

56

Springer Series in Solid-State Sciences

Edited by Peter Fulde



Springer Series in Solid-State Sciences

Editors: M. Cardona P. Fulde H.-J. Queisser

- | | |
|---|--|
| 40 Semiconductor Physics An Introduction
3rd Edition By K. Seeger | 53 Two-Dimensional Systems,
Heterostructures, and Superlattices
Editors: G. Bauer, F. Kuchar,
and H. Heinrich |
| 41 The LMTO Method
Muffin-Tin Orbitals and Electronic
Structure
By H. L. Skriver | 54 Magnetic Excitations and Fluctuations
Editors: S. Lovesey, U. Balucani, F. Borsa,
and V. Tognetti |
| 42 Crystal Optics with Spatial Dispersion,
and Excitons
By V. M. Agranovich and V. L. Ginzburg | 55 The Theory of Magnetism II
Thermodynamics and Statistical Mechanics
By D. C. Mattis |
| 43 Resonant Nonlinear Interactions of
Light with Matter
By V. S. Butylkin, A. E. Kaplan,
Yu. G. Khronopulo, and E. I. Yakubovich | 56 Spin Fluctuations in Itinerant Electron
Magnetism By T. Moriya |
| 44 Elastic Media with Microstructure II
Three-Dimensional Models
By I. A. Kunin | 57 Polycrystalline Semiconductors,
Physical Properties and Applications
Editor: G. Harbeke |
| 45 Electronic Properties of Doped
Semiconductors
By B. I. Shklovskii and A. L. Efros | 58 The Recursion Method and
Its Applications
Editors: D. Pettifor and D. Weaire |
| 46 Topological Disorder in Condensed Matter
Editors: F. Yonezawa and T. Ninomiya | 59 Dynamical Processes and
Ordering on Solid Surfaces
Editors: A. Yoshimori and M. Tsukada |
| 47 Statics and Dynamics of Nonlinear
Systems
Editors: G. Benedek, H. Bilz,
and R. Zeyher | 60 Excitonic Processes in Solids
By M. Ueta, H. Kanzaki, K. Kobayashi,
Y. Toyozawa, and E. Hanamura |
| 48 Magnetic Phase Transitions
Editors: M. Ausloos and R. J. Elliott | 61 Localization, Interaction, and
Transport Phenomena
Editors: B. Kramer, G. Bergmann,
and Y. Bruynseraede |
| 49 Organic Molecular Aggregates, Electronic
Excitation and Interaction Processes
Editors: P. Reineker, H. Haken,
and H. C. Wolf | 62 Theory for the Valence of
Fluctuating State
Editors: T. Saso and T. Kasuya |
| 50 Multiple Diffraction of X-Rays in Crystals
By Shih-Lin Chang | 63 Electronic Properties of
Polymers and Related Compounds
Editors: H. Kuzmany, M. Mehring,
and S. Roth |
| 51 Phonon Scattering in Condensed Matter
Editors: W. Eisenmenger, K. Laßmann,
and S. Döttinger | |
| 52 Superconductivity in Magnetic and Exotic
Materials
Editors: T. Matsubara and A. Kotani | |

Tôru Moriya

Spin Fluctuations in Itinerant Electron Magnetism

With 98 Figures

Springer-Verlag Berlin Heidelberg GmbH

Professor Tôru Moriya
Institute of Solid State Physics, University of Tokyo, Roppongi, Minato-ku
Tokyo 106, Japan

Series Editors:

Professor Dr. Manuel Cardona
Professor Dr. Peter Fulde
Professor Dr. Hans-Joachim Queisser
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1
D-7000 Stuttgart 80, Fed. Rep. of Germany

ISBN 978-3-642-82501-9 ISBN 978-3-642-82499-9 (eBook)
DOI 10.1007/978-3-642-82499-9

Library of Congress Cataloging in Publication Data. Moriya, Tôru, 1930—. Spin fluctuations in itinerant electron magnetism. (Springer series in solid-state sciences ; 56). Bibliography: p. Includes index. 1. Magnetism, Band theory of. 2. Electron band theory of metals. 3. Nuclear magnetism. 4. Ferromagnetism. I. Title. II. Series. QC754.2.B35M67 1985 530.4'1 85-7926

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically those of translation, reprinting, reuse of illustrations, broadcasting, reproduction by photocopying machine or similar means, and storage in data banks. Under § 54 of the German Copyright Law, where copies are made for other than private use, a fee is payable to "Verwertungsgesellschaft Wort", Munich.

