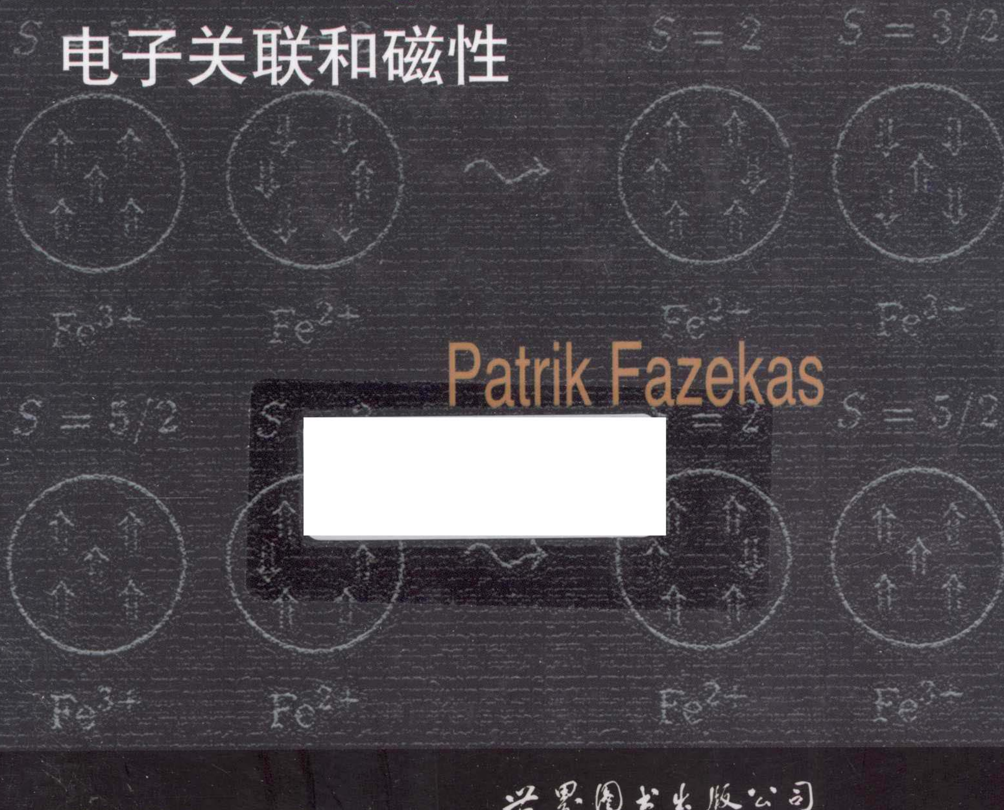
Series in Modern Condensed Matter Physics – Vol. 5

Lecture Notes on Electron Correlation and Magnetism

电子关联和磁性



Patrik Fazekas

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Lecture Notes on Electron Correlation and Magnetism

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Preface

In the academic years 1991–1992 and 1992–1993, the author had the opportunity to give a series of lectures entitled *Electron Correlation and Magnetism* at the Diploma Course organized by the International Center for Theoretical Physics (ICTP, Trieste). The Diploma Course is a one-year teaching program organized for students and young physicists from developing countries, with the intention of standardizing and upgrading their education to a level that is equivalent to that expected in the developed countries. The staff sought to achieve this by elaborating one-term courses to give a solid background in one of the standard subjects, but which also open ways into areas of current interest thereby enabling the students to begin research work.

The one-term, 4-hours-a-week course on magnetism presented a challenge known to all physicists in the field: research interests in the past half a century have been dominated by the effects of strong electron–electron interaction, while standard solid state physics textbooks remain within the bounds of band theory which is a suitable language for weakly correlated systems, and then add a chapter on Heisenberg magnets whose very existence is in contradiction with the rest of the material, and gets never properly justified. The usual way of clarifying these matters is to go through a formal education in many-body theory, and to learn about strong correlation effects piecemeal from its applications (and breakdowns). This, however, is usually the beginning of the professional career of a theoretician, and it may not be the most recommendable approach for others. One takes a long time to discover that there is a unified, non-formal way of thinking about strong correlation phenomena that has long been shared by experimentalists and theoreticians in the field; it can be called elementary and should be accessible to all – but it cannot be found in the well-known textbooks.

