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Contract Nonr - 2216(11). Theory of Solids.

Final Technical Report

4/1/60 - 7/31/69

Since the inception of the Department of Physics at the then new San Diego campus of the University of California, the Office of Naval Research, through its support of studies in the theory of solids, has played an important part in the development of one of the country's major solid state groups. Before discussing in detail the work done under Navy auspices we would like to give a brief review of the development and present status of the entire solid state effort in San Diego. During the years 1960-61, four senior faculty members were appointed: G. Feher, W. Kohn, B. T. Matthias and H. Suhl. They initiated programs in electron and nuclear spin resonance, magnetic and superconductivity materials and general theory of solids. Another senior appointment, in 1967, of J. Wheatley, led to an additional major program on the properties of He^3 and He^4 and ultra-low temperature physics in general. The following younger faculty members have joined the solid state group since its inception: W. Black (ultra-low temperatures); D. Fredkin (theory); J. Goodkind (coherence effects in superfluids); S. K. Ma (theory); S. Schultz (resonances and waves in metals); L. Sham (theory); H. Shore (theory). Although there is no formal organization tying all these activities together, there exist very strong informal interactions between them. We believe that the total effort of these faculty members, together with their graduate students (about 40)

and postdoctorals (about 12) constitutes a significant contribution to the national effort of research and education in solid state physics.

The research results obtained with the support of this contract are contained in the 57 technical reports listed in Appendix I. They cover a wide range of topics mostly in the electron theory of solids. Among the main subject areas we mention especially the following:

I. Electronic Phase Transitions in Solids.

Electronic phase transitions caused by the Bose condensation of electron-hole pairs have been of interest to us since the beginning of this contract. Technical reports 1, 43, 45, 46, 47, 48, 53, 55, and 57 deal with this subject. This subject is intimately related to the area of metal-to-insulator transitions in which our group has been one of the most active in the country.

II. Theory of the Inhomogeneous Electron Gas.

This line of research was started in a paper by Hohenberg and Kohn (Technical Report 23) and continued in Technical Reports 26, 27, 28, 30, 31, 35, 36, 37, 40, 44. It has also been widely applied by other researchers, such as J. C. Slater, F. Herman, Bennett and Duke, etc. for calculations of the electronic structure of atoms, molecules, solids and solid surfaces. We ourselves have currently an active program on the structure of metal surfaces under way which is based on this approach.

III. Fermi Surface Images.

This line of research goes back to a 1959 paper by W. Kohn, pointing at the existence of anomalous kinds in the phonon and spin wave spectra of metals which reflect the shape of the Fermi surface. Technical Reports 5, 8, and 9 deal with this subject which has also found wide application by other theoretical and experimental physicists.

IV. Many Electron Effects in Simple Metals.

Here our group has made contributions to the general progress in many body effects in simple metals. See Technical Reports 1, 2, 6, 7, 10, 18, 21, 22, 29, and 56.

V. Disordered Structures and Metal Defects.

This area which we consider to be of continuing great importance has occupied us since the beginning of this contract. We have currently under way a program of developing a new small cluster theory of disordered structures. Previous work is contained in Technical Reports 4, 7, 16, 25, 28, and 52.

The following graduate students have received their Ph.D. degrees with support of this contract. The addresses in parentheses indicate their present locations. E. J. Woll (Harvard University); C. Majumdar (Tata Institute of Research, India); M. P. Greene (Brown University); B. Tong (University of Western Ontario); C. Y. Young (M. I. T. Lincoln Laboratory); W. H. Butler* (Auburn University, Alabama); J. Rudnick* (University of Washington).

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* Final examinations scheduled for September 1969.

Other students either temporarily associated with this contract or currently working towards their degree are: J. Frohberg, M. Lumming, L. Campbell, A. Bagchi, B. Nickel, T. Wu.

In addition, during the period of this contract a large number of postdoctoral fellows have conducted research and received, in effect, postdoctoral education by participation in this program. Many of the foreign scholars received all or part of their support from sources within their own countries. Following is a list of their names and current affiliations: S. Nettel (Renselaer Polytechnic Institute); E. Daniel (University of Strassbourg); S. Vosko (Westinghouse Research Laboratory); A. Houghton (Brown University); J. Des Cloiseaux (CEN, France); J. J. Pearson (Lockheed Corporation); R. B. Griffiths (Carnegie-Mellon University); L. J. Sham (University of California, San Diego); D. Mermin (Cornell University); V. Celli (University of Virginia); L. Dworin (Northeastern University); T. M. Rice (Bell Telephone Laboratories); M. T. Beal-Monod (Faculté des Sciences, Orsay, France); J. Zittartz (University of Cologne, Germany); U. Schotte (University of Dormstadt, Germany); D. Sherrington (Imperial College, London, England).

This program in the theory of solids is now being continued with the support of a new contract from the Office of Naval Research (Nonr N00014-69A-0200-600. and a grant from the National Science Foundation.