© Springer-Verlag Berlin Heidelberg 1985
Originally published by Springer-Verlag Berlin Heidelberg New York in 1985
Softcover reprint of the hardcover 1st edition 1985

The use of registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

2153/3130-543210

Preface

Ferromagnetism of metallic systems, especially those including transition metals, has been a controversial subject of modern science for a long time. This controversy stems from the apparent dual character of the *d*-electrons responsible for magnetism in transition metals, i.e., they are itinerant electrons described by band theory in their ground state, while at finite temperatures they show various properties that have long been attributed to a system consisting of local magnetic moments. The most familiar example of these properties is the Curie-Weiss law of magnetic susceptibility obeyed by almost all ferromagnets above their Curie temperatures.

At first the problem seemed to be centered around whether the *d*-electrons themselves are localized or itinerant. This question was settled in the 1950s and early 1960s by various experimental investigations, in particular by observations of *d*-electron Fermi surfaces in ferromagnetic transition metals. These observations are generally consistent with the results of band calculations.

Theoretical investigations since then have concentrated on explaining this dual character of *d*-electron systems, taking account of the effects of electron-electron correlations in the itinerant electron model. The problem in physical terms is to study the spin density fluctuations, which are neglected in the mean-field or one-electron theory, and their influence on the physical properties.

There have been two main streams in the research in this direction. One has been to study the local moments in metals or the possibility for the itinerant electrons to exhibit spin density fluctuations that are described at least approximately as a set of local magnetic moments. This approach attained remarkable success in the 1960s from a qualitative point of view and has been extended further since then.

The other stream of research has been to improve the mean-field theory by taking into account the spatially extended spin density fluctuations in contrast with the local moment picture. This line of approach, represented by the random-phase approximation, was, however, not successful until the early 1970s when a self-consistent theory of coupled modes of extended spin fluctuations was advanced and the difficulties of the random-phase approximation were removed. This improved theory was remarkably successful when applied to weakly ferromagnetic metals where the long-wavelength components of spin fluctuations are the predominant thermal excitations.

For example, this theory postulates a new mechanism, without local magnetic moment, for the Curie-Weiss susceptibility. The theoretical and experimental investigations in this decade have well established the picture and theory of extended spin fluctuations in weakly ferro- and antiferromagnetic metals; there is now a new class of magnets at the opposite extreme to the quite familiar local moment systems.

This success has given a breakthrough to the theory of itinerant electron magnetism, since it is quite natural to expect that the properties of many metallic magnets are distributed between these mutually opposite extremes. Thus the latest investigations are focused on the intermediate regime between the extremes, to which most metallic magnets including Fe, Co, and Ni are considered to belong. The concept of spin fluctuations is now generalized to include both the local and extended moment limits and a theory of interpolation between them is expected to lead to a unified description of magnetism.

This monograph is intended to review the above-mentioned developments in the field of itinerant electron magnetism. The important steps in the theoretical developments in this area are treated, emphasizing recent theories including the latest attempts at a unified theory. We try to clarify as far as possible to what extent the subject is understood at present and what still has to be examined and clarified in future.

Since the emphasis is on the finite-temperature properties of magnets, important topics relating to the underlying electronic structures were largely omitted: the band-structure calculation, many-body effects in the ground state, and the experimental and theoretical investigations of photoemission which have marked significant progress in recent years. This specialization of topics seems reasonable in view of the size of the volume and of the author's knowledge. Also it is justifiable to discuss important concepts, giving a general picture of magnetism, without going into too fine details of the underlying electronic structure, as has actually been seen in the past theoretical developments.

