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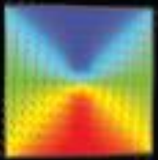

THEORY OF MAGNETISM
Application to Surface Physics

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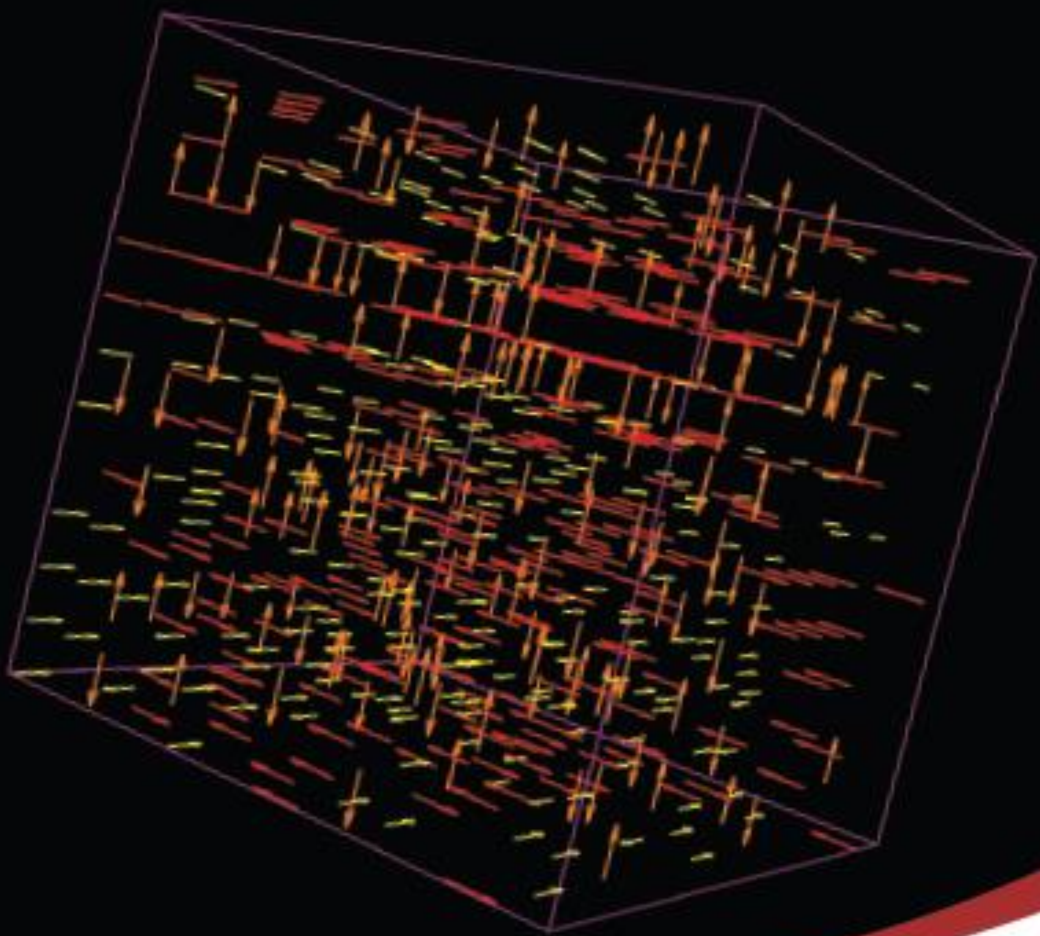

World Scientific

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THEORY OF MAGNETISM

Application to Surface Physics

Lectures, Problems and Solutions

WORLD SCIENTIFIC (2014)

Foreword

The book is intended for graduate students and researchers who wish to learn main properties of magnetic materials in the bulk state and at the nanometric scale such as thin films and multilayers. The book provides fundamental theories and methods of simulation to study and to understand these properties in an explicit manner. Exercises and problems are given for each chapter to help the reader apply the methods to discover new related phenomena and applications which are complementary to the lecture. Detailed solutions are provided for self-learning.

In the first part of the book, fundamental methods in magnetism are presented. The magnetism of systems of independent electrons and atoms is studied in chapter 1. The system of interacting electrons is studied in chapter 2 by the Hartree-Fock approximation which leads to the exchange interaction dependent on spin. This explains the origin of magnetic exchange interaction in magnetic materials. In chapter 3, we introduce the Heisenberg Hamiltonian which was the starting point of the modern theory of magnetism. The demonstration is made by using the method of second quantization. For readers who are not at ease with operator handling, this chapter can be omitted at the first reading of the book. The mean-field theory of systems of interacting spins is developed in chapter 4 where basic notions on the phase transition are given. The spin-wave theory, or theory of magnons, is studied in chapter 5 where detailed calculations of the magnon dispersion relation and low-temperature properties are shown. The Green's function method adapted for the study of magnetic systems is presented in chapter 6. This technique which can be applied in the whole range of temperature is complementary to the spin-wave theory. The phase transition theory is described in chapter 7 with the introduction of important concepts such as the Landau-Ginzburg theory, the renormalization group and the finite-size scaling. Monte Carlo simulation methods for the phase transition are described in chapter 8. Numerical methods constitute nowadays the third approach, next to theory and experiment, to study complicated and complex systems. Simulations are in particular necessary for testing theories and for quantitative comparisons with experiments.

