join us for extended periods of time (e.g., M. Gell-Mann and F. Zachariasen from Cal. Tech., R. Dashen from Princeton, and L. van Hove from CERN, among others). In addition to their

work with T-8, several of these visitors have made significant contributions to other Laboratory groups; for example, S. Meshkov of N.B.S. made an in-depth review of the LAMPF program in weak interactions and F. Low of MIT had extensive discussions with members of CTR.

In like manner, members of T-8 have been invited to consult and to speak at other institutions and have interacted strongly with other groups in the Laboratory. Indeed one member of T-8 has a joint appointment with T-1 and is working on fast breeder reactor safety. Also we have performed calculations for a P-Division group working at LAMPF on pion production in proton-proton collisions; we have discussed with the LAMPF personnel the analysis of data from pion-nuclear elastic scattering experiments, and have stressed the importance of looking for rare pion decays at LAMPF. Perhaps one of the most ambitious projects of this nature is the Advanced Research Committee, a division-wide committee run by a member of T-8. This committee reviews various LASL programs with the idea of informing the Division of their status, of stimulating new fields of potential interest to the LASL, and of galvanizing the breadth and depth of experience in T Division to keep the Laboratory at the forefront of research and development.

II. RESEARCH HIGHLIGHTS

A. Bhabha High Spin First-Order Wave Equations

Stable high spin particles exist in nature (in particular, the spin $3/2$ Ω^- is stable under the strong and electromagnetic interactions, only being unstable under the weak interaction), yet no relativistic field equation has been found which even in principle could describe them.

The historical origins of this problem trace back the work of Dirac, Fierz, and Pauli in the 1930's. Already then there were indications that a consistent theory for particles with spin greater than 1 (in units of $\hbar$) might not be possible. The work of Johnson and Sudarshan in 1961 showed just how deep this problem is by demonstrating that even for the case of spin 3/2 (in the Rarita-Schwinger formalism), simply introducing ordinary minimal coupling to the electromagnetic field of necessity introduces noncausal propagation.

In order to understand, by example, just how far a high-spin field theory can be pushed before possible diseases occur, we have undertaken a major investigation into the properties of the Bhabha first-order wave equations for arbitrary spin.¹¹⁻¹⁴ The Bhabha system was chosen for study by us for two reasons. The first is that it is a first-order wave equation, which yields a more direct quantum mechanical interpretation than second-order equations. In particular, it covers in the same first-order formalism both half-integer-spin particles and integer-spin particles. In fact, the slight differences in the handling of these two types of particles showed how indefinite metrics and built-in subsidiary components for integer spin are related and should be handled. Because of these and related properties, the Bhabha system has afforded much insight into the general problems of high-spin systems: causality, the number of independent components of the fields, multimass and multispin fields, indefinite metrics and their possible interpretation.

It turns out that the Bhabha system is very well behaved. We have obtained the P, C, and T transformation properties, the mass and spin composition of the fields, and the Poincaré generators. In all these results, it has been found that the integer-spin case follows analogously to the half-integer-spin case once proper care

has been taken of the built-in subsidiary components (Sakata-Taketani transformations). We have just finished demonstrating causality with minimal electromagnetic coupling in both the c- and q-number theories. Also, the connection of the indefinite metric and the generalized Foldy-Wouthuysen transformation will soon be discussed. Many of these well-behaved properties trace their origins to the fact that the Bhabha system treats in a special combination multimass and multispin fields. This perhaps indicates that proper high-spin fields should be multimass and multispin multiplets, as internal symmetry advocates would have. Further, the main problem that remains, the indefinite metric, is also tantalizing in interpretation. An indefinite metric by its nature is a slight modification of orthodox quantum mechanics. That too is suggested by recent discussions of the exceptional groups for the internal symmetry of particles.

A second reason for looking at this system is that the simplest special cases of the Bhabha system of equations are the Dirac equation for spin-1/2 and the Duffin-Kemmer-Petiau (DKP) equation for spin-0 and spin-1. We have, with coworkers, proposed the DKP formalism as being a better (in the sense of agreement with experiment) description of mesons in symmetry breaking situations. The latest work in this direction, with B. G. Kenny and D. C. Peasless of the Australian National University, has been to argue that by using a modified Han-Nambu model, the ratios of the decay widths $\pi(V \rightarrow e^+ e^-)$, where $V = (\rho, \omega, \phi, \psi, \psi')$, can be explained if the vector mesons obey the DKP instead of the standard Proca formalism.

B. Algebraic Structure in Particle Physics

We have been investigating the possibility that octonions may be useful in understanding the algebraic structure underlying the internal symmetries of the hadron spectrum. (The octonions form an 8-dimensional algebra which generalizes the complex numbers.) Two directions of research are being followed. In the first, unified theories of quarks and leptons have provided the primary focus for

speculations. The automorphism groups of the octonions and of the 3 by 3 matrices of octonions are the exceptional Lie groups, which naturally incorporate "color," in a way suggested by F. Gursey. (Color is a new quantum number postulated for quarks dynamics.) These groups can then be investigated in the context of unified gauge theories. One stumbling block has been that these theories all predict that baryons can decay into leptons.

A second way that octonions may be relevant was already suggested by P. Jordan in 1932. He pointed out that the algebra of density matrices in quantum mechanics could be generalized to that of hermitian matrices defined over the octonions. Originally this line of research was dropped because only the 3 by 3 matrices provided a consistent generalization. However, the internal symmetry structure of particle physics is finite, and so we may speculate that these "exceptional observables" may be relevant. So far our main results have been more mathematical, but they may be useful in finding significant physical identifications.

C. Abnormal States in Nuclear Matter and Field Theory

Until recently the related problems of predicting bound states in relativistic quantum field theories and of constructing a "first-principles" theory of nuclear matter have remained beyond the range of available calculational techniques. In the past two years, however, several studies applying a variety of new semi-classical and variational methods have produced substantial insight into these problems. Without doubt the most exciting result of these studies is the possible existence of quantum bound states strikingly different in their qualitative properties from normal nuclear matter or from the fundamental field oscillations calculable by perturbation theory. Such states, we call, for want of a better word, "abnormal."

In field theories of elementary particles, the abnormal states

are rough analogs of the "soliton" solutions to nonlinear wave equations and are thus conceptually related to such diverse topics as self-induced transparency in lasers, wave propagation in shallow water, and the Fermi-Pasta-Ulam problem in statistical mechanics! In nuclear matter theories, two distinct abnormal states have been suggested:

1. Deeply-bound, "super-heavy" nuclei with equal numbers of neutrons and protons; and
2. "pion-condensed" nuclear matter, in which, crudely speaking, a macroscopic density of pions coexists with neutrons and protons.

We investigated several aspects of these "abnormal" states and, in particular, studied the possibility that very high density, neutron-rich matter -- as might be found, for example, in a neutron star -- exists in a "pion-condensed" state. At high density this state might be energetically favored over normal matter since the "reaction" which creates pions in the medium, $n \rightarrow p + \pi^-$, substantially reduces the Fermi energy in the neutrons.

Since $\langle \pi^\pm \rangle \neq 0$ in "pion-condensed" matter, such matter would have rather remarkable microscopic properties -- parity and charge conservation would be "spontaneously broken" and the matter would be superconducting. Its macroscopic properties could be similarly interesting. We considered three different aspects of the proposed "pion-condensed" states:

1. the general theoretical framework in which to analyze the properties of abnormal matter;
2. the detailed phenomenology necessary to decide whether such abnormal states can actually exist; and
3. the experimental detectability and observational consequences of such states.

We made substantial progress on the first two problems. After illustrating the occurrence of pion condensation in a simple model relativistic field theory,³ we established that the possible

existence of this abnormal state is in fact a consequence of a model-independent symmetry [chiral $SU(2) \times SU(2)$] which is quite accurately exhibited by low-energy elementary particle systems.^{1,2} To understand more thoroughly the phenomenology of this state, we studied the experimental details of low-energy pion-nucleon interactions. In this endeavor we held mutually beneficial discussions with the LAMPF personnel conducting low-energy pion-nucleon scattering experiments (Experiment No. 96). Our analysis revealed a potentially important omission in previous treatments of pion condensation. We are currently preparing an article discussing the implications of these findings. Further, we initiated a series of calculations on the observable astrophysical implication of the existence of a neutron star in the pion-condensed state.

As an integral part of this research effort we were involved in numerous discussions with other theoretical groups working on similar topics. To further these discussions, we organized a "Workshop on Abnormal States in Nuclear Matter," which was held at the LASL on January 13 and 14, 1975, and attended by physicists from Columbia, Illinois, the Institute for Advanced Study, LASL, MIT, Stanford, and SUNY at Stony Brook.

D. Local Currents as a Field Theory

The theory of local currents provides a concentrated focus for particle physics in all its aspects from phenomenology to constructive field theory. For example, recent electromagnetic experiments at SLAC and neutrino experiments at NAL can be interpreted as direct measurements of the matrix elements of local currents and products of local currents between special states. Moreover, local currents are accepted as the basic concept for a quantitative description of strong, weak, and electromagnetic interactions, and recently a link between weak and electromagnetic interactions via a neutral current has been proposed by Weinberg.

The work in current algebra embodies a class of attempts to understand the mathematical structure of theories of local currents. The idea here is to use the local currents as dynamical variables and to construct complete theories by writing the Hamiltonian as a function of the currents. The Hamiltonian is expected to become mathematically well defined when an appropriate representation of the equal-time algebra is employed. Since the successful completion of such a program for a nontrivial Hamiltonian would amount to a consistent and precise description of a relativistic dynamics of interacting particles, it is perhaps not surprising that only incomplete results are available in the relativistic case.

We have worked on formulating complete quantum theories in terms of local currents in the nonrelativistic case, with notable success for (1) the many body problem in the thermodynamic limit and (2) nonrelativistic quantum mechanics where the electromagnetic field is present.

1. Nonrelativistic many-body theory

For nonrelativistic many-body theory in the thermodynamic limit, the local currents consist of the particle number density and the flux density of particles.

This problem is of interest for several reasons. It is an example of a system with an infinite number of degrees of freedom and has many similarities with relativistic quantum field theory. This suggests that the techniques developed for dealing with the non-relativistic many-body problem can be generalized to treat the relativistic quantum fields.

Moreover our approach is a reformulation of many-body quantum mechanics in terms of physical observables (the local currents). This can lead to new insight for physical systems such as a quantum gas or fluid.

The Hamiltonian for an interacting system has been expressed in terms of the currents. The representation of the local currents is determined by a generating functional. We have derived two coupled functional equations for determining the generating functional appropriate for a given interaction in order that the Hamiltonian be a well-defined operator.¹⁸ In addition, each functional equation was expressed as a set of coupled integral equations for the correlation functions.

These equations form an infinite hierarchy in which one correlation function depends on the higher ones. This leads to the closure problem of finding a method of truncating the equations in order to deal with them more readily. We have developed an approximation scheme for handling this problem.¹⁹ It is based on restricting our attention to a finite volume and introducing the mathematical concept of an approximating sequence of representations. In a finite volume, the number of degrees of freedom can be truncated in a physically meaningful manner. The scheme is a generalization of a Jastrow-type approximation which has been used by other physicists to study liquid helium. The framework we developed is helpful in understanding the physical nature of the approximation involved and its range of validity.

2. Local currents and the electromagnetic field

Recently, we have begun to study how one might extend our previous results on formulating nonrelativistic quantum mechanics in terms of local currents so as to include the electromagnetic field. We have found that the charge density, the momentum density, and the components of the electromagnetic field form a closed Lie algebra, and that the Hamiltonian can be written in terms of these operators. The result is a manifestly gauge invariant and path independent formulation of quantum electrodynamics. Among the questions we plan to study are:

1. the way in which the gauge invariance of the underlying canonical theory is expressed in this formulation;

2. whether an indefinite metric is required; and
3. how these results can be generalized to include magnetic monopoles.

E. Quantum Electrodynamics

Despite the unparalleled success of quantum electrodynamics as a predictive algorithm, several fundamental questions about the structure of the theory remain unresolved. For example, do the problems of runaway solutions and preacceleration which afflict the classical theory of radiation reaction appear in quantum electrodynamics as well?

Such questions of consistency were of central importance in the discussions at the 1948 Solvay Conference, however, the very success of the renormalized perturbation theory methods then being developed by Feynman, Schwinger, and Tomonaga diverted attention from these points.

We have recently looked at these longstanding problems and developed an approach to the related questions of electrostatic self-mass, runaway solutions, and preacceleration. The approach is based on the Heisenberg equation of motion derived from the Hamiltonian describing a nonrelativistic electron coupled to the quantized electromagnetic field. Although this model does not display the full complexity of relativistic quantum electrodynamics, its classical counterpart is already beset by the problems of internal consistency which we set out to resolve. Specifically, in the classical Lorentz-Dirac theory of radiation reaction, a nonrelativistic point electron interacting with its self-field and subject to an external force $\vec{F}(t)$ obeys the equation of motion

$$m_0 \ddot{\vec{R}}(t) = \vec{F}(t) = \delta m \ddot{\vec{R}}(t) + \frac{2e^2}{3c} \dddot{\vec{R}}(t), \quad (1)$$

where δm is the (divergent) electrostatic self-mass of the electron.

This theory of radiation reaction suffers from a number of defects besides the fact that $\delta m = \infty$. First, Eq. (1) admits runaway solutions, i.e., solutions for which the acceleration of a particle increases exponentially even in the absence of external forces; second the solutions violate causality, i.e., the particle accelerates before a force acts.

