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国外物理名著系列 10

(影印版)

Quantum Theory of Magnetism
Magnetic Properties of Materials

(3rd Edition)

磁性量子理论
——材料的磁学性质
(第三版)

R. M. White



科学出版社
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国外物理名著(影印版)系列序言

对于国内的物理学工作者和青年学生来讲,研读国外优秀的物理学著作是系统掌握物理学知识的一个重要手段。但是,在国内并不能及时、方便地买到国外的图书,且国外图书不菲的价格往往令国内的读者却步,因此,把国外的优秀物理原著引进到国内,让国内的读者能够方便地以较低的价格购买是一项意义深远的工作,将有助于国内物理学工作者和青年学生掌握国际物理学的前沿知识,进而推动我国物理学科研究和教学的发展。

为了满足国内读者对国外优秀物理学著作的需求,科学出版社启动了引进国外优秀著作的工作,出版社的这一举措得到了国内物理学界的积极响应和支持,很快成立了专家委员会,开展了选题的推荐和筛选工作,在出版社初选的书单基础上确定了第一批引进的项目,这些图书几乎涉及了近代物理学的所有领域,既有阐述学科基本理论的经典名著,也有反映某一学科专题前沿的专著。在选择图书时,专家委员会遵循了以下原则:基础理论方面的图书强调“经典”,选择了那些经得起时间检验、对物理学的发展产生重要影响、现在还不“过时”的著作(如:狄拉克的《量子力学原理》)。反映物理学某一领域进展的著作强调“前沿”和“热点”,根据国内物理学研究发展的实际情况,选择了能够体现相关学科最新进展,对有关方向的科研人员和研究生有重要参考价值的图书。这些图书都是最新版的,多数图书都是2000年以后出版的,还有相当一部分是2006年出版的新书。因此,这套丛书具有权威性、前瞻性和应用性强的特点。由于国外出版社的要求,科学出版社对部分图书进行了少量的翻译和注释(主要是目录标题和练习题),但这并不会影响图书“原汁原味”的感觉,可能还会方便国内读者的阅读和理解。

“他山之石,可以攻玉”,希望这套丛书的出版能够为国内物理学工作者和青年学生的工作和学习提供参考,也希望国内更多专家参与到这一工作中来,推荐更多的好书。



中国科学院院士
中国物理学会理事长
2007年3月20日

To Sara

Preface

Perhaps as many as ten years ago a colleague of mine pointed out to me that the Second Edition of this book was “out of print”. I mentioned this to my editor, who at that time was Helmut Lotsch, and he enthusiastically encouraged me to write a Third Edition. Thus began the long process that has finally resulted in this new edition. My primary goal was to get the book back into print, not necessarily to rewrite a new book. But I have taken the opportunity to change emphasis on some material as a result of recent developments and to add new material. For example, an entire chapter on thin film magnetic multilayers has been added.

The rationale for a book on magnetism is as valid today as it was when the first two editions were published. Magnetic phenomena continue to be discovered with deep scientific implications and novel applications. Since the Second Edition, for example, Giant Magneto Resistance (GMR) was discovered and the new field of “spintronics” is expanding rapidly. In addition, magnetic properties are often an important clue to our understanding of new materials. High temperature superconductors are a good example. The “parent” (undoped) compounds are antiferromagnetic. Their magnetic properties, studied by susceptibility measurements, nuclear magnetic resonance, neutron scattering, etc., have provided insight to the superconducting state. The purpose of this book is to provide a framework for understanding magnetic phenomena.

This framework is built upon linear response theory. In particular, mean field theory, or the random phase approximation, is used to determine the response of materials to magnetic fields. This approach provides a physical description of most magnetic phenomena. But it is not as powerful and elegant as other approaches applied to many interesting problems represented by magnetic systems. For example, I do not cover the renormalization group or the techniques used to obtain exact solutions to lower dimensional systems. Thus, this book may be thought of as a poor man’s theory of magnetic phenomena.

