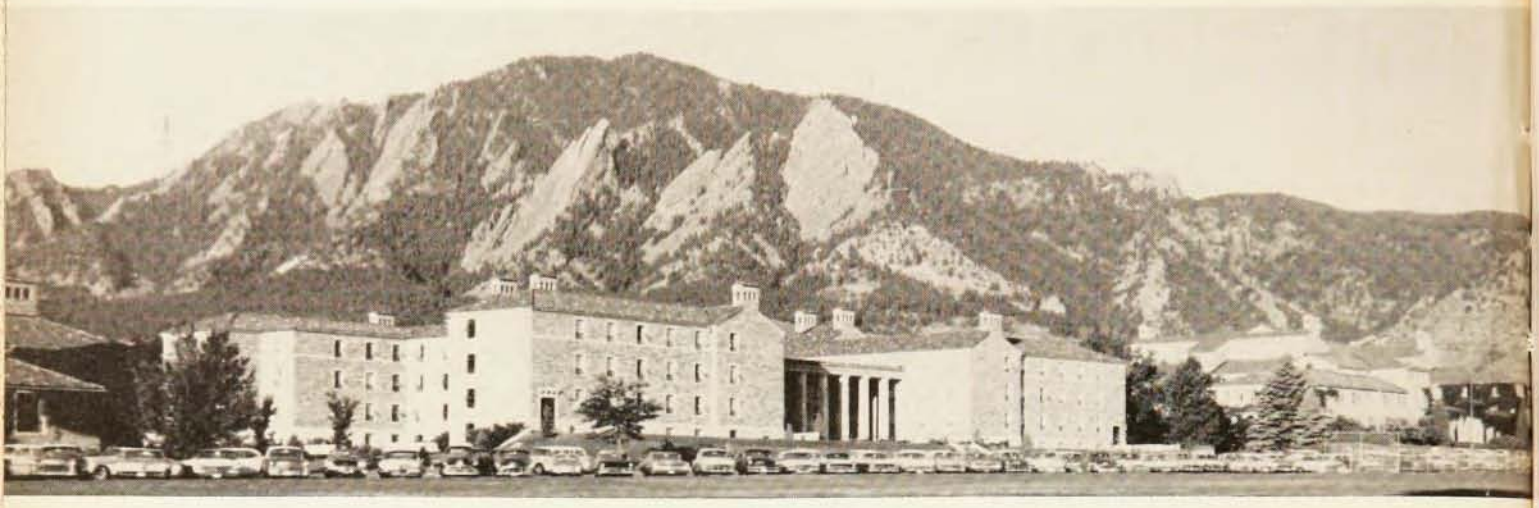

The University of Colorado's Libby Hall, headquarters for the conference.

Boulder Conference on MOLECULAR QUANTUM MECHANICS

By ***Klaus Ruedenberg***

IN this country there have been conferences on molecular quantum mechanics in 1951 on Shelter Island, New York, and at Austin, Texas, in 1955. The 1959 conference was held, with the support of the National Science Foundation, from June 21 to June 27 on the campus of the University of Colorado at Boulder. About one hundred molecular scientists from a dozen nations congregated there in order to review the advances which have been made in their field during the past four years.

The scientific pace of the meetings, held in the chemistry auditorium, was far from leisurely. About sixty half-hour contributions were fired off in rapid succession, at the rate of a dozen a day, in the course of a five-day week. The material presented was limited to new aspects of contemporary research on the electronic structure of molecules and, as a result of the steering committee's screening, was in general excellent. As the week progressed, the focus of interest was gradually shifted from mathematical intricacies of solutions of the many-body Schrödinger equation to an analysis of the physical and chemical significance of such solutions, and from there to problems of electronic spectra and electronic aspects of vibration, rotation, and magnetic resonance spectra. At the end there was even a physicochemical experimental demonstration to bring everybody firmly down to earth. Then, in the harmonious setting for the concluding after-banquet paper, C. A. Coulson tackled the delicate task of harnessing the wide-flung interests into a team of common purpose.

Thursday afternoon was designated as "William Moffitt Memorial Session". Dr. Coulson gave an address in W. Moffitt's honor, and his former students presented a series of papers on subjects lately of interest to him.