These difficulties can be seen explicitly in the general solution to Eq. (1), which is

$$\ddot{\vec{R}}(t) = e^{t/\tau} \left[\ddot{\vec{R}}(0) - (1/m\tau) \int_0^t e^{-t'/\tau} \vec{F}(t') dt' \right], \quad (2)$$

with $\tau = 2e^2/3mc^3$.

The runaway behavior can be suppressed with the choice

$$\ddot{\vec{R}}(0) = (1/m\tau) \int_0^\infty dt' e^{-t'/\tau} \vec{F}(t') \quad (3)$$

in which case Eq. (2) reduces to

$$\ddot{\vec{R}}(t) = \frac{1}{m} \int_0^\infty ds e^{-s} \vec{F}(t + s\tau). \quad (4)$$

The acausal nature of this solution is obvious, since the particle samples the force for a time τ into the future. However, Eq. (4) correctly describes classical radiation damping insofar as it has been tested. Consequently the view is generally adopted that, since preacceleration occurs over such a short time scale ($\tau \sim 10^{-23}$ s for an electron), the acausal effects belong in the domain of quantum theory, which is where one has to look for a resolution of the problem.

In our work²¹ we have started from the operator form of Maxwell's equations and the Lorentz force equation which follows from the standard Hamiltonian governing the interaction of a nonrelativistic electron with a quantized electromagnetic field. We derived a quantum

mechanical operator equation of motion for a point electron which reduces to Eq. (1) in the correspondence limit (i.e., $\hbar \rightarrow 0$) and showed that (i) the electrostatic self-mass of a point electron is zero in quantum mechanics; (ii) the equation of motion does not admit runaway solutions; (iii) the correspondence limit of the solution of the quantum mechanical equation likewise does not display runaways; and (iv) the solutions do not display acausality. These calculations thus show how nonrelativistic quantum electrodynamics manages to suppress the runaways, conforming to requirements which presumably follow from the general principles of quantum mechanics, and in addition possesses a physically reasonable correspondence limit.

In future work, we plan to investigate how, if at all, these results are modified when the electron is treated relativistically, and how these results can be understood using standard perturbation theory methods.

F. Scaling in Nonrelativistic Systems (Nuclei and Liquids) and the Approach to Scaling

Although the quark model was originally motivated by the spectroscopy of the observed hadrons, it was given a boost in the late 1960's by the so-called deep inelastic electron scattering experiments performed at SLAC. In these experiments (the spiritual descendants of Rutherford's), highly energetic electrons (~ 10 GeV) were scattered at large momentum transfers from nucleons. The pattern of scattered electrons showed some remarkable characteristics: (a) those elastically scattered (i.e., where the nucleon remains intact) behaved like the alpha particles in Rutherford's experiment, thus confirming the nonelementarity of the nucleon. This is usually expressed by saying that the elastic form factor of the nucleon, $G(q^2)$, falls rapidly with increasing q^2 [an elementary particle would have $G(q^2) = 1$ for all values of q^2]. (b) The inelastic scattering on the other hand behaved as if the electrons were being

scattered by point scattering centers. It was only natural to associate these constituents with the quarks of Gell-Mann. Subsequent experiments at CERN and NAL with neutrino beams have brilliantly confirmed this hypothesis. Technically this phenomenon is referred to as Bjorken scaling since elementarity shows itself here as a scaling phenomenon. The analog of the dimensionless form factor for inelastic scattering, F , depends here on two variables q^2 and ν , the electron energy loss. (Note that in elastic scattering $\nu = q^2/2M$, M being the nuclear mass. So what was a two-variable problem reduces to one-variable only; thus G depends only on q^2 .) Experimentally, it was found that $F(q^2, \nu)$ depends only on the one-dimensional variable $x \equiv q^2/2M\nu$; this is Bjorken scaling. Physically this can be understood on dimensional grounds by noting that structureless quarks have no spatial extent and thus cannot introduce a dimensional parameter into the problem.

We have been examining nonrelativistic systems to see whether similar effects occur there, even though the energies are much smaller than the target masses, M_T .²⁶ Indeed one can prove analogous scaling laws for these systems which appear to be satisfied empirically. The most useful scaling law is in terms of the variable $y \equiv (2M - q^2)/2Mq$ from which one can abstract useful information concerning the target wave function. In electron scattering from nuclei, such scaling laws appear to be reasonably well behaved although the interpretation is somewhat clouded by rather sparse data and by the structure of the nucleons themselves. Perhaps more striking is the case of thermal neutron scattering from liquid helium at $\sim 10^6$ K which exhibits almost perfect scaling. The nonrelativistic theory also allows one to estimate the rapidity of the approach to scaling, i.e., how big does q^2 have to be for scaling to occur. This is generally governed by the correlation function which, for a many body system such as liquid helium, is oscillatory. Experiments do indeed exhibit an oscillatory approach to scaling. When one applies such a model to the nucleon system, one expects the approach to scaling to be smooth since the quark correlation function should behave

rather similarly to the elastic form factor $G(q^2)$ which itself is smooth. Surprisingly, experiment seems to bear this out even in its quantitative aspects, showing that the nucleon behaves as if it were a bag of quarks even in its approach to scaling.

We have also examined the approach to scaling in more general models based, for instance, on analogs to finite energy sum rules and have shown under rather general circumstances how the behavior of the elastic form factor together with gauge invariance in large part determine the approach to scaling.

G. Models for the Photoproduction of the ψ 's

Not long after the discovery of the new ψ particles at SLAC, groups at SLAC, NAL, and Cornell showed that they could be photoproduced in the same way that the conventional vector mesons (ρ , ω , ϕ) can. From such experiments it is possible to estimate both the total cross section and the ratio of elastic to inelastic scattering in ψN scattering; these turned out to be ~ 1 mb and $\sim 1\%$, respectively, both numbers being unusually small for interpreting ψ as a hadron. We have investigated, together with Dennis Sivers and John Townsend of SLAC, various models for the extraction of these numbers from the data. These models were either of the quark - antiquark bound state or multiperipheral type. In all cases we found that the kinds of extrapolations naively assumed in estimating these numbers were most likely incorrect and that, in general, dynamical corrections tended to increase these numbers to be of a more hadronic nature. Several experimental tests of our ideas were suggested and in particular the use of nuclear targets was emphasized.²⁸ A model independent lower bound of ~ 300 μ b for the photoproduction cross section of new states (possibly charmed) was derived using an inequality based on unitarity and Zweig's rule.

H. Theories of Multiparticle Production

The recent opening of large accelerators with proton beams having momentum in excess of 100 GeV/c has given rise to a new type of phenomena in elementary particle physics, namely, the production of a large and varying number of particles (mainly pi-mesons) from a single high-energy collision.

At lower energies, particle collisions are known to produce a small number n of specific final products. In these processes, called exclusive reactions, one measures the momenta of all the final particles. The $n+2$ particle Green's function of the field theory describes this process.

At very high energies where 20 or more particles may be produced in one reaction, it is no longer feasible to measure the momentum distribution of all the final products. Instead, one measures the so-called inclusive reactions, e.g., one considers the reaction $p + p \rightarrow \pi + \text{anything}$ and measures only the single particle momentum distribution. Standard quantum field-theoretic tools have not proven useful in describing these data. Because of the complexity of these processes, many investigators have introduced statistical and hydrodynamical models to describe multiparticle production. In the hydrodynamical model, one assumes that a high-energy collision deposits a large amount of energy into the pion field; the energy is localized in a small region of space-time. The subsequent history of the energy density is treated hydrodynamically and from this one determines the distribution of produced pions. These techniques have had considerable success in fitting single particle spectra at low transverse momentum. However, there is an overabundance of large transverse momentum events as compared with the prediction of this model. Moreover the produced particles seem to cluster in momentum space (i.e., phase space is not populated uniformly) which leads one to suspect that collective phenomena are quite important.

The thrust of investigations in T-8 has been twofold. First we have explored the range of applicability of phenomenological models (the cluster and hydrodynamical models). Second, we have developed a transport theory of multiparticle processes which bridges the gap between fundamental field theories and phenomenological models. The transport theory allows a direct calculation of multiparticle production inclusive cross sections once given a fundamental theory. It also allows one to discuss collective behavior and the hydrodynamic properties of prehadronic matter.

1. Quantum transport theory of multiparticle production

A new unified approach to multiparticle production processes in high elementary particle collisions has been developed.^{4,5,6} The method involves casting the field theoretic description of the process in a form reminiscent of traditional transport theory. The inclusive differential cross sections are expressible in terms of covariant Boltzmann functions $F(p,R)$, etc., whose equations of motion depend on the nature of the interaction. (More precisely one obtains a hierarchy of coupled integro-differential equations for the multiparticle distribution functions.)

The idea of the method is easily expressed for the scattering of a nonrelativistic particle by a potential well. Wigner's replacement for the Boltzmann function,

$$\tilde{f}(p,R,t) = \int \frac{d^3 \underline{r}}{(2\pi)^3} e^{-i \underline{p} \cdot \underline{r}} \psi^* \left(\underline{R} - \frac{1}{2} \underline{r}, t \right) \psi \left(\underline{R} + \frac{1}{2} \underline{r}, t \right) \quad (5)$$

has the usual properties

$$\int d^3 p f(p,R,t) = n(\underline{R},t) \quad (6)$$

$$\int d^3 R f(p,R,t) = n(p,t)$$

where $n(R,t)$, $n(p,t)$ are respectively the number densities in position and momentum space.

The function f , defined in Eq. (5), obeys an equation of motion (determined by the Schrodinger equation) very similar to the Boltzmann transport equation. The scattering problem is to find f for late times given $f = f_0$ for $t \rightarrow -\infty$, where f_0 is known in terms of the initial wave packet. The scattering cross section may be determined from Eq. (6).

The relativistic case is more complicated, particularly in that a hierarchy of new distributions is inevitably introduced. For theories involving a relativistic Bose field ϕ , we define the covariant analog $F(p,R)$ of Eq. (5) by means of a four-dimensional Fourier transform. The single particle inclusive differential cross section is then determined by $F(p,R)$ in analogy to the non-relativistic case. F is to be determined by solving transport equations specific to the theory. These solutions typically involve closure approximations of unknown validity. The most interesting result to date has been the discovery of collective modes in the produced final state which could be the origin of "clustering" effects seen in recent experiments.

2. Transport and hydrodynamic aspects of multiparticle production

The transport theory described above when solved for $F(p,R)$ provides a direct evaluation of the single particle distribution function $E \frac{dN}{d^3p}$ via the reduction formula

$$E \frac{dN}{d^3p} = (p^2 - m^2) F(p, q = 0) \quad (7)$$

where $F(p,q) = \int e^{iq \cdot R} F(p,R) d^4R$. It also allows one to study the hydrodynamical properties of the field produced by looking at the moments of $F(R,p)$

$$\langle : T^{uv}(R) : \rangle = \int F(R,p) p^u p^v d^4p - g^{uv} \langle : L_{int} : \rangle \quad (8)$$

where T^{uv} is the energy-momentum tensor.

To understand how the transport theory is solved, how renormalization works in the context of transport theory, and how one identifies collective modes, we have studied $\lambda\phi^4 + g j\phi$ field theory where the source j has replaced the effect of two nucleons colliding and ϕ is the pion field.^{8,9,10} When we set $\lambda = 0$ (particle production from an external source), we verified that the transport theory gave the same result for the single particle spectra as one would have obtained by directly solving the field theory, i.e.,

$E \frac{dN}{d^3p} = |j(p)|^2$. We also found that when $\lambda = 0$, $\langle T^{uv}(x) \rangle$ had the form of a perfect fluid

$$\langle T^{uv}(x) \rangle = (\epsilon + p) u^u u^v - p g^{uv} \quad (9)$$

where $\epsilon(x)$, $p(x)$, $u^u(x)$ are respectively the collective energy density, pressure, and fluid 4-velocity. Moreover, after the current acted, one could identify the fluid velocity u^u with the physical pion velocity. A Lorentz contracted source led to the experimentally observed flat distribution of pions in $\frac{dp_{||}}{E}$. Thus we verified in this model many of the assumptions of the successful phenomenological model of Landau, i.e., the perfect fluid description of the pre-hadronic matter and the ability to identify the hydrodynamic variables with particle variables. We then looked at the effect of the $\lambda\phi^4$ interaction treated in the random phase approximation ($\langle \phi^3 \rangle = \langle \phi \rangle \langle \phi^2 \rangle$) in the transport theory and directly in field theory. The renormalization procedure was identical for the transport theory and the field theory and we found that the collective excitation of the pion field found in the inclusive process (from the transport theory) could be identified with the bound state found in the exclusive channels (from the field theory). Thus the transport equations are complementary to the more usual Green's function equations of field theory. The transport approach allows for direct calculation of the inclusive processes, whereas the Green's functions of the field theory are tailored to calculate the exclusive processes.

3. Clustering effects in high-multiplicity hadronic final states

There are about 15 particles produced in a typical high-energy hadron collision. This large number of degrees of freedom greatly complicates the choice of variables for describing the final states. Moreover, the data are often averaged over events with different multiplicities (different numbers of final particles) and may also contain large backgrounds. Nevertheless, one goal of an analysis of this data is to assess the amount and type of structure of the quantum mechanical probability density. For example, one would like to learn whether a typical hadronic event consists of a number of independently emitted objects (resonances or single hadrons), or whether there are collective effects in which many or most of the final state particles participate. It has become necessary to use rather sophisticated statistical methods to deal with such questions, especially in view of the fact that the constraints of phase space such as energy momentum conservation tend to mask dynamical effects.