I should like to thank Professors Y. Ishikawa, Y. Masuda, S. Ogawa, G. Shirane, H. Yasuoka, and K. R. A. Ziebeck for discussions and correspondence regarding the experimental results discussed here. I have benefited from many stimulating discussions with my colleagues who have taken part in the theoretical developments discussed here. My special thanks go to Dr. Y. Takahashi for critical reading of the manuscript and his resulting useful comments on it. I am greatly indebted to Mrs. K. Fujii for her constant help in typing and re-typing the manuscript and drawing figures.

Tokyo, January 1985

T. Moriya

Contents

1. Introduction	1
1.1 Local Magnetic Moment and the Weiss Theory of Ferromagnetism	1
1.2 Magnetic Moments of Atoms	3
1.3 Heisenberg Localized Electron Model	4
1.4 Itinerant Electron Model	5
1.5 Localized vs Itinerant Electron Models	7
1.6 Random-Phase Approximation Theory of Spin Fluctuations in Itinerant Electron Magnets	8
1.7 Local Moments in Metals	9
1.8 Self-Consistent Renormalization Theory of Spin Fluctuations and Weakly Ferro- and Antiferromagnetic Metals	10
1.9 Unified Picture of Magnetism	12
1.10 Organization of the Book	13
2. Mean-Field Theory of Itinerant Electron Magnetism	15
2.1 Model Hamiltonians	15
2.2 Ferromagnetism	18
2.3 Antiferromagnetism	22
2.4 Spin-Density Waves	25
2.5 Stability of Various Spin Orderings	28
3. Dynamical Mean-Field Theory of Spin Fluctuations	30
3.1 Stoner Excitations and Spin Waves in Ferromagnetic Metals	30
3.2 General Spin Fluctuations and Dynamical Susceptibilities	36
3.3 Critical Spin Fluctuations	37
3.4 Antiferromagnets	39
3.5 Limitations of the Hartree-Fock-RPA Theory	42
4. Self-Consistent Renormalization (SCR) Theory of Spin Fluctuations	44
4.1 Expressions for the Free Energy of an Interacting Electron System	45
4.2 Paramagnon Theories	47
4.3 SCR Theory of Ferromagnetic Metals	50
4.3.1 Curie Temperature and Magnetic Susceptibility Above T_C	51

4.3.2 Analytical Explanation of the New CW Law	54
4.3.3 Magnetization Below T_C	58
4.3.4 Rotationally Invariant Treatment	59
4.4 Phenomenological Mode-Mode Coupling Theory	61
4.5 SCR Theory of Antiferro- and Helimagnetic Metals	65
4.6 Physical Origin of the New Curie-Weiss Susceptibility	68
4.6.1 Temperature Variation of the Mean-Square Local Amplitude of Spin Fluctuation	68
4.6.2 Spatial Spin Correlation	70
4.7 Coexistence of and Phase Transitions Between Ferro- and Antiferromagnetism	72
4.8 Quantitative Aspects of the SCR Theory for Weak Itinerant Ferromagnets	77
5. Physical Properties of Weakly and Nearly Ferro- and Antiferromagnetic Metals	82
5.1 Properties of Spin Fluctuations	82
5.2 Thermal Expansion	87
5.3 Specific Heat	91
5.4 Nuclear Spin Relaxation	95
5.4.1 Weakly and Nearly Ferromagnetic Metals	96
5.4.2 Weakly and Nearly Antiferromagnetic Metals	99
5.5 Electrical and Thermal Resistivities and Magnetoresistance	101
5.5.1 Weakly and Nearly Ferromagnetic Metals	102
5.5.2 Antiferromagnets	106
5.6 Coupling Between Spin and Charge Density Fluctuations	107
6. Local Magnetic Moments	109
6.1 Local Moments in Insulator Magnets	109
6.2 Metal-Insulator (Mott) Transition	111
6.3 s - d or s - f Exchange Model	113
6.4 Local Moment Formation in Metals	114
6.4.1 Virtual Bound State	114
6.4.2 The Anderson Model	116
6.4.3 The Wolff-Clogston Tight-Binding Model	119
6.5 Physical Properties of a Single Local Moment in Metals	121
6.6 Interaction Between a Pair of Local Moments in Metals	123
6.7 Local Moment Description of Magnetic Transition Metals	127
7. A Unified Theory and Its General Consequences	129
7.1 General Considerations Toward a Unified Theory	129
7.2 A Phenomenological Description of the Unified Theory	136
7.3 General Mechanism for the Curie-Weiss Susceptibility	137
7.3.1 A Mean Mode-Mode Coupling Theory of Magnetic Susceptibility	137

