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FINAL REPORT

Magnetic Effects in Solids

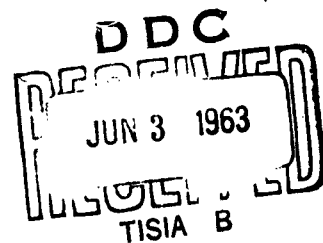covering the period

June 1, 1960 to June 1, 1963.

Contractor: The Regent of the University of California

ONR Project No. NR 018-105

Contract No. Nonr 233(63)

Report prepared by David I. Paul, Project Director.

FINAL REPORT

Magnetic Effects in Solids

The contract on Magnetic Effects in Solids, ONR Project No. NR 018-105, Contract No. Nonr 233(63) was begun on June 1, 1960 and terminates June 1, 1963. The Project Director would like to take this opportunity to thank the Office of Naval Research for their very kind aid and cooperation in this research during the entire period.

This Final Report complies with U.S.Navy, ONR Physics Branch Unclassified Reports Police ONR:421:FBIhds requesting a final report summarizing all work accomplished under the contract.

A. List of all Technical Reports published including all papers published in professional journals during the period June 1, 1960 to June 1, 1963.

1. Theory of Magnetism and the Ground State Energy of a Linear Chain II - Configuration Interaction Effects by David I. Paul, Physical Review 120, 463, (1960). Work on this paper was completed prior to June, 1960.

2. Some Exact Solutions to the Two Dimensional Spin Wave Hamiltonian by David I. Paul, Journal of Mathematics and Physics, 40, 249, (1961). Also submitted as Technical Report No. 1.

3. Developments in the Energy Band Methods for Solids, March 1958 - April 1961, by Mr. Donald Bullock. Submitted as Technical Report No. 2 dated May 25, 1961.

4. Interaction of Antiferromagnetic Spin Waves with a Bloch Wall by David I. Paul, Physical Review 126, 78, (1962). Also submitted as Technical Report No. 3.

5. Nuclear Magnetic Resonance within an Antiferromagnetic Bloch Wall by David I. Paul, Physical Review 127, 455, (1962). Also submitted as Technical Report No. 4.

6. Spin Waves and Nuclear Magnetic Resonance Enhancement in NiF_2 Domain Walls by David I. Paul. Scheduled for publication in the Physical Review, July 1, 1963. Also submitted as Technical Report No. 5.

7. A Perturbation Theory of the Heisenberg Antiferromagnet by Donald L. Bullock. This constitutes the doctoral dissertation of Donald L. Bullock. Also submitted as Technical Report No. 6.

Paper No. 1 is the second of a series of two papers investigating the nature and causes of ferromagnetic and antiferromagnetic behavior from

a fundamental quantum mechanical point of view. Paper No. 2 considers some two dimensional aspects of the problem. Papers Nos. 3 and 7 were done by Donald Bullock as a graduate student studying for his doctoral degree in theoretical solid state physics. Papers Nos. 4, 5, and 6 form a series of three papers on the effect of Bloch Walls in magnetic substances. All of the above Technical Reports have been distributed previously and constitute a presentation, summary, and discussion of the above work.* For convenience and completeness, Appendix A of this final report contains an abstract of each of these papers.

B. List of papers presented at meetings of the American Physical Society during the period June 1, 1960 to June 1, 1963:

1. Paper presented at the annual New York meeting of the American Physical Society entitled "The Spin Wave Theory of Ferromagnetism for a Two Dimensional Lattice" by David I. Paul, Bulletin of the American Physical Society, II, 6, No. 1, Pt. 1, RA-11, (Feb. 1, 1961).

2. Paper presented at the annual Solid State Division meeting of the American Physical Society at Baltimore, Md. on "Propagation of Antiferromagnetic Spin Waves Through a Bloch Wall" by David I. Paul, Bulletin of the American Physical Society, II, 7, No. 3, 212, PA-3, (March 28, 1962).