It is essentially impossible to interpret the results of a data analysis in a model independent fashion. Therefore, it has become popular to use the average cluster size of cluster-emission models to parameterize the dynamical structure in the probability density. We have analyzed in detail the results of Quigg, Pirila, and Thomas, who study the distribution of rapidity-gap lengths in 200-400 GeV proton-proton collisions. They conclude that the average cluster size is about 3 hadrons. This would suggest that a typical hadronic event consists of the independent production of the well-known (low mass) hadrons and resonances. They use an independent cluster emission model to come to this conclusion, where clusters are produced uniformly over the rapidity interval. We have found that their result is most sensitive to the multiplicity distribution generated by their specific model, and not to the actual structure in the momentum distributions in individual events. We showed this using a semiclassical model in which clusters are emitted according to transverse-momentum-damped phase space, but the multiplicity distribution is constrained to follow the data. Although independent

cluster emission models relate cluster size and the multiplicity distribution, the assumption of independence is violated by the phase-space constraints, and, for example, the rapidity interval is a function of the multiplicity. Thus, we do not take seriously the relation of the multiplicity distribution to the cluster size, but simply take the multiplicity distribution from the data. From this point of view, we conclude that the gap length distribution is quite insensitive to the structure in phase space as parameterized by an average cluster size.

The problem of finding the average cluster size is better tackled by analyzing the semi-inclusive data. We have developed and tested a statistical measure which measures the fluctuation of the distribution of secondaries from event to event. Monte Carlo techniques have been used to check that this measure is more sensitive to the average cluster size than is the multiplicity distribution. It gives a cluster size of 5 or 6 hadrons at 200 GeV. Thus, there is a rich structure in the multiparticle amplitudes, similar to that expected by models with collective modes. This type of behavior is confirmed in the exclusive 6- and 8-body channel measured at 30 GeV, where the event-to-event fluctuations in the momentum distributions are too large to be accounted for by low mass, low-multiplicity resonance formation. These results are reported in two Physical Review articles and one Phys. Rev. Letter.^{23,24,25}

4. Large transverse-momentum production

The relatively large flux of hadrons produced at large transverse momentum ($p_{\perp}$) has been successfully described in terms of a parton picture in which the large $p_{\perp}$ particles come from a hard interaction between the point-like constituents of the incident hadrons. The success of the parton picture has been interpreted as a verification of the quark model. In view of the evidence for the production of large clusters of secondaries, we have investigated whether other models, namely cluster models, can also explain the relatively rare large $p_{\perp}$ events. We have examined a nova-like model

where a single cluster is produced peripherally and decays according to a constant matrix element into the observed secondaries. This model accounts well for the correlations and associated multiplicities observed in the data. However, the total flux falls below the measured flux. This may be an indication that the constant-matrix-element assumption is wrong, and the large p flux may be increased by fluctuations in the momentum due to structure in the matrix element. We have been developing the mathematical machinery to deal with this problem.

1. Astrophysics

1. The photon rest mass

We have obtained a new upper limit on the mass of the photon

$$m \leq 8 \times 10^{-49} \text{ g} \equiv 6 \times 10^{-16} \text{ eV} \equiv 2 \times 10^{-11} \text{ cm}^{-1}, \quad (10)$$

by an analysis of the data obtained by Pioneer 10 of Jupiter's magnetic field, where the photon mass is treated as a free parameter. This limit is the lowest, directly measured limit that has been placed on a possible finite rest mass of the photon.¹⁷

2. The Titius-Bode law and evolution in the solar system

In a short article it has been pointed out that although it is by no means clear that the Titius-Bode law of planetary distances is indeed a "law" (even though there are enticing indications), if one assumes that the law is a "law" and that the planets obey it, then this argues against recent large-scale evolution in the solar system. Put another way: one can believe in the Titius-Bode or in recent large-scale evolution or in neither of them. But it appears difficult to believe in both of them.¹⁵

III. T-8 PUBLICATIONS

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23. R. Slansky and T. Ludlam, "Cluster Size and the Rapidity Gap-Length Distribution," Phys. Rev. Lett. 35, 127 (1975).
24. R. Slansky and T. Ludlam, "Estimates of the Cluster Size in High-Energy Hadron Collisions," Phys. Rev. D12, 59 (1975).
25. R. Slansky and T. Ludlam, "What Do Rapidity Gaps Say About Clustering," (Phys. Rev. D12, 65 (1975)).
26. Geoffrey B. West, "Electron Scattering from Atoms, Nuclei, and Nucleons," Phys. Reports 18C, 5, 264 (1975).
27. G. B. West, "Maybe the Quark Parton Model Can Survive Electron-Positron Annihilation," Phys. Lett. 55B, 195 (1975).
28. D. Siver, J. Townsend, and Geoffrey B. West. "Photoproduction of ψ -Particles," (to be published in Phys. Rev.).

IV. T-8 OUTSIDE TALKS AND SEMINARS

1. P. Carruthers, Seminar on "Quantum Transport Theory of Multiparticle Production," given at the following places, 1975:
 - a. Aspen Center of Physics
 - b. University of Arizona
 - c. Arizona State University
 - d. APS Meeting, Williamsburg, Virginia
 - e. University of California at San Diego
 - f. Coral Gables Conference, Florida
 - g. University of Colorado
 - h. University of Marburg, Germany
 - i. Erice Workshop, Sicily
 - j. Ecole Polytechnique, Paris
2. F. Cooper, Seminar at Erice, Sicily, May 1975, "Hydrodynamic Model of Multiparticle Production."
3. F. Cooper, Seminar at the University of Bielefeld, West Germany, "Hydrodynamic Model of Particle Production," April 1975.
4. F. Cooper, Seminar at the University of Bielefeld, West Germany, "Transport Approaches to Multiparticle Production," April 1975.
5. M. M. Nieto, "Is the Pion a Fundamental Particle Having a Minimal Electromagnetic Interaction," physics seminar given jointly with Felix Boehm of Cal. Tech. at the Aspen Center for Physics, Aspen, Colorado (July 1974).
6. M. M. Nieto, "Limits on the Mass of the Photon: From Benjamin Franklin to Pioneer 10," Physics Department Colloquia given at:
 - a. University of Auckland, New Zealand, March 1975
 - b. University of Canterbury, Christchurch, New Zealand, March 1975
 - c. University of Melbourne, Australia, March 1975
 - d. University of New South Wales, Sydney, Australia, April 1975
 - e. Research School of Physical Sciences, Australian National University, Canberra, Australia, April 1975
 - f. University of Hawaii, Honolulu, May 1975
7. M. M. Nieto, "The History of a Stolen Idea: The Titius-Bode Law of Planetary Distances," colloquia given at:
 - a. Physics Department, Victoria University of Wellington, New Zealand, March 1975
 - b. School of Physics, University of Sydney, Australia, April 1975
 - c. Mt. Stromlo Observatory, Australian National University, Canberra, Australia, April 1975
8. M. M. Nieto, "First-Order Wave Equations for Mesons," Theoretical Physics Seminar, Department of Theoretical Physics, Australian National University, Canberra, Australia, April 1975.

9. M. M. Nieto, "Bhabha First-Order Wave Equations for Arbitrary Spin," Theoretical Physics Seminar, Department of Theoretical Physics, Australian National University, Canberra, Australia, April 1975.
10. R. Slansky, "Off-Shell Effects in the Reaction $p + p \rightarrow n + \rho + \pi^0$," (with W. R. Gibbs, B. F. Gibson, and G. J. Stephenson). Bull. Am. Phys. Soc. 20, 83 (1975). (Anaheim Meeting).
11. R. Slansky, "What Can Rapidity Gaps Teach Us About Clustering?" (with T. Ludlam). Bull. Am. Phys. Soc. 20, 649 (1975) (Washington Meeting).
12. R. Slansky, "Estimates of the Cluster Size in High Energy Hadron Collisions," (with T. Ludlam). Bull. Am. Phys. Soc. 20, 650 (1975) (Washington Meeting).
13. G. B. West, Seminar at University of Washington, Seattle, "Neutron Diffraction from Liquid Helium and the Parton Model," May 1975.
14. G. B. West, Seminar at the University of California, Berkeley, "Scaling in Deep Inelastic Electron Scattering from Nonrelativistic Systems," March 1975.
15. G. B. West, Colloquium at the University of California, Santa Cruz, "Scaling in Deep Inelastic Electron Scattering from Nonrelativistic Systems," March 1975.

GROUP T-9 - NUCLEAR AND OTHER THEORY

C. L. Critchfield, Group Leader

I. INTRODUCTION

In 1964 about 20 staff members in T Division detached themselves from the programmatic work of the Division and took up self-motivated problems in pure research. Some of the fields of research were related to principal interests of the Laboratory, e.g., in nuclear physics, but most were not and ranged from Lie groups to disordered lattices. Twelve of these staff members asked to be recognized as a distinct group and this resulted in the formation of T-9 in August 1964. The Director recognized the group as an important link to the frontiers of scientific research and essential to the vitality of the Laboratory.

Membership in the group increased until August 1971 when T-5 was formed to represent our theoretical support of MP Division (Meson Physics). In recent years, an increased emphasis on basic research has led to the formation of other groups and to a broadened interest within existing groups. As a result, other members of T-9 joined groups which specialized in their individual areas of expertise. Now there are six staff members in T-9.

Two of these are engaged in nuclear theory which is directly applicable to the reactor and weapons program at the LASL. The reduction of nuclear data to a minimum number of parameters, represented in the application of the theory of the R-matrix, is an important task and is being executed by T-9. We are also involved in the application of our tremendous computing facility to a realistic description of nuclear fission, heavy ion reactions, and superheavy nuclei.

A large effort in the group is devoted to creative research of a fundamental nature. We have solved a longstanding paradox in the theory of Mott insulators, are developing a fundamental field theory of nuclei, have developed new models to treat thermal conductivity in solids, and are studying scalar potentials in the Dirac equation and their relation to the quark confinement problem.

Highlights of this work are described in the following section. We are also involved in consulting work for other groups at the LASL and these activities are described in Sec. III.

II. RESEARCH HIGHLIGHTS

A. Heavy Nuclei

Some of the research in T-9 is concerned with the theory of nuclear fission and very heavy ion reactions. Because fission is a basic mechanism in nuclear weapons and nuclear reactors, an understanding of this process is crucial to both our national defense and the solution of our energy needs. Moreover, since very heavy ion reactions may lead to the discovery of new elements and new phenomena with unusual properties, an understanding of this process is essential to keep us abreast in an emerging scientific discipline of potentially important consequences.

Why are fission and very heavy ion reactions of such fundamental importance? Both processes are concerned with changes in the shape of the nucleus and with the number of particles that it contains. In fission, the nuclear shape varies from a nearly spherical ground-state shape, through a cylinder-like saddle-point shape and a dumbbell-like scission shape, to two nearly spherical fragments at infinity. In very heavy ion reactions, the nuclear shape varies from two nearly spherical nuclei at infinity, through the contact point of two nearly spherical touching nuclei, to an amalgamated

system which may either remain fused or disintegrate into a variety of possible shapes.

A new generation of very heavy ion accelerators is currently being constructed in the United States and abroad. This is making available nuclear projectiles that contain up to 100 protons and that have mass numbers up to 250. This is essentially doubling the range of accessible nuclear systems. Thus, for the first time we will be able to study at least transient nuclear systems that contain up to 200 protons and that have mass numbers up to 500. The large Coulomb and centrifugal forces possible in the collision of two such heavy nuclei will deform the system into nuclear shapes that have been inaccessible up to now.

The study of large-scale nuclear shape changes provides important information on four fundamental aspects of nuclei: the nuclear potential energy of deformation, the nuclear inertia, nuclear dissipation, and the nuclear equation of state. At present we have some information about the nuclear potential energy, which can be described approximately as the sum of a smoothly varying macroscopic contribution and a rapidly fluctuating single-particle correction term. Much less is known about the nuclear inertia, which specifies the amount of kinetic energy involved with a given time rate of change of the nuclear shape. Our present knowledge of nuclear dissipation, the transfer of energy of collective motion into internal single-particle excitations, is even more obscure. The basic mechanism by which the energy transfer occurs is even in dispute; it could proceed either by means of two-body collisions between nucleons or alternatively by means of one-body collisions of nucleons with a moving potential wall. Finally, we know very little about the nuclear equation of state, which specifies the pressure inside the nucleus as a function of the nuclear density and internal energy. The increase in nuclear density that is expected in very heavy ion collisions at high bombarding energies should help decide important questions concerning the nuclear equation of state. In addition,

such tantalizing discoveries as nuclear density isomers and pion condensates may occur.

As we enter the new era in nuclear physics stemming from the construction of the new very heavy ion accelerators, these are some of the problems that we are concerned with in T-9. These same problems are being pursued experimentally by members of P Division and CNC Division, and a close collaboration exists between the experimental and theoretical efforts. In this way we hope to advance optimally our overall understanding of several new facets of nuclear physics.

The following subsections outline a few of the advances made within the last year.

1. Fission and heavy ion reactions

Our work on the theory of nuclear fission and heavy ion physics has progressed through the stage of calculating the ground-state properties and fission barriers of a large number of heavy nuclei. We are now using the same methods that were developed in connection with fission theory to calculate the potential energy for heavy ion reactions.