The author has attempted to fill this gap in his own way in the lectures mentioned above. The provision of notes for the courses was compulsory, and the 300-page handwritten version of the manuscript became an internal ICTP publication (DICTP CMP–MN(1,...,8), 1992). Yu Lu (who organized the course) kindly suggested that it should be rechecked, typed, whereupon it might be published by World Scientific, Singapore as *Lecture Notes on Electron Correlation and Magnetism.*

Though eager to accept the offer, I missed a series of deadlines, and was unable to avoid a considerable increase in the number of pages. However, this was made inevitable by (among other things) the nature of the undertaking: gaps in the reasoning had to be filled in, illustrative material collected, and the delay turned out not to be a bad thing bearing in mind the developments of the intervening years. I was astonished to discover that the subject of ferromagnetism which (in teaching) one tends to skip over as the easiest and dullest part of the subject magnetism, had in fact been the least understandable in the standard approach which uses the Hubbard model as its starting point. The developments of 1995–1998 brought significant advances in our understanding of ferromagnetism. Another subject which did not appear (though it should have done) in the older version of my notes, is the role of band degeneracy and orbital ordering, which enjoys great renewed interest.

I had the chance to experiment with new versions of presenting my material in the following years while giving courses for students specializing in solid state physics at the R. Eötvös University (Budapest) in 1993–1995, and at the Technical University of Budapest from 1996 to the present day. Usually, I give a two-semester course with two hours a week. Obviously the material assembled here is too much for that, so it should rather be understood that different versions of the course can be put together around the same central themes. The essential chapters are 4 and 5 (chapters 2 and 3 give background material with somewhat updated emphasis, and may be skipped). Basically, the most important correlation effect is the Mott transition, and spin models of magnetic ordering should be understood as strong-coupling effective Hamiltonians derived from an underlying fermion model. What follows afterwards is a matter of taste. One can continue with Ch. 6, or go straight to either Ch. 7 or Ch. 9. The mean field (Stoner) theories described in Ch. 7 should be supplemented with their criticism, especially with regard to ferromagnetism (see the discussion on p. 458, and Sec. 8.5). Any survey of magnetic ordering phenomena benefits from including a discussion of orbital ordering (sections 5.4 and 8.5). As for chapters 9 and 10, the author found that the Gutzwiller–Brinkman–Rice approach, though it requires a fair amount of preparation, offers the easiest way to discussing how the Mott transition is approached from the metallic side, and thus has some pedagogical advantages. Similarly, the most elementary way to discuss the fractional Quantum Hall Effect is by reference to Jastrow-type correlated many-electron states (Ch. 12).

Occasionally, when the general derivation of a result would have meant an undue burden on the main text, a simplified demonstration is posed as one of the *Problems*, and outlined in the *Solutions*. Searching for these is facilitated by listing the problems as separate *Contents* items.

I am aware of the many omissions, some of which are hard to justify. First, essentially the entire solid state physics could be approached by means of density functional theory (DFT). Some of the problems we consider to be particularly difficult (for instance, the ferromagnetism of iron) have been non-problems for DFT experts for thirty years. However, DFT is an art which one either practices, or one does not; and in the latter case, it is difficult to do anything more than to acknowledge what comes out of the calculations. At least, the author found it difficult to interpret the results by direct insight, or to establish links with the arguments which are straightforward in terms of the Hubbard model framework. Thus DFT is not described in any detail, but one has to keep it in mind that it is a very successful approach within the domain of its applicability. This domain is certainly getting wider, but we prefer to take the view that the Mott insulator and other strong-coupling states had better be described in the strong correlation framework. Second, even within the scope of lattice fermion models, a different author might well have written a completely different book with the same title, in which exactly solvable models (the one-dimensional Hubbard and Heisenberg model, and the Anderson/Kondo impurity problems) would have been dominant themes. In the present text, the emphasis is on motivating the introduction of models, and characterizing their overall behaviour (whenever known), rather than on their exact solution in particular cases. Third, we generally consider lattice problems, and discuss the (admittedly very important) impurity problems only very briefly.

A word should be added about the references which are many but even so, the list should not be regarded as complete, representative, or fair. This is meant to be an introductory text, not a professional review on any of the subjects. To illustrate a point, I usually chose the first source I came across, and did not attempt to survey the literature. I tried to cite reviews, or alternatively some of the latest works on a subject (in the hope that their reference lists lead on to the earlier publications). Nevertheless, I would like to apologize to all whose contributions are not properly represented here.

A book like this cannot be written without a great deal of help from others. Discussions with, and criticism from, colleagues and students have played a decisive role in shaping the text. I am particularly indebted to Attila Virosztek who has carefully read almost the entire manuscript, not seldom in several versions, and kindly pointed out an alarmingly large number of mistakes, inaccuracies, and cases of nebulous formulation. Tamás Kemény and Kazumasa Itai have also given great help by reading and checking most of the text. Karlo Penc has given valuable advice about certain subjects, and also helped me with some of the figures. G. Aeppli, K. Held, M. Jarrell, Y. Tokura and M. Ulmke sent me postscript files of (in some cases, still unpublished) illustrative material, as well as valuable comments. It would be impossible to recall all the occasions when I received assistance from colleagues who commented upon a part of the manuscript, or discussed with me one of the numerous issues, but let me mention at least C. Andreani, A. Asamitsu, D. Baeriswyl, S. Daul, P. Erdős, F. Gebhard, B. Győrffy, J. Hajdu, A. Jánossy, H.-Y. Kee, A. Klümper, J. Kollár, G. Kriza, P. Monachesi, E. Müller-Hartmann, T. Pruschke, T. Sakakibara, P. Santini, H. Shiba, J. Sólyom, A. Sütő, H. Tasaki, I. Tüttő, O. Újsághy and D. Vollhardt. I also thank all the authors who permitted me to display figures from their publications.