One of the challenges of producing this edition was that the previous editions had been type-set, so the material did not exist in a digital format. This

meant retyping everything using LaTeX. I am extremely grateful to Ferna Hartman of Carnegie Mellon for recreating not only the text but the many equations as well. The figures also had to be scanned and new ones created. For this I am grateful to Dr. Chando Park. Sergio Rezende and Vladimir Safonov kindly read the entire manuscript and offered helpful suggestions. I want to thank Jeff Lynn for his comments on the chapter on neutron scattering; Luc Berger for reviewing the section on spin transfer; and Christian Ruegg for reading the section on quantum phase transitions. I would also like to thank the Materials Science and Engineering Department at Stanford, Shan Wang in particular, and the Geballe Laboratory for Advanced Materials for their hospitality during the final stage of writing.

Palo Alto, September 2006

R.M. White

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The Magnetic Susceptibility

Any system may be characterized by its response to external stimuli. For example, in electronics the proverbial “black box” is characterized by its measured output voltage when an input current is applied. This transfer impedance, as it is called, provides all the information necessary to understand the operation of the black box. If we know what is in the black box – for example, the detailed arrangement of resistors, diodes, etc. – then we can predict, through analysis, what the transfer impedance will be.

Similarly, a system of charges and currents, such as a crystal, may be characterized by a response function. In this text we shall be concerned mainly with the response of such a system to a magnetic field. In this case the “output” is the magnetization and the response function is the magnetic susceptibility. A complete analysis of the magnetic susceptibility is virtually impossible since the system consists of about 10^{21} particles. Therefore we usually look to a measured susceptibility for clues to the important mechanisms active in the system and then use these to analyze the system. In order to carry out such a program, we must know what possible mechanisms exist and what effect they have on the susceptibility.

Determination of the susceptibility entails evaluation of the magnetization produced by an applied magnetic field. In general, this applied field may depend on space and time. The resulting magnetization will also vary in space and time. If the spatial dependence of the applied field is characterized by a wave vector \mathbf{q} and its time dependence is characterized by a frequency ω , and if we restrict ourselves for the time being to the magnetization with this wave vector and frequency, we obtain the *susceptibility* $\chi(\mathbf{q}, \omega)$. As we shall see shortly, the magnetization is the average magnetic moment. The magnetic moment itself is a well-defined quantity. The problem, however, is the computation of its average value. In order to compute this average it is necessary to know the probabilities of the system being in its various configurations. This information is contained in the distribution function associated with the system.

We shall see in this chapter that the distribution function depends on the total energy, or Hamiltonian, of the system. Therefore the first step in understanding magnetic properties is the identification of those interactions relevant to magnetism. In Chap. 2 the origin of these interactions is discussed, and they are expressed in a form which facilitates their application in later chapters. The reader is asked to keep in mind that Chaps. 1 and 2 both constitute background material for the theoretical development which begins in Chap. 3. The motivation for the material in these first two chapters should become clear as this theory unfolds.

In the absence of time-dependent fields we may assume that the system is in thermal equilibrium. In this case the distribution function is easily obtained. In Chap. 3 this is used to compute the response of noninteracting moments to a static field. This computation leads to the susceptibility $\chi(\mathbf{q}, 0)$. In Chaps. 4 and 5 the response $\chi(\mathbf{q}, 0)$ of an interacting system of moments to a static field is investigated in the random-phase approximation.

In the presence of time-dependent fields the distribution function must be obtained from its equation of motion. In the case of localized moments this consists of solving the *Bloch equations*. For itinerant moments the distribution function is obtained from a *Boltzmann equation*. In Chaps. 6 and 7 these equations are solved for weakly interacting systems to obtain the generalized susceptibility $\chi(\mathbf{q}, \omega)$. Finally, in Chap. 8 the generalized susceptibility associated with strongly interacting systems is investigated. This function is of particular interest because its singularities determine the magnetic-excitation spectrum of the system.