Our recent work on the dynamics of fission and heavy ion reactions has included both a study of the kinetic energy of collective motion and a study of nuclear dissipation (the transfer of energy of collective motion into internal single-particle excitations). From a comparison of calculated and experimental fission-fragment kinetic energies, we have determined the coefficient of nuclear viscosity to be 0.015 ± 0.005 terapoise. We have also calculated the cross sections for heavy ion-induced compound-nucleus formation by using the criterion that the dynamical trajectory for the fusing system must pass inside the fission saddle-point in a multidimensional space in order to form a compound nucleus.

2. Nuclear equation of state

In an attempt to determine the nuclear equation of state from the high-energy heavy ion experimental data taken at the Berkeley Bevalac, we have developed a relativistic hydrodynamic theory of heavy ion collisions. In this approach the relativistic equations that express the conservation of nucleon number, momentum, and energy for a specified nuclear equation of state are solved numerically by use of finite-difference methods. (See Fig. 26.)

B. Reactions and Scattering of Light Nuclei

The interactions of light nuclei have always been of interest to LASL since among them are the so-called fusion reactions occurring in both explosive and controlled thermonuclear processes. Despite their practical interest, even a phenomenological description of the collision processes has been slow in coming, partially because spin observables could not be measured accurately and completely in the absence of polarized ion sources and targets. A few years ago, a decision was made at the LASL to pursue a basic research program in this area, including the development of the required polarized beams and targets. This program involved a rather large investment but has proven to be extremely worthwhile. In particular, the experimental and theoretical methods and tools developed by members of Groups T-9, T-2, and P Division have yielded quantitative information of considerable practical value.

Two notable examples can be cited from cross-section evaluation work. This work is carried on by T-2, but depends heavily on results obtained in T-9. One is the current evaluation of the ${}^6\text{Li}, n$ total and reaction cross sections. These reactions are extremely important since they are used as standards in neutron measurements and are of potential use in the CTR program. The cross-section evaluations depend critically on $\alpha + t$ elastic scattering and polarization measurements. The exact nature of this relationship was first noticed in T-9 when we studied the level structure of ${}^7\text{Li}$. Moreover, the ${}^6\text{Li}, n$ evaluations

Fig. 26. Characteristic stages in the head-on collision of ^{16}O with ^{107}Ag , calculated with a relativistic hydrodynamic code. The laboratory bombarding energy per nucleon is 2.1 GeV. The projectile, which is initially Lorentz contracted in the incident direction, is represented by heavy points, and the target is represented by light points.

are done with EDA, a computer code originally developed in T-9 for basic research on light nuclear systems. The critical experimental measurements in the $\alpha + t$ system have been made at LASL by members of P Division. Some of these measurements use the recently developed polarized triton source, a unique LASL facility.

The second example, quite startling and unexpected, was the recent discovery of an inaccuracy in the previously accepted value of the d-t reaction cross section in the kilovolt region. Again, this discovery depended on the use of EDA and on the fact that the analysis paralleled the ${}^5\text{Li}$ studies under way in T-9. The $J = \frac{3+}{2}$ resonance turned out to cause significant deviations from the Gamow penetration factor curve at lower energies than anyone had expected. All previous evaluations had missed this fact because they were based on what was thought to be the pertinent information rather than on a comprehensive study of the whole problem. The deviation from the Gamow curve had even been noticed by the experimenters, but they had dismissed it as an unexplained error.

Highlights of our work on the phenomenological description of light nucleon systems are described below. It all involves the development and use of EDA, a multichannel, energy-dependent, partial wave parameter search routine that attempts to find an energy-dependent S-matrix in terms of resonance levels in the R-matrix formalism. EDA guarantees a unitary S-matrix and a physically reasonable energy-dependence of the S-matrix parameters. A typical application involves the simultaneous fitting of one or two thousand data points of differential cross sections and spin polarization experiments of many kinds over a range of energies. A hundred or more parameters may be required to fit all the data.

1. The five nucleon system

We have continued an R-matrix analysis with EDA of the ${}^5\text{Li}$ and ${}^5\text{He}$ compound systems. Our goal is to determine the level structures of the two systems and to explain the Coulomb energy differences

between them. Moreover, in collaboration with members of T-2, we are using the analysis to gain a better knowledge of the d-t and d- ^3He elastic scattering cross sections at low energies. New data, including those obtained by P Division from the new LASL polarized triton source, are part of these evaluations.

2. Study of the ^7Be system

We are studying the states of ^7Be up to ~ 8 MeV excitation by an analysis of the $^4\text{He}(^3\text{He}, ^3\text{He})^4\text{He}$, $^6\text{Li}(p,p)^6\text{Li}$, and $^4\text{He}(^3\text{He}, p)^6\text{Li}$ processes. Seven MeV in the ^7Be system corresponds approximately to the threshold of the $^6\text{Li}^* + p$ channel, which will be incorporated in future work. The $\frac{3}{2}^-$ and $\frac{1}{2}^-$ bound states as well as the known $\frac{7}{2}^-$ and the $\frac{5}{2}^-$ states are all found and are necessary to fit the data. In addition there is some evidence for new $\frac{1}{2}^+$, $\frac{1}{2}^-$, and $\frac{3}{2}^-$ levels.

The parametric description of the levels in ^7Be is simpler than what we have previously found for ^7Li , although the essential level structure is similar. It is likely that this analysis will afford a simpler description of the ^7Li system. It will also give a more accurate prediction of the low energy of the $^6\text{Li}(p, \alpha)^3\text{He}$ cross section, which is of astrophysical interest, for example, as an energy source in very young stars of low density and temperature. This work is being carried out in collaboration with S. Baker and E. K. Biegert of Rice University.

3. Inclusion of photon channels in EDA

An accurate phase-shift analysis of the π -nucleon elastic scattering experiments now under way at LAMPF requires the inclusion of photon channels. We were the first investigators to include photon channels in such an analysis. Originally EDA was used for this purpose in a rather artificial way, i.e., we treated the photon spin as if it were that of a particle of finite mass, and imposed photon longitudinal spin polarization as a constraint on the photon widths in the total channel spin representation. Since the longitudinal polarization is only an asymptotic property, it was necessary to

define the photon reduced widths at an unrealistic channel radius and thus the phase-space energy dependence of the physical width was lost. EDA has now been modified to include multipole photon channels directly.

C. Strong Coupling Field Theory

Calculations in nuclear physics generally start with a Hamiltonian that contains nucleon-nucleon potentials. The nucleon-nucleon potentials are ascribed to the virtual exchange of mesons. It seems natural to attempt to eliminate the intermediate step of representing the mesonic interactions by an internucleon potential and instead calculate directly the properties of a system of nucleons and virtual mesons. This "quantum field theory of nuclei" has been the subject of our investigations during the last five years.

In this theory the interaction between nucleons is regarded as arising from the exchange of scalar and vector (and possibly other) mesons. There are three basic systems of interest: (1) infinite nuclear matter (INM), that is, matter like that occurring in the interior of a large nucleus but infinite in extent; (2) finite nuclei (FN) which are just the nuclei observed in nature; and (3) the single nucleon (SN) where the interest lies in the internal properties of the nucleon itself that arise from its interaction with the meson field. In each system, the aim is to compute the energy, mass, charge distribution, and other observables in terms of the coupling constants and masses that appear in the assumed Hamiltonian for the system. Each of these basic systems can be treated either relativistically with a fully Lorentz-covariant theory or semirelativistically with a theory that describes the mesons relativistically and the bare nucleon nonrelativistically.

The semirelativistic INM, FN, and SN systems were treated several years ago. This past winter fully relativistic treatments of the INM and FN systems were developed and published in Physical Review.^{2,3}

The recent effort this spring has been devoted to the relativistic SN problem. The projection operator technique that led to a successful treatment of the relativistic FN problem also makes the relativistic SN problem tractable. The formal details and some numerical examples have been worked out and are described in Ref. 5.

Previously, only the lowest approximation to the solution of the various problems had been given. We have now developed a scheme for systematically improving the solution. This scheme is like the one-meson, two-meson, etc., approximations used in the early 1950's for the pion-nucleon problem, with the difference that the mesons are added to the clothed nuclear states. The one-meson formalism has been worked out for the semirelativistic SN problem; it is described in Ref. 4. The results are promising, and work continues along these lines.

D. Theory of Mott Insulators

The subject of Mott insulators began, in the late 1930's, with the recognition that certain materials with partially filled d (or f) bands are insulators in spite of the prediction from elementary band theory that they should be metallic. (NiO and CoO are the prime examples; also many other transition-metal oxides, sulphides, and halides, as well as many lanthanide and actinide compounds.) It was later recognized that the ground states of many such insulators are antiferromagnetic, and that the consequent enlargement of the unit cell (as seen, for example, by the spin-up electrons) can produce additional band gaps and thus convert a metal into an insulator. Lattice distortions which lower the lattice symmetry can also lead to insulating band gaps (as in VO_2 , for example). Thus antiferromagnetism and/or lattice distortion (V_2O_3 exhibits both) can explain the low-temperature insulating gaps of a number of materials within the general framework of Hartree-Fock (HF) band theory, so these cases are no longer considered paradoxical. For many antiferromagnetic materials, however, the local moments and insulating

gap persist above the Neel temperature, where the disorder of the local moments precludes a conventional band-theoretic interpretation. It thus appears, phenomenologically, that the electrons responsible for the magnetism are localized instead of itinerant (band-like), in apparent violation of Bloch's theorem. It is these latter materials which are now regarded as the bona-fide Mott insulators.

A year ago we resolved the most obvious difficulties by means of a novel extension of the conventional HF band theory. We generalized the concept of unrestricted HF theory to consider solutions in which the net spin polarization at each one of the N sites can be either "up" or "down," i.e., we assumed the existence of 2^N different HF solutions, corresponding to the 2^N possible Ising spin configurations. Solutions of a numerically solvable model system were presented as evidence that such Ising-HF solutions must actually exist, provided the intra-atomic exchange matrix element is sufficiently large. In applying this HF model to NiO and CoO, we found that the popular local $\rho^{1/3}$ exchange approximation of Slater (the "X α " approximation) is inadequate, whereas the more realistic parameterization scheme of Kanamori, for the 3d-3d intra-atomic matrix elements, does suffice to explain the large (~ 4 eV) gaps observed experimentally.

This year we have refined and extended the above theory in several respects, as described below. We have also prepared a comprehensive report consisting of three manuscripts submitted to Physical Review B.¹⁰⁻¹²

1. Electronic rearrangement effects

One of the theoretical problems has been to determine the bandwidth, or equivalently the principal hopping integrals, for the 3d electrons. Different experimental phenomena in NiO have implied radically different values. We have now achieved a reconciliation of the various experiments, namely Heisenberg exchange coupling, bound polaron hopping, two-magnon and four-magnon production via electron-magnon coupling. This was done by considering several

strong orbital-rearrangement effects, resulting from changes in the 2p-3d covalency and changes in the 2p-4s hybridization, due to the presence of a 3d hole. Simple estimates of these effects have led to semi-quantitative agreement of all of the above data with the effective 3d hopping integrals obtained by Mattheiss from his APW band calculation of NiO.

2. Crystal-field theory

It is well known that the crystal-field or ligand-field theory applies to the low-energy optical exciton absorptions in these materials, but there has been some question about whether this is also the correct approach for understanding the 3d structures observed in x-ray photoelectron spectroscopy (XPS) experiments. We have performed crystal-field calculations to predict the 3d XPS structures of NiO and CoO, doing this in more detail than previous investigators. Particular attention was paid to the choice of parameters and the resulting intensity distributions. This has considerably improved the agreement between theory and experiment to the point where it should now be clear that this approach is empirically valid. Rough arguments about the widths of the various crystal-field structures have provided a qualitative theoretical justification for the present success of crystal-field theory.

3. Formal derivation of the effective spin Hamiltonian

Until now there has been no fully satisfactory formal justification for the Heisenberg-like effective spin Hamiltonians which are widely employed in phenomenological analyses of the magnetic behavior of magnetic insulator materials. The superexchange theory is formally and semi-quantitatively satisfactory for isolated clusters involving two magnetic cations, but theories of bulk systems with a macroscopic number of magnetic cations have always run afoul of one aspect or another of the "nonorthogonality catastrophe." We have now resolved this formal problem by means of a linked-cluster perturbation theory of open-shell systems, a formalism which has been widely used in studies of low-energy nuclear spectra.

This formalism preserves rotational invariance in spin space for s-band systems. Furthermore, it is sufficiently general to properly handle the effects of spin-orbit coupling, Hund's rule coupling ($S > \frac{1}{2}$), and crystal-field degeneracy, as encountered for example in CoO. There is also a significant by-product from this formally exact perturbation theory: it demonstrates that the small differences among the total HF energies of our 2^N different Ising-HF configurations are all consistent with the superexchange theory of Anderson, to within the accuracy of HF approximations. A direct proof of this result is not possible within the framework of our Ising-HF model because one runs into a type of nonorthogonality catastrophe.

E. Thermal Conductivity and Kapitza Resistance

1. The self-consistent reservoir model

Several years ago we invented the self-consistent reservoir model for nonequilibrium thermal properties of crystals. This model simulates nonharmonic interactions (electron-phonon, phonon-phonon) by stochastic interactions of each atom with its own heat bath. The temperature of each heat bath is determined self-consistently by requiring that there be no energy current in the steady state to or from any of the reservoirs except those at the boundaries of the system. The principal virtues of the SCR model are that it is fairly realistic and that in some cases it can be solved exactly. The model yields quantum mechanical Langevin equations with random force terms whose autocorrelations are determined by the local temperatures.