3. Paper presented at the annual Solid State Division meeting of the American Physical Society at St. Louis., Mo., on Bloch Walls and Nuclear Magnetic Resonance in Weak Ferromagnetic Materials by David I. Paul, Bulletin of the American Physical Society II, 8, No. 3, O-7, 227, (March 26, 1963).

4. Paper presented at the meeting of the American Physical Society in Washington, D.C., on Perturbation Theory of the Antiferromagnetic Ground State by Donald L. Bullock, Bulletin of the American Physical Society, II, 8, No. 4, VA-9, 382, (April 23, 1963).

*A complete set of the publications listed above are attached to this report for distribution to the Physics Branch, Office of Naval Research, Washington 25, D.C., and also the Office of Naval Research Branch Office, Pasadena 1, California.

C. Names of graduate students associated with this contract:

1. Donald L. Bullock - Received his doctoral degree during
   the Spring semester 1963. His doctoral dissertation
   presented as Technical Report No. 6 under this contract.

2. Bruce Grover - Mr. Grover had a research assistantship
   under this contract for the academic year September 1962 -
   June 1963. In conjunction with the project director, David
   Paul, he has been considering the effect of Bloch walls on
   the canted antiferromagnet, $KMnF_3$. Work to date on this
   substance is incomplete. Mr. Grover hopes to continue
   investigating this subject.

The Project Director and those graduate students associated
with this contract again thank the U.S. Office of Naval Research
for their support of this research.

This Final Report was prepared on May 27, 1963, and is
herewith respectfully submitted.

David I. Paul

David I. Paul, Project Director

APPENDIX A

Abstracts of all paper and technical reports for period June 1, 1960 to June 1, 1963.

1. Theory of Magnetism and Ground State Energy of a Linear Chain II - Configuration Interaction Effects by David I. Paul.
We continued the investigation, begun in the previous paper of this series, on the ground state energy of a one dimensional chain of atoms from the point of view of orthogonal atomic wave functions. Thus, the exchange integral is positive and the configuration interaction between polar and nonpolar states is included. Our results are extended to include the condition of a large amount of overlap among the unperturbed nonorthogonal atomic functions resulting in a strong interaction between the orthogonalized non-polar and polar energy states for the case of two electrons having their spins oriented opposite to all other electron spins. These results indicate that for this case the energy of the unmagnetized state is lower than that obtained when all the electron spins are parallel and that the system is nonferromagnetic.

2. Some Exact Solutions to the Two Dimensional Spin Wave Hamiltonian by David I. Paul
In this paper we have presented some exact solutions for the Dirac Spin Wave Hamiltonian of a two dimensional periodic rectangular array of N atoms. Each atom in its isolated state is considered to have one outer electron which is in an s state - all other electrons being in closed shells. We have shown that if the number of spin waves are less than or equal to the number of atoms in either of the two lattice directions, exact solutions exist in which the spin waves behave as independent particles subject to Fermi statistics. The energy eigen-values for these solutions are rigorously additive and are exactly the same as those obtained by Bloch although the number of allowed eigen-states are more restricted.

3. Developments in the Energy Band Methods for Solids, March 1958 - April 1, 1961 by Mr. Donald Bullock.
Since the completion of Callaway's review (J. Callaway, Adv. Solid State Physics, Vol. 7, p. 99 (1958) of the energy band method for solids, considerable efforts have been made to improve the state of the theory. This report consists of a review of the new developments in this field. However, no attempt is made to cover the development of the allied field concerned with the calculation of the correlation and exchange energy of a many electron system, such as is contained in the theories of Bohm and Pines (Physical Review 92, 609, 626, (1953), and M. Gell-Mann and K. Brueckner, (Physical Review 106, 364 (1957). The discussion is divided into two parts. The first is concerned with the development of the band theory as it applies to the transition metals. The second takes up the development in other areas such as the alkali metals, polyvalent metals, heavy metals, and semiconductors. A bibliography is also contained in this report.

