Meetings

Physics: Atomic, Molecular, and Solid-State

Reports of calculations that lend new understanding to the genetic code and magnetism were among the highlights of the 1968 international symposium on atomic, molecular, and solid-state physics. The real significance of the symposium, a joint project of the University of Florida and Uppsala University, Sweden, was in the revelation that quantum theorists are now able to make highly accurate calculations on the structure of matter. This year's symposium marks the emergence of theoretical research in solid-state physics and quantum chemistry into a new era of confidence and maturity. More than 160 scientists from throughout the world attended.

Per-Olov Lowdin, director of the University of Florida's Quantum Theory Project and professor of quantum chemistry at Uppsala, said quantum theorists, by their papers presented at the symposium, "showed the ability to calculate with confidence properties that have not yet been attainable by laboratory measurement." In fact, it is now a question of calculating very refined details, according to Lowdin. Theorists at the symposium argued over small differences between theory and experiments in the band theory of solids.

Quantum biology is an area which recently has loomed into the spotlight in the quantum field. One of the pioneers in this new field, Madame Alberte Pullman (Paris), discussed recent progress in quantum biochemistry; in her invited survey lecture, she stressed the importance of intermolecular forces for the recognition process between molecules in determining how and whether they may fit together. She reported the results of some calculations on various types of pairings of nitrogen bases that occur in the DNA molecule in the living cells in contrast to the crystallized materials.

The idea of the role of the protons in the genetic code as forming the essential part of the genetic message was first formulated by Per-Olov Lowdin 6 years ago. Most of the work has since been carried out by the Uppsala and University of Florida projects. Now this idea is being pursued by several research centers, including the Quantum Theory Group of the Center for Theoretical Biology at the State University of New York at Buffalo.

One of the most renowned researchers in this field is Robert Rein, chairman and principal cancer research scientist in the Department of Experimental Pathology, Roswell Park Memorial Institute, and Center for Theoretical Biology and Department of Biophysics, State University of New York at Buffalo.

Rein remarked that scientists are now beginning to understand the concept of DNA transfer. He reported on his calculations showing how nitrogen bases are bonded and stacked in forming DNA (deoxyribonucleic acid) and at what temperature DNA "melts." In reporting on his "theory of intermolecular interactions," Rein pointed out that they "include hydrogen bonding and stacking, and play a significant role in the stabilization of ordered macromolecular configurations. Thus the calculation of these forces often represent a first step toward a quantitative theory of macromolecular stability.

"The physical nature of these forces are peculiar in the sense that the interacting molecules are not strictly separable electronically nor is the dipole approximation of the conventional London technique applicable. We were thus concerned with the development of more appropriate computational methods for the treatment of interactions in the weakly overlapping range. These methods have been applied to the study of various interactions in DNA. For example, the stacking interactions between the bases for all possible configurations have been calculated. Other interesting applications of the technique involve the study of the energetics of the Crick Wobble hypothesis and the energetics of various hydrogen bonding schemes. Further aspects of hydrogen bonding were also under investigation and included an analysis of the proton vibrational states in the hydrogen bonds connecting the DNA bases.

"As a first step in the investigation of water structure and solvation effects, a study of hydrogen bonding between water molecules was begun.

"Another area of our research interest is in the development of theories which connect the microscopic interaction energies with macroscopic observations. To this end we used an extension of the Ising model to analyze experimental melting curves on synthetic DNA-like polymers. The stacking energies obtained from this analysis are in good agreement with the values calculated by quantum mechanical methods," Rein reported.

W. Macintyre, a University of Colorado chemist, reported some interesting results on the replication plane of the DNA molecule which may help to explain why the genetic code stays unchanged for millions of years.

Arthur J. Freeman, professor and chairman of physics at Northwestern University, reported on the work he and the University of Florida's Donald Ellis have done in the field of magnetism. "We have made significant advances in obtaining accurate solutions of polyatomic systems," Freeman said. "We are able to solve the complicated equations for the motion of electrons in these systems by means of a numerical integration technique on a high-speed digital computer." Freeman reported having "effectively solved the so-called many-center integral problems since the electron executes complicated motions around the different nuclei of the atoms.