The bulk of the work was done in the years 1994–1997 at my home institute, the Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences. I gratefully acknowledge that during this period, I received financial support from the Hungarian National Research Foundation, under Grant No. OTKA T-014201. Since the beginning of this year, I have been supported by Grant No. OTKA T-025505.

I am indebted to World Scientific for their ongoing encouragement and support.

Special thanks do I owe to my wife for her constant support during all these years.

Budapest, September 1998 *Patrik Fazekas*

Contents

Chapter 1

Introduction

1.1 Magnetism and Other Effects of Electron–Electron Interaction

Magnetism is a vast subject and only a small part of it can be dealt with in these notes. Our first aim is to learn how to describe the effect of an external magnetic field H on the behaviour of a solid substance. In the limit of weak fields, the strength of the response is measured by the susceptibility

$$\chi = \frac{M}{H},$$

where M is the magnetization density. Generally, we can probe the system by a field which is space-, and time-dependent. Decomposing both H and M into Fourier-components, the relevant response function is the wavevector-, and frequency-dependent generalized susceptibility $\chi(\mathbf{q}, \omega)$ which should tell us all we want to know about the weak-field behaviour of the system. But what lies beyond? Need we worry about what happens in stronger fields?

The calculation of the magnetization requires solving a quantum-mechanical eigenvalue problem where the interaction of the probe with the external field is added to the Hamiltonian. The microscopic energy scale of this interaction is $\mu_B H$, where

$$\mu_B = \frac{e\hbar}{2mc} \approx \begin{cases} 9.27 \times 10^{-21}\mathrm{erg G^{-1}} & \text{(CGS)} \\ 9.27 \times 10^{-24}\mathrm{J T^{-1}} & \text{(SI)} \end{cases}$$

is the Bohr magneton. (G stands for 'gauss', while T for 'Tesla'). μ_B is very nearly equal to the spin magnetic moment of an electron in vacuum.

Let us try to get a feeling for the energy scale $\mu_B H$. In condensed matter physics, one often uses the electron volt 1eV $\equiv 1.6\times10^{-19}$J as the energy unit. Furthermore, it is useful to relate energies to equivalent temperatures, remembering that Boltzmann's constant is $k_B = 1.38\times10^{-23}\text{JK}^{-1} = 8.6\times10^{-5}\text{eVK}^{-1}$; thus 1eV corresponds to the temperature 11604K. 5T $\equiv 5\times10^4$G is a standard laboratory field; the corresponding interaction energy is of the order $\mu_B H \sim 3$K which is, by solid state standards, rather small. Let us recall that typical bandwidths are 1–10eV$\sim 10^4$–10^5K; the larger Coulomb matrix elements are in the same range; phonons are characterized by Debye temperatures $\theta_D \approx$100–1000K; even the spin–orbit coupling tends to be quite a bit stronger than $\mu_B H$. Common values of $\mu_B H$ are in the same range as (conventional "low-temperature") superconducting T_cs; indeed, the suppression of superconductivity by a sufficiently strong magnetic field is a long-known phenomenon. However, apart from that, it might seem that practicable magnetic fields cannot cause a drastic change in the behaviour of solids.

That would be a rash conclusion because it may happen that all the other terms in the Hamiltonian conspire to produce a set of more-or-less degenerate levels and, for (nearly) degenerate levels, any perturbation is a large perturbation. For instance, all the Bloch states on the Fermi surface are degenerate, and they are not even approximate eigenstates once an external field is turned on. The study of the resulting plethora of galvanomagnetic phenomena is a science in itself. – It is even possible to create situations where the coupling to the magnetic field is the dominating term of the Hamiltonian: such will be the case with the Quantum Hall Effect.

Another case when laboratory fields can have drastic effects arises when the Fermi temperature T_F turns out be very small, say, in the range 1–10K. There can be diverse reasons for this; marginal band overlap in semimetals like Bi can be one such reason. We will be more closely interested in a different situation, namely when strong electron correlations cause the system to develop narrow effective bands, as in *heavy fermion materials*.

Conventionally, one speaks of weak magnetism when the magneti-