We have solved these equations analytically for a simple cubic homogeneous crystal, yielding thermal conductivity as a function of λ (the parameter describing the strength of coupling to the reservoirs), of temperature, and of the atomic mass and harmonic force constants. At low temperatures the results have the correct temperature dependence and, for a reasonable choice of λ , the right magnitude. At high temperatures one would expect λ to depend on T , since it simulates

complicated and highly temperature-dependent processes. We obtain general agreement with experiment for physically realistic choices of temperature dependence for λ .

2. SCR and the binary disordered chain

For steady-state heat flow in more complicated inhomogeneous systems the equations can be solved numerically. The binary disordered chain (one-dimensional harmonic crystal) has been much discussed because it is not known whether its thermal conductivity (in the limit of an infinitely long chain) is zero, finite, or infinite. The SCR chain for finite N has been solved for any value of λ and the limit $\lambda \rightarrow 0$ numerically estimated. Our results makes it plausible that a finite thermal conductivity exists for $N \rightarrow \infty$; the SCR model shows promise of being a useful tool to attack this problem.

3. Kapitza resistance

A more practical application of the SCR model is to the theory of Kapitza conductance. When heat flows from a metal, for example, into liquid helium, there is a discontinuity in temperature at the boundary. The magnitude of the discontinuity is proportional to the heat current and increases rapidly as the temperature decreases. The proportionality constant is called the Kapitza resistance.

Because of its applications in low temperature technology, understanding the Kapitza resistance has practical importance. For example, it constitutes a major hindrance to the efficient cooling of superconducting magnet coils or transmission lines.

The present theory is inadequate, as evidenced both by the fact that it often disagrees with observation by one or two orders of magnitude, and by its very shaky foundations, being based largely on an analogy of the phonon system with a classical gas. The phonons are imagined to carry heat, as the molecules in a gas do, and are influenced by one another only by relatively infrequent collisions. According to this theory, the phonons are partly transmitted and partly reflected at the boundary depending on the acoustic mismatch.

In the SCR model for a simple Kapitza system, the basic postulate of the acoustic mismatch theory turns out to be false. In the neighborhood of the boundary, the heat is not carried by individual phonons at all, but by excitations involving coherent superpositions of many phonons; that is, the density matrix is not diagonal in the phonon representation in the Kapitza system, although it is in the homogeneous case. (See Fig. 27.)

Our method for solving the SCR equations is at present limited to the situation in which the systems on both sides of the interface are simulated by simple cubic lattices with the same lattice spacing and the same λ although the masses and force constants can be different. These constraints limit the present role of the SCR system to that of providing a benchmark against which to test theories which are not thus restricted, except in the fortunate situations in which those conditions on the structure and dynamics are nearly satisfied.

Molecular dynamical-type numerical experiments have also been performed on one-dimensional Kapitza systems. These calculations, in which the computer solves (stepwise in time) the classical equations of motion for the anharmonic crystal, confirm the results of the SCR model, notably that heat is not carried by independent phonons in the neighborhood of the inhomogeneity.

F. Pion Channeling in Crystalline Solids

When a beam of particles hits a crystalline solid, its interaction depends on the beam direction relative to the crystalline axes and planes. The beam propagates preferentially along certain axes and in certain planes; this is called channeling. Experiments have been proposed for LAMPF to study the channeling of positive and negative pions whose energies are not quite high enough for them to be considered classically. Little theory exists for quantum-mechanical channeling; since the projectiles used in most experiments (protons and heavier) behave classically at the energies involved, only the

Fig. 27. Normalized Kapitza conductance α as a function of the ratio of sound velocities (c_1/c_2) in the two media and the ratio of densities (ρ_1/ρ_2). The dashed lines are the results of the usual acoustic mismatch theory in which Bose-Einstein densities with different temperatures are assumed for the phonons incident from each side. The solid lines are the results of a correction to this theory in which more realistic skewed densities are allowed. The correction is very large where the two materials are similar, but quite small where the acoustic mismatch is extreme. This latter theory still assumes that the phonons are incoherently superposed. Disagreement with experiment is most drastic in the high mismatch regime ($\rho_2 c_2 / \rho_1 c_1 < .1$). Relaxation of the incoherent superposition constraint by the SCR method has shown to result in significant increase in α in this range, although quantitative calculations to compare with experiment have not been performed by reasons discussed in the text.

classical theory has been much developed. We have solved the Schrodinger equation for some simple instances of pion channeling, and have concluded the deviations from classical behavior will usually be small but in some cases easily observable.

G. Random Packing of Powder

Some ceramics and metallurgy groups at the LASL are concerned with properties of powders which consist of mixtures of different sizes and shapes of particles of different materials. Void fractions and densities, average number of contacts, and size of interstices, for example, are important. The general problem is impossibly difficult to consider analytically, but some simple cases are tractable numerically. The random packing of monosized spheres is one case which can be simulated on the computer and yields results which agree reasonably well with experimental observations. No exact analytical theory exists even for this case, let alone the case of mixtures of two sizes of spheres. We have devised a computer algorithm for building random packings of binary mixtures as well as general size distributions. However computer memory severely limits the size disparity which can be allowed. We have tried analytically to consider cases of more practical interest (mixtures of particles with continuous size distributions) by a semi-statistical approach involving a requirement that, as the random packing is built up by sequential addition of particles from the size distribution, the nature of the distribution in and near the surface be stationary. A number of parameters occur in the theory; it is hoped that it will at least yield a formula which can be fit to experimental data.

H. Scalar Potentials in the Dirac Equation

A thorough study of scalar potentials in the Dirac equation for spin 1/2 particles has been completed and possible application to new quark models of hadrons (strongly interacting particles) are now under investigation.^{13,14} These new models are designed to confine quarks, i.e.,

since quarks have never been observed in nature, models using quarks as fundamental building blocks should predict that bound states of quarks (the observed particles) appear in nature, but never individual quarks. One such model, known as the "bag," confines quarks by a scalar pressure which itself contains part of the mass of the system. An alternative model confines the quarks in a scalar potential so that all the mass comes from the energy of the quarks. The latter model has attracted the attention of Feynman and Gell-Mann among others.

We have discovered that the Dirac equation (which quarks are assumed to obey) can be solved analytically when the potential increases linearly with radius and that the solutions are closely related to those for the harmonic oscillator. This is a very desirable feature in such models. We have recently obtained numerical results for nucleons and related our results to the MIT "bag" model. (A comment on this work is soon to appear in Phys. Rev. D.) Current efforts are aimed at applying our work to other hadrons.

III. INTER-DIVISIONAL ACTIVITIES

Members of T-9 have performed a number of important consulting functions for groups in other Divisions. J. R. Nix has consulted with P Division and CNC-Division on their fission and heavy ion experiments. As mentioned earlier, D. C. Dodder has been deeply involved in the experimental program of light nuclear research carried on by P-Division Office and P-9, providing predictions of experimental results as a guide in experimental design. Dodder has also consulted with members of MP-4 concerning π -nucleon elastic scattering. In this work he predicted results, consistent with earlier experiments, for use in evaluating preliminary results at LAMPF and estimated the sensitivity of physical parameters to experimental accuracies.

W. M. Visscher served on the Accelerator Development Committee at LAMPF (meeting about weekly) and consulted with various MP members about beam-dynamical problems in the LAMPF linac (linear accelerator).

In particular the idea of alternating phase focusing was restudied. Alternating phase focusing, if it works, would use the RF in the cavities to focus the beam both longitudinally (bunching) and radially, eliminating the need for focusing magnets. This would make linacs smaller, cheaper, and easier to use (important considerations since there are already some proposals to build linacs for pion cancer therapy). However, radial and phase acceptances appear to be small for economical design parameters and therefore the effects of construction and RF errors need considerable study before one can say whether or not the scheme is practical.

IV. T-9 PUBLICATIONS

1. M. Bolsterli, W. R. Gibbs, B. F. Gibson, and G. J. Stephenson, Jr., "Galilean-Invariance Ambiguity in the Nonrelativistic Pion-Nucleon Absorption Operator," Phys. Rev. C10, 1225 (1974).
2. M. Bolsterli, "Relativistic Second-Order Energy in Infinite Fermion Matter," Phys. Rev. D11, 312 (1975).
3. M. Bolsterli, "A Relativistic Second-Order Energy Functional for Finite Fermion Systems," Phys. Rev. D11, 784 (1975).
4. M. Bolsterli, "Variational Procedure in a Strong-Coupling Theory," (submitted to Phys. Rev. D).
5. M. Bolsterli, "Meson Field Interaction with a Dirac Particle Source," (submitted to Phys. Rev. D).
6. B. H. Brandow, "A Localized-Orbital Theory of Mott Insulators," J. Solid State Chem. 12, 397 (1975).
7. B. H. Brandow, "Formal Derivation of Effective Spin Hamiltonians for Macroscopic Magnetic Insulator Systems," presented at American Physical Society Meeting, Denver, CO (April 1975). Bulletin A.P.S. 20, 502 (1975).
8. B. H. Brandow, "Onset Criteria for Insulating Electronic Transitions in Three-Dimensional Systems," to be published in J. Phys. C.
9. B. H. Brandow, "Perturbation Theory of Effective Hamiltonians," Invited paper at International Topical Conference on Effective Interactions and Operators in Nuclei, Tucson, Arizona (June 1975); to be published by Springer-Verlag in Lecture Notes in Physics, Vol. 40.
10. B. H. Brandow, "Localized-Orbital Descriptions of Mott Insulators I: Local Moment Hartree-Fock Theory," (submitted to Phys. Rev. B).

11. B. H. Brandow, "Localized-Orbital Descriptions of Mott Insulator II: Electronic Properties of NiO, CoO, and MnO," (to be published).
12. B. H. Brandow, "Localized-Orbital Description of Mott Insulators III: Orbital Bases and Perturbation Theories (to be published).
13. C. L. Critchfield, "Scalar Potentials in Dirac's Equation," (to be published in Journal of Mathematical Physics).
14. C. L. Critchfield, "Scalar Binding of Quarks," (submitted to Phys. Rev. D, to be published).
15. C. L. Critchfield and J. L. Gammel, "Rational Approximants for Inverse Functions of Two Variables," Presented at International Conference on Padé Approximants, University of Colorado (June 1972); Rocky Mountain Journal of Mathematics 4, 339 (1974).
16. D. C. Dodder, G. M. Hale, R. A. Nisley, K. Witte, and P. G. Young, "Models Based on Multichannel R-Matrix Theory for Evaluating Light Element Reactions," Presented by H. T. Motz at the EANDC Topical Discussion on Critiques of Nuclear Models and Their Validity in the Evaluation of Nuclear Data, Tokyo (March 1974) (to be published in Proceedings).
17. P. Moller and J. R. Nix, "Calculation of Fission Barriers with the Droplet Model and Folded Yukawa Single-Particle Potential," Nucl. Phys. A229, 269-291 (1974).
18. P. Moller, S. G. Nilsson, and J. R. Nix, "Calculated Ground-State Properties of Heavy Nuclei," Nucl. Phys. A229, 292-319 (1974).
19. J. R. Nix and A. J. Sierk, "Potential-Energy Surfaces for Heavy-Ion Collisions," Physica Scripta 10A, 94-100 (1974).
20. K. T. R. Davies, S. E. Koonin, J. R. Nix, and A. J. Sierk, "Macroscopic and Microscopic Approaches to Nuclear Dissipation," Proc. Int. Workshop III on Gross Properties of Nuclei and Nuclear Excitations, Hirschegg, Kleinwalsertal, Austria (January 1975); Technische Hochschule Darmstadt report AED-Conf-75-009-000 (1975), pp. 8-21.
21. T. Kodama, R. A. M. S. Nazareth, and J. R. Nix, "Exact Calculation of the Penetrability for a Very Simple Two-Dimensional Barrier," Proc. Int. Workshop III on Gross Properties of Nuclei and Nuclear Excitations, Hirschegg, Kleinwalsertal, Austria (1975); Technische Hochschule Darmstadt report no. AED-Conf-75-009-000 (1975), pp. 145-147.
22. J. R. Nix, "Summary of Theoretical Talks," Proc. Int. Workshop III on Gross Properties of Nuclei and Nuclear Excitations, Hirschegg, Kleinwalsertal, Austria (1975); Technische Hochschule Darmstadt report no. AED-Conf-75-009-000 (1975), pp. 252-254.

23. J. R. Nix and A. J. Sierk, "Potential-Energy Surfaces and Dynamical Trajectories for Fission and Heavy-Ion Reactions," Proc. XIII Int. Winter Meeting on Nuclear Physics, Bormio, Italy (January 1975) (in press).
24. A. J. Sierk and J. R. Nix, "Complete Fusion Cross Sections in Heavy-Ion Reactions," Bull. Am. Phys. Soc. 20, 69 (1975).
25. J. R. Nix, "Relevance of Clustering in Heavy Ion and Fission Studies," Bull. Can. Assoc. Phys. 31, 22 (1975).
26. H. W. Meldner, G. A. Cowan, J. R. Nix, and R. W. Stoughton, "How to Detect the Heaviest Man-Made Isotopes," Phys. Rev. C (to be published).
27. A. A. Amsden, G. F. Bertsch, F. H. Harlow, and J. R. Nix, "Relativistic Hydrodynamic Theory of Heavy-Ion Collisions," Phys. Rev. Lett (to be published).
28. F. H. Harlow, A. A. Amsden, and J. R. Nix, "Relativistic Fluid Dynamics Calculations with the Particle-in-Cell Technique," J. Comp. Phys (to be published).
29. William M. Visscher, "Kapitza Resistance in the Presence of a Heat Current," (unpublished data).
30. William M. Visscher, "Transport Processes in Solids and Linear Response Theory," Phys. Rev. A10, 2461 (1975).
31. M. Rich and William M. Visscher, "Disordered Harmonic Chain with Self-Consistent Reservoirs," Phys. Rev. B11, 2164 (1975).
32. William M. Visscher and M. Rich, "Stationary Nonequilibrium Properties of a Quantum-Mechanical Lattice with Self-Consistent Reservoirs," Phys. Rev. A (to be published, August 1975).
33. William M. Visscher, "Computer Studies of Transport Properties in Simple Models of Solids," to appear in Vol. 15 of Methods in Computational Physics: Solid State Physics (Academic Press).
34. William H. Weihs, "Meson Couplings from Conserved Vector Current and Partially Conserved Axial-Vector Current," Phys. Rev. D10, 1970 (1974).
35. William H. Weihs, "Relative Rotation of Axes under Successive Lorentz Transformations," Am. J. Phys. 43, 39 (1975).