7.3.2	General Expressions for the Curie Temperature and Susceptibility	139
7.3.3	Spin Correlations and Magnetic Susceptibility	141
7.4	Possibility for Systematic Analyses of Experimental Results	148
7.5	Temperature Variation of the Local Amplitude of Spin Fluctuation	152
7.5.1	General Remarks	152
7.5.2	Temperature-Induced Local Moments	153
7.6	Limitations of the Adiabatic Approximation	156
8.	Functional Integral Theory	157
8.1	Basic Formalism	157
8.2	Local Moment in Metals	163
8.3	Band Magnetism – A General Formalism	166
8.4	Methods of Calculating the Free Energy Functional	170
8.4.1	A Closed-Form Expression for $\psi[\xi, \eta]$	170
8.4.2	Long-Wavelength Approximations	173
8.5	A Unified Description of Magnetism in Narrow-Band Systems	174
8.6	Approximation Methods of Evaluating the Functional Integrals	177
8.6.1	Unified Theory	178
8.6.2	Molecular Field (Single-Site) Approximation	179
8.6.3	Choice of Forms for the Interaction Hamiltonian	181
8.7	Results of Numerical Calculations	181
8.7.1	Ferromagnetic Transition Metals α -Fe, Co, Ni	182
8.7.2	Antiferromagnetic Transition Metals	185
8.7.3	FeSi, Nearly Ferromagnetic Semiconductor	185
8.7.4	Temperature-Induced Local Moments in CoS_2 , CoSe_2	187
8.7.5	Magnetovolume Effects	189
8.8	Supplementary Discussions on Various Approaches and Physical Pictures	192
8.8.1	The Hartree-Fock Theory for Excited States with Spatially Varying Spin Density	192
8.8.2	Local Band Theory	193
8.8.3	Persistence of Exchange Splitting of the Band Above T_C	193
9.	Spin Fluctuations in d-Electron Systems	194
9.1	Spin Fluctuations and Neutron-Scattering Measurements	194
9.2	Local Moment Systems	196
9.2.1	Heusler Alloys	196
9.2.2	EuO	197
9.3	Substances Close to the Local Moment Limit	198
9.3.1	MnPt_3 , FePd_3	198
9.3.2	FePt_3	199
9.4	Substances Close to the Weakly Ferro- and Antiferromagnetic Limits	200

9.4.1	MnSi	200
9.4.2	Cr	200
9.5	Substances in the Intermediate Regime: q -Space Description	203
9.5.1	Fe ₃ Pt	203
9.5.2	CeFe ₂	204
9.5.3	γ -Mn, γ -(FeMn), γ -Fe	204
9.5.4	α -Mn	204
9.6	Ferromagnetic Transition Metals Fe, Co, and Ni	205
9.7	Some Systematic Trends in Paramagnetic Scattering	210
10.	Toward a Unified Theory of Dynamical Spin Fluctuations	214
10.1	General Considerations	214
10.2	Green's Function Theory of Dynamical Susceptibilities	216
10.3	Effect of Electron Lifetime on RPA-SCR Spin Fluctuations	219
11.	Concluding Remarks	223
References		225
Subject Index		237