Appendix I

"Theory of Solids" Contract No. Nonr-2216 (11)

Technical Reports

Starting date: April 1, 1960 to July 31, 1969

Technical Reports

Starting date: April 1, 1960 to July 31, 1969

1. Giant Fluctuations in a Degenerate Fermi Gas, Walter Kohn and Stephen J. Nettel.

2. On the Momentum Distribution of an Interacting Electron Gas, E. Daniel and S. H. Vosko.

3. Band Structure of Semi-conductors, Walter Kohn.

4. Specific Heat and Spin Susceptibility of Dilute Alloys, A. Houghton.

5. Image of the Fermi Surface in Spin Wave Spectra of Rare Earth Metals, Edwin J. Woll, Jr. and Stephen J. Nettel.

6. Cyclotron Resonance and de Haas-van Alphen Oscillations of an Interacting Electron Gas, Walter Kohn.

7. Evaluation of Kubo's Formula for the Impurity Resistance of an Interacting Electron Gas, J. S. Langer.

8. Images of the Fermi Surface in Phonon Spectra of Metals, E. J. Woll, Jr. and Walter Kohn.

9. Images of the Fermi Surface in Phonon and Spin-Wave Spectra, E. J. Woll, Jr.

10. Thermal Conductivity of a System of Interacting Electrons, J. S. Langer.

11. Spin-Wave Spectrum of the Antiferromagnetic Linear Chain, Jacques des Cloizeaux and J. J. Pearson.

12. Orthogonal Orbitals and Generalized Wannier Functions, Jacques des Cloizeaux.

13. A Class of Energy Levels for the Heisenberg Linear Chain, I. Robert B. Griffiths.

14. A Class of Energy Levels for the Heisenberg Linear Chain, II. Levels Near the Antiferromagnetic Ground State, Robert B. Griffiths.

15. Theory of the Insulating State, Walter Kohn.

16. Orbital Susceptibility of Dilute Alloys, Walter Kohn and M. Luming.

17. A Proof that the Free Energy of a Spin System is Extensive, Robert B. Griffiths.

18. A Calculation of the Phonon Frequencies in Sodium, L. J. Sham.

Technical Reports (continued)

19. Spontaneous Magnetization in Idealized Ferromagnets, Robert B. Griffiths.

20. Free Energy of the Antiferromagnetic Linear Chain, Robert B. Griffiths.

21. Instability in the Quantum Helicon Dispersion Relation, N. David Mermin and V. Celli.

22. Long Wavelength Oscillations of a Quantum Plasma in a Uniform Magnetic Field. II. Vittorio Celli and N. David Mermin.

23. The Inhomogeneous Electron Gas, P. Hohenberg and Walter Kohn.

24. Time-Dependent Correlations in a Solvable Ferromagnetic Model, N. David Mermin.

25. Resistivity of Solid and Liquid Sodium, Michael P. Greene and Walter Kohn.

26. Thermal Properties of the Inhomogeneous Electron Gas, N. David Mermin.

27. Quantum Density Oscillations in an Inhomogeneous Electron Gas, Walter Kohn and L. J. Sham.

28. Continuity Between Bound and Unbound States in a Fermi Gas, Walter Kohn and C. Majumdar.

29. Annihilation of Positrons in Metals, C. K. Majumdar.

30. Exchange and Correlation Effects in an Inhomogeneous Electron Gas, Walter Kohn and L. J. Sham.

31. Self-Consistent Equations Including Exchange and Correlation Effects, Walter Kohn and L. J. Sham.

32. Superconductivity in One and Two Dimensions, T. M. Rice.

33. Free Energy of an Anharmonic Crystal, L. J. Sham.

34. Existence of Energy Gaps in the Spectrum of a One-Dimensional Atomic Chain, Lowell Dworin.

35. Application of a Self-Consistent Scheme including Exchange and Correlation Effects to Atoms, B. Y. Tong and L. J. Sham.

36. One-Particle Properties of an Inhomogeneous Interacting Electron Gas, L. J. Sham and Walter Kohn.

37. A New Formulation of the Inhomogeneous Electron Gas Problem, Walter Kohn.

Technical Reports (continued)

38. Transverse Conductivity of a Degenerate System of Landau Electrons and Optical Phonons, Lowell Dworin.

39. Many-Particle Derivation of the Effective-Mass Equation for the Wannier Exciton, L. J. Sham and T. M. Rice.

40. Electronic States in Metals, Walter Kohn.

41. Superconductivity in One and Two Dimensions, II. Charged Systems, T. M. Rice.

42. Theory of the Shallow Impurity States in Semiconductors, L. J. Sham.

43. Absence of Long-Range Overhauser Spin-Density Waves in One or Two Dimensions, David C. Hamilton.

44. Electronic Structure from the Standpoint of the Inhomogeneous Electron Gas, Walter Kohn.

45. Anisotropy Effects in the Excitonic Insulator, Johannes Zittartz.

46. Theory of the Excitonic Insulator in the Presence of Normal Impurities, Johannes Zittartz.

47. Transport Properties of the "Excitonic Insulator." I. Electrical Conductivity, Johannes Zittartz.

48. Transport Properties of the "Excitonic Insulator." II. Thermal Conductivity, Johannes Zittartz.

49. Spatial Variations of the Order Parameter in Superconductors Containing Magnetic Impurities, Jean Heinrichs.

50. Unified Perturbation and Variational Methods for the Study of Responses to Time Dependent and Time Independent Interactions, Jean Heinrichs.

51. Superconductivity in One and Two Dimensions. II. Charged Systems, T. M. Rice.

52. Strain Effects in Dilute Alloys, M. T. Beal-Monod and Walter Kohn.

53. Speculations about Grey Tin, D. Sherrington and Walter Kohn.

54. Dielectric Properties of the Wigner and Related Dipole Lattices, Amitabha Bagchi.

55. Frequency-Dependent Dielectric Function of a Zero-Gap Semiconductor, D. Sherrington and Walter Kohn.

Technical Reports (continued)

56. Tomonaga's Model and the Threshold Singularity of X-Ray Spectra of Metals, K. D. Schotte and U. Schotte.

57. Two Kinds of Bosons and Bose Condensates, D. Sherrington and Walter Kohn.

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