The chairman of the conference, Robert G. Parr of the Carnegie Institute of Technology, who was responsible for the total organization and for many details, carried out his task with notable success and deserves particular thanks. He was assisted by a steering committee consisting of the local chairman, J. de Heer (University of Colorado), J. O. Hirschfelder (University of Wisconsin), J. H. McMillan (National Science Foundation), R. S. Mulliken (University of Chicago), R. Pariser (E. I. du Pont de Nemours and Company), J. C. Slater (Massachusetts Institute of Technology), and W. T. Simpson (University of Washington). Simpson took over the chairmanship in Prof. Parr's absence during the last part of the conference.

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SINCE the proceedings of the conference appear in the April 1960 issue of the *Reviews of Modern Physics,* the following survey is merely intended as a sketch of the main themes of discussion.

The sessions on the first days dealt with contemporary attacks on the many-electron problem. It emerged that for many nonrelativistic *two*-electron problems there exist now extremely accurate calculations for the ground state. Solutions for the atomic systems H^-, He, Li^+, etc., up to Ne^{8+} were given with an accuracy of 0.01 ev, and for the H_2 molecule a calculation of the entire potential energy curve was presented with an accuracy of 0.0002 ev. Furthermore, very accurate calculations of the ground state of the coulombic *three*-body systems $e^+e^-e^-$, $p^+p^+\mu^-$, $d^+d^+\mu^-$ were reported.

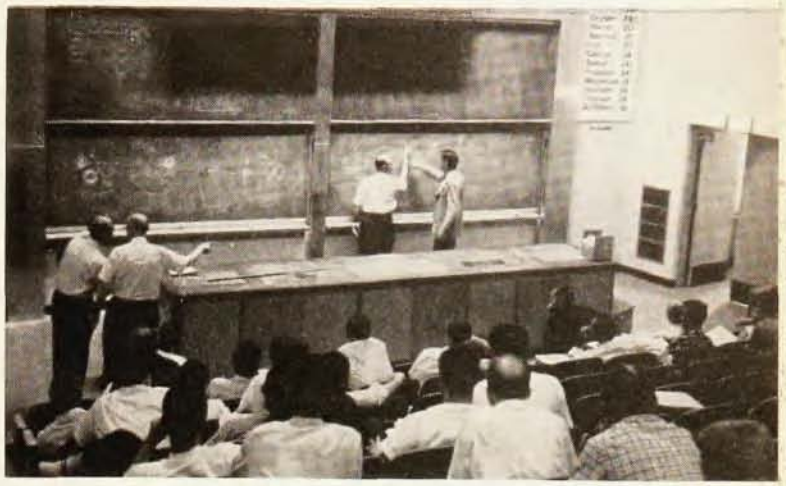
While these high-precision results were obtained by including explicitly the dependence upon *all* interparticle distances, the calculations reported for systems containing more than two electrons were based on superposing antisymmetrized products of one-electron functions. The work on atoms was mainly concerned with establishing self-consistent field solutions in analytic form for certain simple cases. The work on diatomic molecules ranged from self-consistent field calculations to more elaborate methods involving various degrees of configuration interaction. A fair number of investigations concerning small *poly*atomic molecules indicated that progress in that direction is also forthcoming. In spite of the limitations in accuracy still inherent in present approaches, the results reported were most encouraging in that they demonstrated the feasibility of a great number of reliable calculations which, because of their complexity, had been considered unmanageable less than a decade ago.

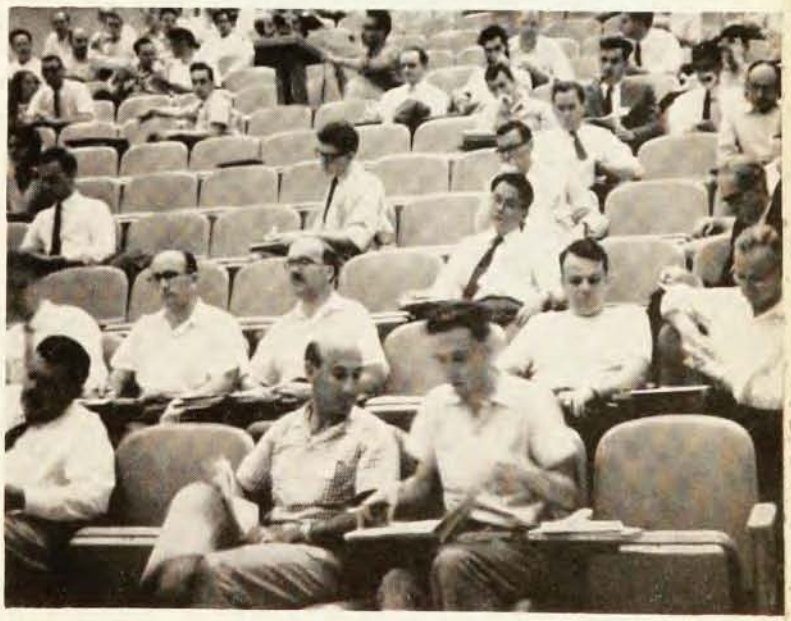
In view of these advances concerning the unrelativistic Schrödinger equation, a contribution which was of importance demonstrated the considerable magnitude of the *relativistic* corrections in atoms and molecules.