With the development of thin film deposition techniques it became possible to fabricate inhomogeneous magnetic materials, particularly thin films. Chapter 9 describes some of the phenomena associated with such structures.

One of the most powerful techniques for studying the spatial and temporal behavior of magnetic materials is neutron scattering. While pulsed and “cold” sources have expanded the range of neutron studies since the first edition of this book, the scattering description provided in Chap. 10 remains valid.

The next few sections introduce the basic quantities with which we shall be concerned throughout this text. Since these quantities may be defined in various ways, the reader may find it informative to compare other approaches (especially the classic work [1]).

1.1 The Magnetic Moment

Let us begin by discussing the magnetic moment. To see why this particular object is of interest let us consider the classical description of a system of charges and currents. Such a system is governed by Maxwell’s equations. The appropriate forms of these equations in a medium are the so-called *macroscopic Maxwell equations*, which are obtained from the microscopic equations by averaging over a large number of particles, see [2]. The microscopic equation

in which we shall be particularly interested is the one representing Ampere's law, which has the differential form

$$\nabla \times \mathbf{h} = \frac{4\pi}{c} \mathbf{j} + \frac{\partial \mathbf{e}}{\partial t}. \quad (1.1)$$

We define the average fields

$$\begin{aligned} \langle \mathbf{h} \rangle &\equiv \mathbf{B}, \\ \langle \mathbf{e} \rangle &\equiv \mathbf{E}. \end{aligned} \quad (1.2)$$

Here $\langle \dots \rangle$ is a spatial average over a region which is small compared with the size of the sample, yet large enough to contain many atomic systems (the lower limit to the macroscopic domain would typically be 10 nm).

When we write $\mathbf{B}(\mathbf{r})$ or $\mathbf{E}(\mathbf{r})$, the coordinate \mathbf{r} refers to the center of the region over which the average is taken. Thus the first equation of (1.2) might have been written as $\mathbf{B}(\mathbf{r}) = \langle \mathbf{h} \rangle_{\mathbf{r}}$. In this description it is assumed that any spatial variations are large in comparison with interatomic spacings. The actual details of the averaging will be discussed in Sect. 1.2. With this notation the macroscopic version of (1.1) becomes

$$\nabla \times \mathbf{B} = \frac{4\pi}{c} \langle \mathbf{j} \rangle + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t}. \quad (1.3)$$

The objective now is to calculate the average current density. To do this we separate the total current density into two parts, that associated with conduction electrons and that localized at an ionic site. The average value of the conduction electron current density is the *free current density* \mathbf{j}_{free} .

The ionic current density may be further separated into two contributions. First of all, the ion may possess an electric-dipole moment which is characterized by a *dipole charge density* ρ_{dip} . If this charge density is time dependent, there is a *polarization current density* \mathbf{j}_{pol} which satisfies the continuity equation

$$\nabla \cdot \mathbf{j}_{\text{pol}} = -\frac{\partial \rho_{\text{dip}}}{\partial t}. \quad (1.4)$$

Taking the average of this equation and assuming that the average commutes with the time and space derivatives, we obtain

$$\left\langle \sum_{\text{ions}} \mathbf{j}_{\text{pol}} \right\rangle = \frac{\partial \mathbf{P}}{\partial t}, \quad (1.5)$$

where the sum is over those ions within the averaging volume and \mathbf{P} is the electric polarization defined by

$$\left\langle \sum_{\text{ions}} \rho_{\text{dip}} \right\rangle = -\nabla \cdot \mathbf{P}.$$

The second contribution to the ionic current density arises from the internal motion of the ionic electrons. Since this current density \mathbf{j}_{mag} is stationary, $\nabla \cdot \mathbf{j}_{\text{mag}} = 0$. This is the current density responsible for the *magnetic moment* \mathbf{m} of the ion. If the center of mass of the ion is at \mathbf{R} , the magnetic moment is defined as

$$\mathbf{m} = \frac{1}{2c} \int d\mathbf{r} (\mathbf{r} - \mathbf{R}) \times \mathbf{j}_{\text{mag}}. \quad (1.6)$$