In essence, he said, "We're trying to understand the origin of the magnetism of the compounds of iron and other similar systems." Freeman presented, for the first time, a highly refined technique for solving the so-called Schroedinger equation, which is fundamental to all quantum mechanics. Freeman also presented a paper on his own studies dealing with magnetism in the so-called rare earth metals, such as gadolinium and europium. In effect, he showed that the origin of magnetism in the rare earth metals is the same as in iron.

Another scientist, Wlodzimierz Kolos,

a visiting professor at the University of Chicago from the University of Warsaw, Poland, reported results proving his ability to make the most accurate computations to date on the simplest molecules, particularly the hydrogen molecule. Using a large computer at the University of Chicago, Kolos has been able to determine the stability and size of the molecule by making accurate computations of its binding energy.

Some new ideas on the treatment of electron scattering by atoms were reported by Frank H. Harris of Stanford University and Harvey H. Michels, United Aircraft Research Laboratories, East Hartford, Connecticut. The results reported on simple systems agree well with results of other methods and the new ideas seem to have great promise and application to much more complicated situations, even electron scattering by molecules.

Bernd T. Matthias, University of California, La Jolla, put forth some theories, followed by substantiating data, to show that superconductivity is more complex than was previously thought. He reported experimental evidence for the existence of at least four types of superconductors. Some had isotope effects; others had negative or positive characteristics; and some had no isotope effects.

Matthias discussed the mechanism of phonon interaction, the valence-electron mechanism found in certain transition metals, the *f*-electron mechanism in lanthanum and uranium, and finally the new exciting results found in metal borides.

The quantum theory institute, held annually at the University of Florida since 1960, opens in December for 4 weeks on the Florida campus. It then moves to Sanibel Island for 3 weeks. The final week is divided between the institute and the symposium.

During the last week, scientists held a discussion on the role of the scientist in modern society. These observations were made:

1) Society does have a right to know where its money is being spent; thus it is necessary that a certain amount of science must be applied to practical results.

2) The scientist also must be given a degree of time to pursue knowledge for the sake of knowledge itself.

3) There is a danger that society's demand for application may result in government and industry reducing support for basic research.

4) Scientists need a strong organization that will provide them with negotiating strength and the tool to tell their story to the public.

5) The better students are being attracted to the more exotic fields of science, and the basic sciences are suffering as a result.

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Calendar of Events

Courses

Images and Words, Santa Cruz, Calif., 1–13 July. Intended for photographers, writers, editors, historians, museum curators, and others who need a basic knowledge of the principles and techniques involved in making and procuring photographs for publication, preparing captions, and combining them with text. Fee: $175 (does not include housing and meals). (University of California Extension, Santa Cruz 95060)

NATO Advanced Study Institute in Psychogenetics, University of Birmingham, England, 5–18 September. Is intended primarily for graduates in psychology or genetics or allied fields. Discussions and practical work will cover the main approaches to the problems of behavioral inheritance as displayed in a variety of organisms, including man. (Professor P. L. Broadhurst or Professor J. L. Jinks, P.O. Box 563, University of Birmingham, Birmingham 15, England)

Iterative Analog Computation, Rolla, Mo., 24–28 June. Topics will include the configurations and control of the operational amplifier, digital logic components, the interface components which establish analog logic communications, and process engineering problem solutions on the parallel hybrid computer. Participants should hold at least a bachelor's degree and should be familiar with programming and operating analog computers. Fee: $175. (Extension Division, University of Missouri-Rolla, Rolla 65401)

Current Trends in Automatic Control Theory, St. Louis, Mo., 19–24 Aug. Included will be some of the latest topical areas of modern control theory. The prerequisite mathematical level will be a good M.S.; however, lectures will be conducted in a manner suitable for stimulating advanced research workers. (Dr. G. L. Esterson, Box 1048, Institute for Continuing Education in Engineering and Applied Science, Washington University, St. Louis, Mo. 63130)

Analysis of Settlement in Soils, Madison, Wis., 17–21 June. The course, which is intended for practicing engineers and contractors, will consider approaches to the determination of stresses and displacements in soil masses, as well as methods of analyzing total soil settlement. Fee: $150. (Dr. Dwight D. Zeck, Course Coordinator, University of Wisconsin-University Extension, 432 North Lake St., Madison 53706)