One afternoon was devoted to new types of approaches to the many-body problem which have been under development in recent years. The treatment of electron correlation in macroscopic systems by the plasma model was reviewed, and refinements of the Thomas-Fermi statistical model for possible application to molecules were discussed. Further contributions considered ways of exploiting more effectively the density matrix formalism, e.g., for finding a two-body variational principle of the n-body problem and for decomposing large systems into smaller fragments. Intermolecular forces were also discussed.

At midweek the topic turned to questions involving physical significance of the new-fangled elaborate calculations. The question of "atoms in molecules" was treated with the aim of improving the methods which try to achieve a cancellation of intra-atomic correlation energies between atoms and molecules. Furthermore an interpretation was proposed on how the physical nature of the chemical bond could be analyzed on the basis of complex wave functions.

The Thursday morning session proved that investiga-





Sessions were held in the University's chemistry auditorium during the week-long international conference. The discussion at the blackboard pictured in the top photograph is between B. Pullman (France) and H. C. Longuet-Higgins (England).

Photos by B. M. Axilrod

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tions of delocalized pi electrons in conjugated systems continue to furnish significant insights and stimulating suggestions for molecular systems in general. From several contributions it emerged that the old problem of bond alternation in long conjugated chains is finally becoming theoretically understood. Derivations of increasing sophistication were presented for the existence of properties, such as pairing of states and insignificance of certain overlap terms, which were originally deduced from the simple Hückel model. The power of such methods in matters of ultraviolet spectra was again exhibited by the prediction and verification of remarkable relations between the spectra of alternant hydrocarbons and their positive and negative ions.

In addition to a variety of other electronic spectra, electronic aspects of biochemical questions were reviewed.

It was refreshing to learn in the remaining days that, besides the classical ultraviolet spectra, electronic effects in other spectroscopic domains have become objects of serious theoretical investigations. Concerning electronic-vibronic interactions, analyses were given on several problems: on the question of forbidden electronic transitions becoming allowed via vibrational coupling, on the instability of the geometrical confirmation of degenerate electronic states (Jahn-Teller effect) in conjugated hydrocarbons, on the coupling between vibrational, electronic, and spin angular momenta concomitant with the bending of triatomics, and on the use of the Hellmann-Feynman theorem for serious calculations of interatomic force constants.

In the microwave field there was presented an excellent review of recent experimental results concerning barriers to internal rotation. An independent theoretical treatment emphasized the challenge which still exists here for the theory. Microwave spectra due to intermolecular tunneling were also discussed, and so were hyperfine interactions and quadrupole coupling.

The domain of paramagnetic resonance spectra was represented by a report on negative spin densities in pi-electronic radicals. Metallic reflections in molecular crystals, as well as optical activity and rotatory dispersion, were topics of further contributions. Finally there was an interesting attempt to outline a uniform view of many of these effects by characterizing them as "weak interactions" which yield important information on electronic wave functions without materially disturbing them.

A regrettable circumstance was the absence of any paper on ligand field theory of inorganic complexes.

In conclusion it was felt that new theoretical methods and ideas which have come into being during the past decade are beginning significantly to transform the theory of molecules. In the last lecture, the audience was, however, reminded that essential insights have come and must still be expected to come from conventional chemical and physical methods. The concomitant experimental demonstrations made a fitting conclusion for a meeting which had started out with purely mathematical concerns about the Schrödinger equation.