A convenient representation for \mathbf{j}_{mag} which has zero divergence and satisfies (1.6) is

$$\mathbf{j}_{\text{mag}} = -c\mathbf{m} \times \nabla f(|\mathbf{r} - \mathbf{R}|), \quad (1.7)$$

where $f(|\mathbf{r} - \mathbf{R}|)$ a smoothly varying function centered at \mathbf{R} which goes to 0 at the ionic radius and is normalized to 1. In Chap. 2 we shall see that this function has a quantum mechanical interpretation. Then

$$\left\langle \sum_{\text{ions}} \mathbf{j}_{\text{mag}} \right\rangle = c \left\langle \sum_{\text{ions}} \nabla f(|\mathbf{r} - \mathbf{R}|) \times \mathbf{m} \right\rangle = c \nabla \times \left\langle \sum_{\text{ions}} f(|\mathbf{r} - \mathbf{R}|) \mathbf{m} \right\rangle. \quad (1.8)$$

The last average in (1.8) is the magnetization \mathbf{M} , defined by

$$\mathbf{M} \equiv \left\langle \sum_{\text{ions}} f(|\mathbf{r} - \mathbf{R}|) \mathbf{m} \right\rangle. \quad (1.9)$$

Combining these results, we may now write (1.3) as

$$\nabla \times \mathbf{B} = \frac{4\pi}{c} \mathbf{j}_{\text{free}} + \frac{4\pi}{c} \frac{\partial \mathbf{P}}{\partial t} + 4\pi \nabla \times \mathbf{M} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t}. \quad (1.10)$$

Defining

$$\mathbf{H} = \mathbf{B} - 4\pi \mathbf{M} \quad (1.11)$$

and

$$\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P}, \quad (1.12)$$

we have the familiar result

$$\nabla \times \mathbf{H} = \frac{4\pi}{c} \mathbf{j}_{\text{free}} + \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t}. \quad (1.13)$$

Thus we see that the magnetization which appears in the macroscopic Maxwell's equations is the average of the ionic magnetic moment density. Since $f(|\mathbf{r} - \mathbf{R}|)$ is normalized to the volume the magnetization is the magnetic moment per unit volume.

As an example of the use of definition (1.6), let us neglect the possibility of nuclear currents and consider only the electron currents within the ion. Then

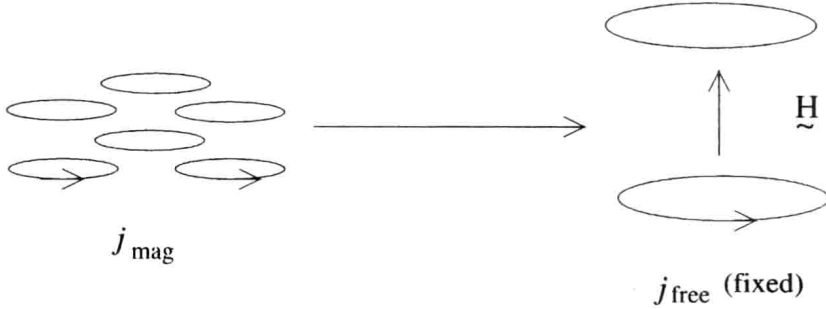


Fig. 1.1. Geometry envisioned in deriving the magnetic energy

$$\mathbf{j}_{\text{mag}}(\mathbf{r}) = \sum_{\alpha} e v_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}), \quad (1.14)$$

where e is the charge on the electron, which is $-|e|$, and \mathbf{v}_{α} is the velocity of the α th electron. From (1.6) we find for the total magnetic moment of the ion

$$\mathbf{m} = \frac{e}{2c} \sum_{\alpha} \mathbf{r}_{\alpha} \times \mathbf{v}_{\alpha}. \quad (1.15)$$

Recalling that the orbital angular momentum of an electron is

$$\mathbf{l}_{\alpha} = \mathbf{r}_{\alpha} \times m \mathbf{v}_{\alpha}, \quad (1.16)$$

we have

$$\mathbf{m} = \sum_{\alpha} \frac{e}{2mc} \mathbf{l}_{\alpha}. \quad (1.17)$$

Since $e = -|e|$, we see that the orbital magnetic moment of an electron is in the opposite direction to its orbital angular momentum.