V. T-9 OUTSIDE TALKS AND SEMINARS

1. C. L. Critchfield, "Harmonic Potentials in Dirac's Equation," seminar presented at the Physics Department, University of Houston, Houston, TX (November 1974).
2. C. L. Critchfield, "Harmonic Potentials in Dirac's Equation," seminar presented at the Physics Department, California Institute of Technology, Pasadena, CA (December 1974).

3. D. C. Dodder, "Low-Lying Levels of Five-Nucleon Systems," Invited talk at the American Physical Society Meeting, Knoxville, TN (June 1975); Bulletin A.P.S. 20, 6 (Series 2) p. 821 (1975).
4. G. G. Ohlsen, et al., (including D. C. Dodder), "Elastic Scattering of 7-12 MeV Tritons by Alpha Particles," presented at the American Physical Society Meeting, Washington, DC (April 1975).
5. J. R. Nix, "Fundamental Research at Los Alamos," presented at the Astronomy Seminar, Juiz de Fora, Brazil (August 1974).
6. J. R. Nix, "Macroscopic Nuclear Potential Energy," lecture presented at the Brazilian Center for Physical Research, Rio de Janeiro, Brazil (August 1974).
7. J. R. Nix, "Nuclear Dynamics," lecture presented at the Brazilian Center for Physical Research, Rio de Janeiro, Brazil (August 1974).
8. J. R. Nix, "Theory of Nuclear Fission, Superheavy Nuclei, and Heavy-Ion Reactions," colloquium presented at the Brazilian Center for Physical Research, Rio de Janeiro, Brazil (August 1974).
9. J. R. Nix, "Single-Particle Corrections," lecture presented at the Brazilian Center for Physical Research, Rio de Janeiro, Brazil (September 1974).
10. J. R. Nix, "Fission Barriers for Heavy Nuclei," lecture presented at the Brazilian Center for Physical Research, Rio de Janeiro, Brazil (September 1974).
11. J. R. Nix, "Superheavy Nuclei," lecture presented at the Brazilian Center for Physical Research, Rio de Janeiro, Brazil (September 1974).
12. J. R. Nix, "Heavy-Ion Physics," lecture presented at the Brazilian Center for Physical Research, Rio de Janeiro, Brazil (September 1974).
13. J. R. Nix, "Calculation of Fission Barriers," seminar presented at the Institute of Physics, University of Sao Paulo, Sao Paulo, Brazil (September 1974).
14. J. R. Nix, "Unified Theory of Nuclear Fission and Heavy-Ion Reactions," seminar presented at the Argentinian Atomic Energy Commission, Buenos Aires, Argentina (September 1974).
15. J. R. Nix, "Dynamics of Heavy-Ion Reactions," presented at the Physics Department Colloquium, Florida State University, Tallahassee, FL (October 1974).
16. J. R. Nix, "Superheavy Nuclei," Colloquium presented at the Physics Department, University of Manitoba, Winnipeg, Canada (February 1975).

17. J. R. Nix, "Compound-Nucleus Cross Sections," seminar presented at the Nuclear Chemistry Division, Lawrence Berkeley Laboratory, Berkeley, CA (March 1975).
18. J. R. Nix, "Dynamics of Fission and Heavy-Ion Fusion Reactions," Colloquium presented at the Cyclotron Institute, Texas A&M University, College Station, TX (April 1975).
19. J. R. Nix, "Calculation of Compound-Nucleus Cross Sections," presented at the Workshop on Deep Inelastic Processes and Compound Nucleus Formation in Heavy Ion Reactions, Stony Brook, New York (April 1975).
20. J. R. Nix, "Superheavy Nuclei," Colloquium presented at the Physics Department at the University of Virginia, Charlottesville, VA (April 1975).
21. C. A. Coulter and William M. Visscher, "Planar Channeling Theory: Quantum and Classical," presented at the Meeting of American Physical Society, Denver, CO (April 1975).
22. William M. Visscher and M. Rich, "Stationary Nonequilibrium Properties of a Quantum-Mechanical Lattice with Self-Consistent Reservoirs," presented at the Meeting of American Physical Society, Anaheim, CA (January 1975).

GROUP T-10 - THEORETICAL BIOLOGY AND BIOPHYSICS

George I. Bell, Group Leader

I. INTRODUCTION

Group T-10 was formed at the beginning of this year to consolidate work being done by four staff members on the theoretical interpretation of problems in the biological sciences. In general, emphasis has been given to the mathematical modeling of real problems in cellular and molecular biology and in biophysics. Much of the work has involved close collaboration with biomedical research workers in H Division, the University of Colorado Medical Center, or elsewhere as noted.

During its brief existence, T-10 has become widely recognized as the center for mathematical immunology. We were originally attracted to immunology about five years ago when it appeared that, thanks to a sound theoretical framework together with quantitative experimental methods, immunology was about to be transformed from a medical art to a biological science. Indeed, immunology is now by far the most extensively studied field of mammalian biology.

The human immune system is composed of about 10^{12} cells (largely lymphocytes) and 10^{20} molecules (antibodies produced by the lymphocytes) which detect the presence of foreign molecules (antigens) or foreign cells and hasten their elimination from the body. There is great diversity in the immune system with a typical vertebrate being able to produce probably on the order of 10^6 different kinds of antibody molecules. Moreover, the immune system is a learning system; each animal learns to produce best those antibodies which it needs to cope with dangerous bacteria and viruses in its environment. The nature of this learning is explained by the clonal selection theory. The lymphocytes arise by division of stem cells in the bone marrow.

According to the clonal selection theory, as a lymphocyte matures, it becomes committed to produce one and only one kind of antibody molecule and it begins to insert these molecules into its surface where they can function as specific receptors for complementary antigen molecules. When an animal is invaded by an antigen, the antigen molecules will stick to the surfaces of those lymphocytes which have complementary antibodies exposed in their surfaces. This sticking will, under appropriate conditions, stimulate the lymphocyte cells to proliferate and to produce large amounts of antibody. The antigen thereby selects complementary cells (or clones of cells) for proliferation. Thus, the animal will have more lymphocytes which are able to respond to the stimulating antigen, i.e., the animal "learns" to deal with antigens to which it is exposed. This learning process is the basis of all vaccination procedures.

The clonal selection theory is generally accepted as providing a valid outline of an immune response. However, at the molecular and cellular level, many key questions remain unanswered despite intensive study and are in need of theoretical analysis. For example, it has been found that, under some experimental conditions, contact between antigen and responsive lymphocytes will lead to paralysis or cell death; under other conditions, the contact leads to proliferation and antibody secretion. Among the relevant conditions are (i) the presence of other cells, especially other lymphocytes which have matured in the thymus and adherent cells, and their prior experience with antigen; (ii) the presence in the medium of other molecules derived from thymus-derived lymphocyte cells; and (iii) the molecular structure of the antigen, including the number and spacing of sites which can bind antibodies. It is difficult if not hopeless to sort out the contributions of all these factors without theoretical models and analysis. Moreover there are many clinical situations in which the immune response is ineffective or even self-destructive. To cite one instance: many cancer patients are making an immune response of sorts against their tumors but it is clearly ineffective except perhaps in preventing metastases. Why it is ineffective and

what can be done by way of immunotherapy to improve the patients' prospects are central questions being studied by many hundreds of experimental scientists and clinicians. We believe that a parallel theoretical effort will be recognized as necessary within the next few years.

Our theoretical work in immunology has concentrated on three areas: (1) analysis of key experimental techniques or assays in immunology, (2) modeling of the interaction between antigens and the receptors on lymphocyte surfaces, and (3) modeling of the regulation and function of an immune response. Progress continued in each of these areas during the year. In particular, we were able to elucidate the conditions under which a certain assay, the "hemolytic plaque assay," can be used for identifying those cells in a clone which are producing altered antibody molecules.⁴ According to the clonal selection theory, such cells should be the exception rather than the rule, but recent experiments indicate they may be an important exception whereby the immune system generates new and more effective antibodies. We also derived an improved theory for the aggregation of lymphocyte receptors by antigen, which may be the key event in triggering the lymphocyte immune response.

Our efforts in theoretical immunology have received considerable recognition. During the year we presented several invited talks and prepared an invited paper² for an immunology journal. Our assistance was requested in establishing a program in theoretical immunology at the National Cancer Institute (NCI) and in response, one of our staff members will be spending the next year at NCI's Laboratory of Theoretical Biology.

Research has continued in collaboration with experimental scientists in H Division and at the University of Colorado Medical Center. This has included a continuing study of the effects of ionizing radiation on DNA,⁶ which are believed to constitute the main biological lesions produced by low levels of radiation and to be responsible for genetic mutations and cancer.

In addition, several important studies in molecular biology were carried out. In particular it was shown that an apparent orderliness in the sequence of bases (chemical building blocks) in DNA has a surprisingly high probability of arising by chance.

Finally, it should be noted that over the past several years Alan Perelson has invented, with George Oster at Berkeley, a new method for treating complex systems of reacting chemicals. In this method, analogies with electrical network theory were exploited. A number of improvements and clarifications were carried out¹⁵⁻²² this year as well as the preparation of a review article,²⁰ and the publication of a comprehensive presentation of the method.^{13,14}

II. RESEARCH HIGHLIGHTS

A. Immunology

1. The hemolytic plaque assay

In the earliest version of this, the most important assay in cellular immunology, a layer of red blood cells (RBC) was covered by a layer of lymphocytes, some of which were secreting antibodies which would bind to the red cells. After suitable incubation, a plaque, i.e., a region of red cell destruction, became visible around each lymphocyte which was secreting anti-RBC antibodies. The assay was first used to enumerate the number of cells in an animal which secrete antibody against RBC. Later it was found that various antigens could be chemically coupled to the RBC so that the assay could be used to detect cells secreting antibodies of other specificities. Moreover plaque formation could be inhibited by introducing free antigen into the medium; i.e., at high enough concentrations, the free antigen binds the majority of antibody molecules and renders them unavailable for binding to red cells. From inhibition data it was sometimes possible to deduce antigen-antibody equilibrium constants.

During the preceding year, we developed a mathematical model of plaque formation in which antibody secretion, diffusion, and binding

to free antigen or to RBC are taken into account. With this model we were able to clarify the experimental conditions in which antigen inhibition of plaque formation is a valid assay for antigen-antibody affinity. It should be noted that these conditions are by no means obvious and that their understanding really requires the use of the mathematical model together with experimental results. For example, to inhibit plaque formation for the type G antibody, it is essential that the spacing of antigen determinants on the red cells be small enough and that multivalent attachments of an antibody molecule to a red cell be highly probable.

The assay has recently been used by Alistair Cunningham at the Australian National University with mixed populations of red cells (e.g., from a sheep and a goat). He found that most of the cells in a clone give plaques of one morphology: either clear indicating antibody binding to both kinds of red cells; cloudy indicating binding to only one kind of cell; or sombrero (a clear center with a cloudy brim) indicating unequal binding to the two red cell populations. However, Cunningham found that there is a startlingly high probability (~ 3% per mitosis) that a clone will produce plaques of altered morphology. His interpretation was that cells with a new antibody specificity were present as if generated by a process of somatic mutation (mutation in the body cells as opposed to the germ plasm). We have used our theory to show that, while plaque morphology can also be affected by secretion rates, it was probably a valid indicator of altered antibody specificity in Cunningham's assay.⁴ These experiments are the first clear revelation of somatic generation of antibody diversity and thus of basic importance. Their interpretation had been widely doubted.

DeLisi is currently preparing a monograph on our theoretical interpretation of the hemolytic plaque and related assays.

2. Interactions of lymphocytes with antigens

A typical B lymphocyte has of the order of 10^5 bivalent antibody molecules (receptors) on its surface. These molecules can move in

the plane of the cell membrane and hence, when the cell is exposed to a solution of multivalent antigen molecules, it is possible for an antigen-receptor lattice to form on the cell surface. Such lattice formation has been observed and is known as "patching." It may represent a critical stage in the activation of lymphocytes by antigen.¹ (Fig. 28.)

During the present year we extended our theoretical models of patching to accommodate the experimentally important competition between multivalent and monovalent antigens² and to include a better treatment of the antigen valence and of the kinetics of lattice formation (Fig. 29). In these models critical conditions for patch formation are derived; they involve the receptor number and mobility, the antigen concentration and valence, and the antigen receptor reaction-rate constants. Experiments to test the predictions have been suggested. These are likely to indicate some revisions in the models.