4. Interaction of Antiferromagnetic Spin Waves with a Bloch Wall by David I. Paul.

The interaction of an antiferromagnetic spin wave with a 180° Bloch wall is studied from the theoretical point of view. Our formulation includes the anisotropy and exchange energies of the crystal together with the characteristics of the wall such as its stiffness and viscosity. The anisotropy is assumed to be of a general orthorhombic form. We show that there exists a bound wall excitation branch as well as a free spin wave excitation branch, and we derive a restrictive set of relationships between the excitations on two different sublattices. Further, we show that there exist special values of the energy for which the spin waves are degenerate and the restrictions no longer apply. Finally, we determine the change of phase of the spin waves on passing through the Bloch wall as a function of the wavelength, demonstrate that the phase change decreases as the wavelength increases, and compare our results with those of the analogous ferromagnetic case.

5. Nuclear Magnetic Resonance Within an Antiferromagnetic Bloch Wall by David I. Paul.

In the previous paper by the author,(4 above), the bound spin wave excitation spectrum existing within an antiferromagnetic Bloch wall was derived. We calculate, here, the effect of this energy excitation spectrum on the line width and relaxation times of the magnetic resonance of nuclei existing within the wall. A relaxation time, T_1, caused by excitation of the transverse components of the electron spin by the resonance field, is shown to be smaller in antiferromagnets than in ferromagnets due to the larger minimum wall excitation energy. The line width due to indirect coupling of the nuclear spins through the virtual excitation of a spin wave, however, proves to be increased by the square root of the ratio of the anisotropy to the stiffness parameters compared to the uniform antiferromagnet. A second nuclear line width, resulting from the variation of the deviation of the longitudinal component of the electron spin from the center to the edge of the wall is also calculated. Numerical results are obtained and, where possible, compared with experiment.

6. Spin Waves and Nuclear Magnetic Resonance Enhancement in NiF_2 Domain Walls by David I. Paul.

In this paper, we obtain the allowed magnetic resonance modes or spin waves in the canted antiferromagnet NiF_2 in the presence of a Bloch wall. Our formulation includes the anisotropy and exchange energies of the crystal together with the characteristics of the wall such as its stiffness, mass, and viscosity. From the dispersion equations, we show that there exists a bound wall excitation branch having a lower excitation energy than the free spin wave excitation branch. Further, we have calculated the effective nuclear magnetic resonance field enhancement due to the bound wall excitation branch as a function of the parameters of the crystal and the Bloch wall and shown that our results are equivalent to those obtained experimentally by

Paper No. 6 continued
R. Shulman, (Suppl. Jrnl. Appl. Physics, 32, 126S, 1961). Finally,
we compare this enhancement with that of a pure antiferromagnet -
demonstrating that the canting is essential for this process.

7. A Perturbation Theory of the Heisenberg Antiferromagnet by Donald
Bullock.
The antiferromagnetic ground state for typical one, two, and three
dimensional interlocking sublattice systems and arbitrary spin is
treated. The results are reported in terms of series expansions
generated by means of a modified Rayleight-Schrodinger perturbation
theory, which is proposed and developed in this dissertation. The
modification is a process whereby the definition of the zero order
Hamiltonian is changed through the prediction and inclusion of
certain infinite classes of terms, whose first members appear in
the original perturbation series. The final zero order Hamiltonian
obtained is the Ising model. Explicit expressions for the ground
state parameters are given through fourth order for the linear
chain, plane quadratic, and simple cubic lattices with arbitrary
spin. The calculation is carried through to determine the energy
series through six orders for the linear chain with spin one-half.
A comparison with experimental determinations of the long range
order in real antiferromagnets is made. In addition, the problem
of the first excited states is considered. A perturbation calcula-
tion similar to that performed for the ground state is carried out
for the partition function of the Heisenberg antiferromagnet. The
low temperature terms of this expansion are shown to be related
to the energies of the ground state and first excited states. The
calculation of the first excited state energies is carried out to
second order. A complete analysis of the relationship of this
perturbation method for the ground state and first excited states
with the spin wave treatment of the same states is also contained
in this dissertation.

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