We shall find it convenient to adopt a more general definition of the magnetic moment than that given by (1.6). This definition is based on the energy of the magnetic system (magnetic energy is discussed in [3] and [4]). The form of the magnetic energy depends upon the definition of the magnetic system. Let us define our magnetic system by the ionic magnetic current density \mathbf{j}_{mag} . This excludes the free currents, \mathbf{j}_{free} , which are assumed to be fixed and are the source of an external field \mathbf{H} in which our magnetic ion is to be located.¹ We now want to know the change in energy of this magnetic system when the field \mathbf{H} is applied or, equivalently, we may think of bringing the currents \mathbf{j}_{mag} in from infinity to a position in the field (see Fig. 1.1).

The energy difference results from the work done by the magnetic currents as they accommodate to the increasing external field. Since the magnetic field itself does no work on moving charges, we must use the induced electric field

¹ The magnetic field \mathbf{H} is understood to be the field in vacuum. Strictly speaking, this is the magnetic induction or flux density, \mathbf{B} . But in vacuum and in cgs units, $\mathbf{B} = \mathbf{H}$. It has become common practice to denote the field in vacuum as \mathbf{H} .

which is present while the external magnetic field is being turned on (due to the relative motion). This is given by

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t}. \quad (1.18)$$

The work done by the magnetic currents in a time δt is

$$\delta W = \int \mathbf{j}_{\text{mag}} \cdot \mathbf{E} d\mathbf{r} \delta t. \quad (1.19)$$

Making use of the representation (1.7) for \mathbf{j}_{mag} , integrating by parts, and then using (1.18), we obtain

$$\delta W = - \int f(|\mathbf{r} - \mathbf{R}|) \mathbf{m} \cdot \delta \mathbf{H} d\mathbf{r}. \quad (1.20)$$

If the field \mathbf{H} is uniform over the ionic dimension, $\delta \mathbf{H}$ may be taken outside the integral. Since \mathbf{m} is just a constant vector and $f(|\mathbf{r} - \mathbf{R}|)$ is normalized to unity,

$$\delta W = -\mathbf{m} \cdot \delta \mathbf{H}. \quad (1.21)$$

This work corresponds to Kittel's "scheme A" for applying the field [4]. Kittel also calculates the work needed to create the magnetized material in zero field in the first place ("scheme B"). The work associated with scheme A is important because this is the work that results in the change in the energy of the system given by its quantum mechanical eigenvalues [4].

Neither of these results give the *total* change in energy of the system when the magnetic material is introduced into the field since they do not include the work done by the source in keeping \mathbf{j}_{free} fixed. Jackson shows that the total change in energy is given by

$$W = \frac{1}{2} \int \mathbf{M} \cdot \mathbf{H}_0 d\mathbf{r},$$

where \mathbf{H}_0 is the field (\mathbf{B}_0) in the absence of the magnetic material, and the $\frac{1}{2}$ arises from an assumed linear relation between \mathbf{M} and \mathbf{B} .

The resulting change in the energy of the magnetic system is $\delta E = W$. Thus from (1.21)

$$\mathbf{m} = -\frac{\partial E}{\partial \mathbf{H}}. \quad (1.22)$$

As an example of the application of this definition, consider the ionic system of electrons which gave rise to the current density of (1.14). In the presence of a uniform field \mathbf{H} , which may be obtained from a vector potential \mathbf{A} by $\mathbf{H} = \nabla \times \mathbf{A}$, the energy of such a system is

$$E = \sum_{\alpha} \frac{1}{2} m v_{\alpha}^2 + \sum_{\alpha} e \phi_{\alpha}, \quad (1.23)$$