B. Molecular Biology

1. Radiation damage to nucleic acids

We have continued cooperative efforts with H Division on the effects of ionizing radiation on nucleic acid polymers and oligomers in solution.⁶ The experimental data obtained in Group H-9 were of three kinds. From optical absorption data we obtained the frequency of some, but not all damage to the monomers. From chromatographic data together with a theoretical model we obtained the molecular weight distributions of the damaged polymers. Finally, the temperature distribution of the binding of damaged-to-intact nucleic acid polymers was measured. The temperature distribution depends both on the length of the damaged segments and on other molecular damage which does not lead to polymer termination.¹² By making a self-consistent analysis of all these data, it was possible to obtain the incidence of various damaging events per unit radiation dose and to distinguish events leading (i) to chain termination, (ii) to altered base pairing and hence altered stability of the double helix, and

Fig. 28. Binding of multivalent antigen to cells. Multivalent antigen is assumed first to combine reversibly with a cell receptor, with forward and reverse rate constants k_a and k_d . Then irreversible binding is established to further receptors with rate constant k_i .

Fig. 29. Relative rate of lattice formation with hapten inhibition. (Hapten is a substance that binds with antibody.) The ordinate is proportional to the rate of lattice formation. The abscissa K_c is the equilibrium constant for antigen binding to a single receptor (K) times the concentration of free antigen (c). Y is the ratio of hapten binding to antigen binding. As Y increases, the rate of lattice formation decreases.

(iii) to base lesions not affecting helix stability. Moreover, from experimental results with radical scavengers present, it was possible to separate the effects due to each of the three most prominent radiation-induced free radicals in aqueous solution, namely the hydrated electron, OH^- and H^+ .

2. Nucleic acid sequence and structure

The activity of many of the genes in bacterial DNA has been found to be modulated by the very specific and tight binding of certain protein molecules (repressors) to certain operator regions of the DNA. It appears as if the base sequence in an operator region may favor a local three-dimensional folding of the molecule so as to distinguish that region from all others. Moreover, in small single-stranded RNA molecules, there is considerable self-complementarity and local folding. It has therefore been suggested that strong evolutionary pressures must have selected those base sequences that can form local three-dimensional structures. However we have shown that, even in random base sequences, there is a surprisingly high probability of self-complementarity and order. Therefore caution should be observed in interpreting DNA and RNA sequence significance.

3. Macromolecular processes

The motion of macromolecules, such as repressor molecules in cells, is treated customarily as a diffusion process. However recent advances in fluid dynamics theory indicate that it may be important to account for many-particle velocity correlations which lead to a persistence of molecular motion. We have developed a theory along these lines, applied it to the kinetics of operator-repressor interaction, and obtained improved agreement with experiment.

C. Analysis of Clinical Data

1. Incidence of chromosomal abnormalities

In recent years, it has been discovered that many human disorders,

ranging from mongolism to some forms of leukemia, are caused by or at least associated with specific gross chromosomal abnormalities. It is therefore important to see whether such abnormalities are caused by environmental factors and if so, which ones. For the past ten years, all babies born in Denver have been checked for abnormal numbers of sex chromosomes or of chromosome 21 (involved in mongolism). Over a hundred individuals with such abnormalities have been identified. We have been collaborating with scientists at the University of Colorado in interpreting these data. A careful statistical analysis has indicated that, with high confidence, approximately half of the abnormalities occur in epidemics, i.e., as time clustered events.⁷ These may be caused by specific and identifiable environmental factors, which are of course being sought.

III. T-10 PUBLICATIONS

1. G. I. Bell, "On Signals Generated by the Binding of Multivalent Antigens to Immunocompetent Cells," in Mammalian Cells; Probes and Problems, AEC report CONF-731007 (1975).
2. G. I. Bell, "B Lymphocyte Activation and Lattice Formation," Transplant. Rev. 23, 23 (1975).
3. G. I. Bell, et al., "Preliminary Report - Study of Fast Reactor Safety Test Facilities," Los Alamos Scientific Laboratory report LA-5978-MS (1975).
4. C. DeLisi and G. I. Bell, "Plaque Morphology as an Antibody Specificity Marker; The Physical Chemical Foundations of the Marker," Immunochemistry (in press).
5. C. DeLisi, "The Kinetics of Hemolytic Plaque Formation. V. The Influence of Geometry on Plaque Growth," J. Theor. Biol.. (in press).
6. F. N. Hayes, D. E. Hoard, P. N. Dean, and W. B. Goad, "Degradation of Nucleic Acid in Aqueous Solution by Ionizing Radiation. II. Analysis of the Contribution of Various Water Radicals to the Loss-of-Ultra-Violet Absorption by Thymidylate Solutions During X-irradiation," Int. J. Radiat. Biol. 26, 511-522 (1974).
7. W. Goad, A. Robinson, and T. T. Puck, "Incidence of Aneuploidy in a Human Population," Am. J. Human Genetics (in press).

8. S. L. Shapiro, A. J. Campillo, V. H. Kollman, and W. B. Goad, "Excitons in DNA," Optics Communications (accepted for publication).
9. B. Goldstein and C. DeLisi, "Immunodiffusion in Cells Containing Erythrocyte Antigen. II. Analysis of Experiments Involving the Diffusion of Antiserum from a Circular Well," Immunochemistry (in press).
10. A. Perelson and C. DeLisi, "A Systematic and Graphical Method for Generating the Kinetic Equations Governing the Growth of Aggregates," J. Chem. Phys. 62, 4053-4061 (1975).
11. A. Perelson and C. DeLisi, "Infinite Systems of Coupled Quadratic Nonlinear Differential Equations," SIAM Review (in press).
12. C. DeLisi, "Statistical Thermodynamics of Oligomer Polymer Interactions," Biopolymers 13, 230 (1974).
13. G. Oster and A. Perelson, "Chemical Reaction Dynamics: I. Geometric Structure," Arch. Rational Mech. Anal. 55, 230-274 (1974).
14. A. Perelson and G. Oster, "Chemical Reaction Dynamics: II. Network Structure," Arch. Rational Mech. Anal. 57, 31-98 (1974).
15. G. Oster and A. Perelson, "Chemical Reaction Networks," IEEE Trans. Circuits and Systems CAS-21, 709-721 (1975).
16. A. Perelson, "Bond Graph Sign Conventions," Trans. ASME, J. Dynamic Systems, Measurement, and Control 97, 184-188 (1975).
17. A. Perelson, "Bond Graph Junction Structures," Trans. ASME, J. Dynamic Systems, Measurement, and Control 97, 189-195 (1975).
18. A. Perelson, "Discussion of Properties of Bond Graph Junction Structure Matrices," J. Dynamic Systems, Measurement, and Control (in press).
19. A. Perelson, "Description of Electrical Networks Using Bond Graphs," Int. J. Circuit Theory and Applications (in press).
20. A. Perelson, "Network Thermodynamics: An Overview," Biophysical J. (in press).
21. A. Perelson, "A Note on the Qualitative Theory of Lumped Parameter Systems," Chem. Eng. Sci. (in press).
22. A. Perelson and G. Oster, "On the Application of Network Theory to Nonisothermal Systems," Int. J. Circuit Theory and Applications (accepted for publication).

IV. T-10 OUTSIDE TALKS AND SEMINARS

1. G. I. Bell, "B Lymphocyte Activation and Lattice Formation," presented at the University of Colorado Department of Biophysics, the Basel Institute of Immunology, and the University of London, Tumor Immunology Unit.
2. G. I. Bell, "Models of the Hemolytic Plaque Assay," presented at the Massachusetts Institute of Technology, Cancer Research Center.

3. G. I. Bell, "Mathematical Immunology," presented at the Gordon Conference on Theoretical Biology.
4. C. DeLisi, "Models of the Hemolytic Plaque Assay," presented at Yale University, Columbia University, and the National Cancer Institute.
5. A. Perelson, "The Immune System at the Cell and Population Levels," presented at the University of Chicago.
6. A. Perelson, "Chemical Reaction Networks," presented at the University of California-Santa Cruz.
7. A. Perelson, "Network Thermodynamics Analysis and Models of Gravitational Receptors," presented at NASA Ames Research Center, Conference on Gravity and the Cell.

GROUP T-DOT - OTHER THEORY

I. INTRODUCTION

The group T-DOT (where DOT is an abbreviation for Division Office - Technical) is the administrative assignment for efforts too small to justify the formation of a group, for the gestation of new groups, or for personnel working directly with Division Office staff.

Present work is principally in the areas of statistical physics, astrophysics, and nonlinear differential equations. Highlights of some of this research are described below.

II. RESEARCH HIGHLIGHTS

A. Statistical Physics

1. Computer studies on fluid systems of hard core particles

The interaction between computer studies and purely analytical theoretical investigations in statistical mechanics has proven to be extremely fruitful in advancing our knowledge of the behavior of molecular systems. Often one can most easily test theoretical predictions by comparing them with data from computer studies on simple hard core systems. A successful confrontation then leads to increased confidence in applications of the theory to more realistic models of actual physical interactions.

We have nearly completed an extensive numerical investigation of the self-diffusion process in hard spheres and disks using Monte Carlo and both "equilibrium" and "nonequilibrium" molecular dynamics techniques.¹⁵ Data have been obtained on the velocity autocorrelation function, the Fick's law self-diffusion coefficient, the displacement moments, the van Hove self-correlation function, and the super-Burnett self-diffusion coefficient over a wide range of densities.

The results confirm and strengthen earlier evidence for the long-time tails of the velocity autocorrelation functions, the related divergence of the self-diffusion coefficient for hard disks, and its slow convergence for hard spheres. Our results also support recent theoretical predictions of the divergence of the super-Burnett coefficient for hard disks, and probably for hard spheres as well, although less convincingly. They suggest that the van Hove self-correlation function for hard disks remains non-Gaussian at long times, but are consistent with an approach to Gaussian form in the case of hard spheres. From a fundamental point of view, the most important conclusion is that in general local equilibrium is approached much more slowly than was formerly expected from theory.

In support of this work we have also undertaken theoretical calculations of the long-time limit and the time dependence of the super-Burnett self-diffusion coefficient given by the Boltzmann equation, and of finite system effects on the velocity autocorrelation function and the super-Burnett self-diffusion coefficient. Partial accounts¹⁵ of this work have been presented and published and several additional publications are in preparation.

2. The Ehrenfest wind-tree model

We have studied the mean-free-time and the short-time dependence of the velocity autocorrelation function $\langle V(o)V(t) \rangle$ in the Ehrenfest wind-tree model (point particles scattered by immovable parallel squares). In the case in which the squares are allowed to overlap each other, the mean-free-time was found to disagree with the conventional "exact" theoretical calculation, due to the nonergodic character of this model.

3. Solid ^3He at low temperature

Solid ^3He at low temperatures (below 100 mK) and for molar volumes between $24.25 \text{ cm}^3/\text{mole}$ and $21.0 \text{ cm}^3/\text{mole}$ was thought to behave thermodynamically as a Heisenberg antiferromagnet with nearest neighbor and next nearest neighbor interactions. Until approximately

a year ago, such a theory described all low temperature data quite well. However, during the summer of 1974 new data was published which was claimed to be inconsistent with such a theory. We have shown that such was not necessarily the case and, in fact, the experimental data then reported do not uniquely determine the theory.¹⁰ In March 1975, the results of another experiment were published giving more data at molar volume $24.25 \text{ cm}^3/\text{mole}$. Subsequently we have shown that although all data at any fixed molar volume are still describable with the above-mentioned theory, it is extremely difficult to fit the data at all molar volumes with a reasonable volume dependence of this theory. Therefore, we conclude that if the experiments are correct, a new theoretical model of ^3He seems necessary.

4. One-dimensional magnetic systems

Magnetic systems, in particular cerium magnesium nitrate (CMN), have served as both thermometers and refrigerators in low temperature work. For example, via adiabatic demagnetization, CMN can be used to cool a sample to quite low temperatures. It has been recognized that a one-dimensional magnet holds promise of being a more efficient refrigerator than a three-dimensional magnet such as CMN due to the larger specific heat of one-dimensional magnetic systems. For a number of years, this effect was not taken seriously since the physical world is three dimensional. However, magnetic systems with very weak interactions in two dimensions as compared to the third direction are now quite well known in nature.

We have been conducting a theoretical study of such systems to determine if these essentially one-dimensional systems might serve as a more efficient refrigerator. An abstract has been submitted to the Magnetism and Magnetic Materials meeting of December 9 - 12, 1975. More work is planned and a paper is to be written.

B. Hydrodynamic Turbulence

To date "successful" studies of hydrodynamic turbulence have mostly been statistical in nature. In brief, one assumes an initial

distribution function (over velocity fields) which determines multi-velocity correlation functions. The (non-linear) Navier-Stokes equations of motion then relate various such functions to one another in a typical hierarchical scheme. These equations can be re-expressed through a functional-differential equation that the so-called generating functional of the theory obeys. This generating functional is of identical format to a statistical mechanics partition function, or a field-theoretic path-integral generating functional, and so the statistical theory is amenable to usual high-energy physics diagrammatic techniques.

For the following reasons, our approach has been largely otherwise. Hierarchical equations are notoriously insoluble at present. Diagrammatic techniques constitute a coupling-constant perturbative solution to these equations which are, accordingly, apt to be meaningless for strong coupling (i.e. when non-linearities are deeply significant, rather than fine corrections to a qualitatively accurate initial description.) In the case of Navier-Stokes turbulence, the interplay between a quadratic (transport) non-linearity and a higher order singular perturbation (viscous damping) controls dissipation rates and sets the scales of motion in a way which is, qualitatively, worlds removed from a linearized treatment. Accordingly, a meaningful diagrammatic approach must immediately sum large classes of diagrams to produce "dressed" propagators, etc. simply to achieve a reasonable starting point.

