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Yoshiro Kakehashi

Modern Theory of Magnetism in Metals and Alloys

Springer

Yoshiro Kakehashi
Faculty of Science, Department of Physics
University of the Ryukyus
Nishihara, Japan

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Preface

Metallic magnetism has a long history because there have been continuous discoveries of many intriguing phenomena and difficulties in their theoretical description. One of the long-standing problems has been known as the itinerant vs localized behavior of the magnetism. The ground-state properties of Fe, Co, and Ni such as magnetization and the T-linear specific heat at low temperatures, for example, are explained by the band model, while their finite temperature properties such as the paramagnetic susceptibility and the large specific heat anomaly at the Curie temperature are explained well by the localized model.

The dual property of metallic magnetism led to two paths in theoretical investigations. One is to develop the band theory at the ground state taking into account correlation effects on the one electron potential for electrons. There the density functional theory (DFT) has played an important role. Theoretical improvement of metallic magnetism at the ground state has been achieved as a part of the developments of the DFT in the electronic structure calculations.

Another direction of the development has been to take into account the spin fluctuations in order to describe local-moment behaviors of metallic magnetism at finite temperatures. Theoretical results in this direction until 1980 are summarized in the book by Moriya (*Spin Fluctuations in Itinerant Electron Magnetism* (Springer, Berlin, 1985)). Although spin fluctuation theories have succeeded in describing the local moment behavior at finite temperatures in metallic magnetism, the underlying electronic structure related to the magnetism of a certain individual material seems to be oversimplified. A book which unifies the two paths on the same footing would be valuable for readers to understand the metallic magnetism.

This book aims to describe the theories of metallic magnetism from both viewpoints, namely spin fluctuations and the electronic structure. It attempts to clarify the magnetism from metals to disordered alloys to amorphous alloys.

The book covers most of the traditional topics of metallic magnetism such as electron correlation effects on the ferromagnetism, magnetic excitations, as well as the stability of antiferromagnetism and spin density waves. But it also includes topics which have been developed in the past three decades. The first is the development of the dynamical CPA (coherent potential approximation), which describes

the dynamical spin and charge fluctuations on the basis of the microscopic electronic structure within the single-site approximation. In particular, the first-principles dynamical CPA has reduced the gap between the spin fluctuation theory and the band theoretical approach to a large extent, thus allowing the investigation of the relationship between metallic magnetism and electronic structure. We elucidate this theory in Chap. 3. We also point out in the same chapter that the dynamical CPA is equivalent to the dynamical mean-field theory (DMFT) in the metal-insulator transition.

The second topic is the theory of local environment effects (LEE) in disordered alloys, which goes beyond the single-site CPA theory of magnetism. In Chap. 8, we describe the theory and clarify the magnetic behavior in the vicinity of the magnetic instability of Fe–Ni, Ni–Mn, and Ni–Cu alloys. This chapter also includes the molecular dynamics approach, which automatically determines the complex magnetic structure in metals and alloys. The third topic is the theoretical development of magnetism in amorphous metals and alloys. The finite-temperature theory sheds light on the amorphous magnetism from the viewpoint of spin fluctuations and the LEE, and clarifies how structural disorder drastically changes the magnetic properties of metals and alloys. This development is discussed in Chap. 9. Chapter 1 presents an introduction for the readers who are not familiar with the magnetism.

The frustrated system with heavy effective mass (e.g., YMn_2 and LiV_2O_4) is not described in this book, because it is still under development. Recent topics on the spintronics are also omitted for the same reason. Non-local theory of dynamical spin fluctuations which goes beyond the dynamical CPA is left as a problem of future concern.

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Okinawa Y. Kakehashi
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