In the last five years significant mathematical advances have been made in comprehending chaotic behavior in causal systems themselves, without a priori injection of statistical assumptions. Also, in this same time period, the renormalization group of field theory has been fitted upon systems of a mutually cooperating vast number of degrees of freedom in the form of a regimen with qualitative appeal. This approach consists in a recursive averaging over modes of excitation and transformation to a self-recursive averaging over modes of excitation and transformation to a self-similar system.

Our attempts to formulate a theory of turbulence is aimed at a hybrid of these two bodies of thought.

The first-mentioned, mathematical, advance focuses attention upon asymptotic stability sets that are both chaotic in structure and ergodically evolved through. Such behavior is a believable representation of observed turbulent motion. The stages of onset of turbulence clearly appear to be of a bifurcation character, the theory of which collaterally has been significantly advancing these last years. Accordingly, we have felt the time appropriate to investigate Navier-Stokes-like systems in a non-statistical fashion with an eye towards discovering its chaotic limit sets. We initially investigated simpler, lower dimensionality (but dissipative and nonlinear) Hamiltonian systems. Apart from improving our comprehension of the non-linearity-singular-perturbation interplay, we were very quickly led to a realization of the significance of stability sets in turbulence. Consequently, we began studies of stability sets in discrete recursion relations as these are simpler than differential equations, yet akin in the sense of a difference equation approximant. It has been elsewhere speculated this summer that the specific equation entertained probably possesses "strange attractor" stability sets that might characterize fully developed turbulence. That equation, the well-known population equation,

$$x_{n+1} = \lambda x_n (1 - x_n)$$

crudely resembles the Navier-Stokes equations in its non-linearity structure and is possibly a model for a suitable (averaged) mode of excitation. We have carefully analyzed the rich bifurcation structure but, to date, have not succeeded in quantitatively comprehending its Cantor-like infinite stability sets and have only crudely related it to modes of the actual equations of motion. The bifurcation structure is known to be independent of the exact form of the recursion relation, and we have discovered and are pursuing this independence (or universality) in quantitative ways. Universality

is significant in that it implies that a naively simple equation might prove appropriate to the underlying Navier-Stokes equation.

Along the second line of thought, we explored the applicability of K. Wilson's renormalization group approach. Striking similarities to turbulence arise immediately upon even cursory acquaintance with its critical phenomena applications. The sort of problems hopefully amenable to such treatment are characterized by a vast diversity of length-scales. Although not immediately apparent in statistical studies of turbulence, multiple length-scales are indeed a specialty of turbulence. The most successful phenomenologically inspired theory concerns itself with the so-called "energy cascade". Essentially, energy is fed into the mean flow (the largest scale size in the system) to be dissipated (in relatively inviscid systems) only in the finest scale eddies, these two scales many orders of magnitude removed from one another. Since one anticipates that any motions of roughly similar length and time scales can significantly interchange energy, and since a non-linearity generates higher harmonics, one is led naturally to a picture of a continuous range of length scales of eddies through which energy is successively transported from the largest scale of injection to the microscale of viscous dissipation. While there is much to recommend such a scheme, essentially no theoretical derivation of its presence exists. It is exactly this cascade structure that we would hope to be able to decoct from the Navier-Stokes equation through the auspices of the renormalization group. That is, one hopes that suitably averaged modes obey essentially discrete equations of roughly "nearest-neighbor" coupling to one another, homogenous with respect to average wave number. Such a system of equations has surfaced in the literature with a "derivation" of, at best, heuristic value. However, they generate stable spectra in good agreement with experiment. An honest derivation (of probably slightly different equations) would constitute a true theory of turbulence. In fact it is exactly this system of equations that is structurally similar (though of several variables) to our earlier mentioned population recursion relation. Accordingly, our endeavor has consisted of a variety of "filterings" of different

modes of the Navier-Stokes equations and believable approximations as to which terms initially and tentatively to retain. To date our work has been successful only in a qualitative sense. Nevertheless we are hopeful that a physical scheme and its mathematical implications will be realized through further exploration of these ideas.

C. Astrophysics

1. Stellar opacity data

Thirty-nine tables of stellar opacity data have been prepared for publication in the Astrophysical Journal Supplements. These tables have been requested by workers in the fields of stellar structure, stellar evolution, and stellar pulsation, and some have been used without publication since 1971. Careful study shows that the data are reasonably homogeneous even though the computing programs have undergone considerable modification by the efforts of Group T-4.

2. Cosmic gamma bursts

Several hydrodynamic problems have been done to see if the LASL-discovered cosmic gamma bursts could be due to small relativistically approaching iron pellets which see visible solar photons blue-shifted to x-ray and then scatter these photons, blue-shifted again to the gamma rays that are observed. To match observed pulse durations, the time scale for the receipt of the x-rays in the frame of the pellet is so long that the pellet explodes too rapidly and is too cool and diffuse to produce the observed gamma rays.

3. Color history of Cepheids and R. R. Lyrae stars

The color history through the pulsating periods of Cepheids and R. R. Lyrae stars has been calculated by a radiation transport code in collaboration with C. G. Davis (J-15).^{4,5,6} The purpose is to see how color means can be related to the effective surface temperature of the stars. The relation is vital in determining the masses of these pulsating stars since only the color history is observed but mean effective temperatures are needed in the interpretation of observations.

4. Calculations of strictly periodic stellar pulsation

A large effort has gone into developing a new fast method for calculating strictly periodic stellar pulsation. Following Stellingwerf who has pioneered this technique, initial values of temperature, radii, velocities, and the period are alternately adjusted to be just right for strictly periodic behavior. Much greater speed in reaching limiting amplitudes of pulsations is possible by this method because the complete time behavior no longer needs to be followed. Application of this method is planned for the pulsations of dwarf and white dwarf stars where pulsation growth rates are very slow.

5. Multiple period Cepheid project

Calculations using the older initial value approach are in progress for double mode (therefore non-periodic) pulsations of an R. R. Lyrae variable AC Andromedae. The ratio of the two periods observed simultaneously is related to the star's mass, and non-linear calculations are needed to calibrate the effect of both pulsation modes operating together. This multiple period Cepheid project will be reviewed in an International Astronomical Union Colloquium in Budapest next September.^{7,8}

D. Nonlinear Partial Differential Equations

1. The abstract Cauchy problem

Very recently, we have done preliminary work for forthcoming research on the abstract Cauchy problem:

$$\begin{aligned}\frac{du}{dt} + A(u) &= 0, & t > 0 \\ u(0) &= x, & u \in \text{Hilbert space } H,\end{aligned}$$

where $A(u)$ is a nonlinear operator. This could represent a problem in nonlinear partial DE's. We know that if $A(u)$ is maximal monotone in some sense, then it is the generator of a nonlinear semigroup

$u = T(t)x$, $T(0) = I$, that solves the problem, and vice versa. $T(t)$ is called the solution operator. Of interest is the eigenvalue problem $T(t)V = \lambda(t)V$ for the nonlinear time-dependent solution operator, and what we can find out about it from prior attributes that we can assign to the generator $A(u)$ (aside from being maximal monotone). We have a hunch that the eigenelements of the solution operator have something to do with solitary waves, and that we might be able to get an abstract characterization of solitons in this way. (The importance of soliton-like solutions in quantum field theory, water wave propagation, laser phenomena, and statistical systems is now recognized.)

2. "Superlinear" Hammerstein operators

We are now completing a phase of work on nonlinear Hammerstein operator¹³ of the type we call "superlinear." Under study is the eigenvalue problem

$$\lambda u(s) = \int_0^1 K(s,t)f(t,u(t))d\sigma(t) \quad , \quad \sigma(t) \in \uparrow$$

where $f(t,u)$ has superlinear form, Fig. 30. The idea is to find conditions on the kernel $K(s,t)$ and on the function $f(t,0)$ such that the branches of eigensolutions are devoid of secondary bifurcations and other degeneracies.

Fig. 30

First we studied the discrete case where $\sigma(t)$ is an increasing step function.

We were able to find some conditions and submitted this work to Mathematisches Annalen for publication.

Next we worked on the case where $\sigma(t)$ is continuous increasing. This problem is much more difficult, but again we have found conditions.

Sublinear cases are still to be treated. Also we will attempt to extend these results to other types of non-linear operators.

3. Stationary solutions to the problem of Taylor instability

We have worked on the question of stationary solutions of the problem of Taylor instability. The unstable stationary solutions one obtains in the ordinary cylindrical geometry were investigated.⁶ Then we showed how one might stabilize the interfaces by using a rhombic cylinder as a geometry.

III. T-DOT PUBLICATIONS

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2. A. N. Cox, D. S. King, and J. E. Tabor, "Non-Pulsating Stars and the Population I and II Instability Strips," Proc. of IAU Sym. 59 Stellar Instability and Evolution, Reidel Pub. Co., 1974.
3. A. N. Cox and J. E. Tabor, "A Search for Beta Cephei Pulsation in Extreme Composition Models," Proc. of IAU Sym. 59 Stellar Instability and Evolution, Reidel Pub. Co., 1974.
4. A. N. Cox and C. G. Davis, "Non-Linear Radiation Transport Calculations to Obtain Mean Colors and to Verify the Wesselink Method," Mem. Soc. R. Sci. Liege 8, 209, (1975).
5. A. N. Cox and C. G. Davis, "Mean Colors of Cepheids," Proc. of Goddard Cepheid Modeling Conference and Workshop, 1975 (in press).
6. A. N. Cox and C. G. Davis, "Theoretical Mean Colors of Pulsating Cepheids," Proc. of Multicolor Photometry and the Theoretical H-R Diagram, Dudley Observatory, Report 9, 297, (1975).
7. A. N. Cox and J. P. Cox, "Cepheid Pulsation Theory and Multiperiodic Cepheid Variables," Proc. of IAU Colloquium 29 Multiperiodic Variable Stars, Reidel Pub. Co. (in press).
8. D. S. King, A. N. Cox, and S. W. Hodson, "On the Mass of AC Andromedae," Proc. of IAU Colloquium 29 Multiperiodic Variable Stars, Reidel Pub. Co. (in press).

9. M. Feigenbaum, "The Relationship between the Normalization Coefficient and Dispersion Function for the Multi-group Transport equation," accepted for publication in the Journal of Mathematical Physics and presented at the Fourth Annual Conference on transport Theory, Blacksburg, Virginia, March 10 to 13, 1975.
10. J. D. Johnson and E. C. D. Cohen, "Is Solid ^3He a Heisenberg Antiferromagnet?", accepted for publication in Physical Review B.
11. George H. Pimbley, "Periodic Solutions of Predator-Prey Equations Simulating an Immune Response II," Mathematical Biosciences 21, 251-271 (1974).
12. George H. Pimbley, "Periodic Solutions of Third Order Predator-Prey Equations Simulating an Immune Response," Archive for Rational Mechanics and Analysis 55, No. 2, 93-123 (1974).
13. George H. Pimbley, "A Region of No Secondary Bifurcation for Nonlinear Hammerstein Equations," with N.W. Bazley, J. of Applied Math. & Physics (ZAMP), Vol. 25, 743-751 (1974).
14. George H. Pimbley, "Stationary Solutions of the Problem of Rayleigh-Taylor Instability," accepted, J. of Math. Analysis and Applications, January, 1975.
15. W. W. Wood, "Computer Studies on Fluid Systems of Hard-Core Particles," lecture series presented at the International Summer School on Fundamental Problems in Statistical Mechanics III, Wageningen, The Netherlands, July 29 - August 15, 1974; published in Fundamental Problems in Statistical Mechanics III, E. G. D. Cohen, Editor (North-Holland Publishing Company, Amsterdam, 1975); presented at Physics Department Seminar, University of Maryland, January 28, 1975, and as an invited paper at the Symposium on Molecular Dynamics, American Physical Society meeting, Denver, Colorado, April 1, 1975. Work done in collaboration with J. J. Erpenbeck.

IV. T-DOT OUTSIDE TALKS AND SEMINARS

1. J. D. Johnson and E. G. D. Cohen, "Nuclear Spin Ordering in Solid ^3He ," presented at the May, 1975, Yeshiva Meeting on Statistical Mechanics, Yeshiva University, New York.
2. George H. Pimbley, "Stationary Solutions of the Problem of Rayleigh-Taylor Instability," Lecture given at Dept. of Mathematics, University of Strathclyde, Glasgow, Scotland, October 17, 1974; Mathematical Institute, University of Cologne, Germany, December 4, 1974.

3. George H. Pimbley, "A Region of No Secondary Bifurcation for Hammerstein Operators, "Lecture given at Edinburgh Mathematical Society, Harriot-Watt University. Edinburgh, Scotland, October 18, 1974; Mathematical Institute, University of Oxford, Oxford, England, November 1, 1974; Mathematical Institute, University of Cologne, Germany, November 27, 1974; Mathematical Institute, Ruhr University, Bochum, Germany, December 3, 1974.
4. George H. Pimbley, "Periodic Solutions of Predator-Prey Equations Simulating an Immune Response, "Mathematical Institute, University of Cologne, Germany, December 11, 1974.
5. W. W. Wood, "Self-Diffusion in Hard-Core Fluids", seminar talk, University of Maryland, Physics Department Seminar, January 28, 1975.
6. W. W. Wood, "Cooperative Motions in Hard-Core Fluids", invited paper for Symposium on Molecular Dynamics, American Physical Society Meeting in Denver, April 1, 1975.

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