The second part of the book is devoted to the application of the theory of magnetism to surface physics. In chapter 9 the magnetism at surfaces is shown by methods from the spin-wave theory, the Green's function technique and Monte Carlo simulations. Numerous examples covering typical cases in ferromagnets, antiferromagnets, ferrimagnets, helimagnets and frustrated spin systems are illustrated. Fundamental surface effects are shown and discussed. These simple models allow us to understand qualitatively experimental results observed in often more complicated real systems. The spin transport is described in chapter 10 where basic formulation of the Boltzmann's equation is recalled and recent methods of Monte Carlo simulation to deal with the spin resistivity are explained.

In the third part of the book, we present detailed solutions of problems given in each chapter. Many problems are important topics in magnetism.

An appendix on elements of statistical physics is also included to make the book self-contained. Finally, a simple Monte Carlo program is provided to facilitate the first step in the writing of a simulation program.

The material of this book can be used for one-semester lectures of three hours weekly in a graduate program of physics. An equivalent amount of time is needed for students to solve problems with the help of an assistant.

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Contents

LIST OF PROBLEMS

Chapter 1: Magnetism of Free Electrons and Atoms

1. Orbital and spin moments of an electron: Using the theory of angular momentum, calculate the orbital and spin moments of an electron. Determine the total magnetic moment.

2. Zeeman effect

a) Calculate the magnetic moment per atom for Fe, provided the saturated magnetization under an applied magnetic field equal to $1.7 \times 10^6\ A/m$, the mass density of Fe $\rho = 7970\ kg/m^3$ and the atomic mass of Fe $M = 56$.

b) Calculate ΔE the separation of the energy levels due to the Zeeman effect on the atomic level corresponding to the wavelength $\lambda = 643.8\ nm$ of a cadmium atom. Calculate the variation of frequency $\Delta\nu$ of the initial level.

Numerical application: Calculate ΔE and $\Delta\nu$ for the following fields $\mu_B H = 0.5$, 1, and 2 Tesla.

3. Density of states: Calculate the density of states ρ(*E*) of a free electron of energy E in three dimensions. Show that ρ(*E*) is given by Eq. (A.41}).

4. Fermi-Dirac distribution for free-electron gas:

Electrons are fermions which obey the Pauli's exclusion principle. Microscopic states follow the Fermi-Dirac statistics. The Fermi-Dirac distribution is given by (see Appendix A)

$$f(E,T,\mu) = \frac{1}{e^{\beta(E-\mu)}+1} \qquad (1.82)$$

where μ is the chemical potential, $\beta = \frac{1}{k_B T}$, k_B the Boltzmann constant and T the temperature. The function $f(E,T,\mu)$ is the number of electrons of the microscopic state of energy E at temperature T.
Give the properties of $f(E,T,\mu)$ at $T = 0$. Plot $f(E,T,\mu)$ as a function of E for an arbitrary $\mu(> 0)$, at $T = 0$ and at low T.

5. Sommerfeld's expansion: Demonstrate the Sommerfeld's expansion for a free electron gas at low temperature.

6. Pauli paramagnetism: Calculate the susceptibility of a three-dimensional electron gas in an applied magnetic field ***B***, at low and high temperatures. One supposes that ***B*** is small.

7. Paramagnetism of free atoms for arbitrary **J**: Consider a gas of *N* free atoms of moment **J** in a volume *V*. Find the average of the total magnetic moment per volume unit.

8. Langevin's theory of diamagnetism

9. Langevin's theory of paramagnetism

10. Calculate the variation of the energy gap due to an applied magnetic field in a semiconductor.

11. Paramagnetic resonance

12. Nuclear Magnetic Resonance (NMR).

Chapter 2: Exchange Interaction in an Electron Gas

1. System of two electrons - Fermi hole

2. Theorem of Koopmann

3. Screened Coulomb potential, Thomas-Fermi approximation

4. Paradox of the Hartree-Fock approximation

5. Hydrogen molecule: Calculate the exchange interaction between two electrons of a hydrogen atom.

Chapter 3: Magnetic Exchange Interactions

1. Study properties of a free electron gas with the second quantization.

2. Calculate the energy of an interacting electron gas at the first-order of perturbation with the second quantization.

3. Hubbard model: one-site case

4. Hubbard model on a two-site system

5. Show that [H,N]=0 where N is the field operator of occupation number defined in (3.36) and H the Hamiltonian in the second quantization (3.35).

6. Show that $\Phi(\mathbf{r})N=(N+1)\Phi(\mathbf{r})$ for both boson and fermion cases.

7. Show that $\Phi+(\mathbf{r})$|vac> (``vac" stands for vacuum) is a state in which there is a particle localized at **r**.

8. Using the equation of motion for $\Phi(\mathbf{r})$] with H the Hamiltonian in the second quantization of a system of fermions, show that we can obtain the Hartree-Fock equation by taking a first approximation (linearization).

9. Bardeen-Cooper-Schrieffer theory of supraconductivity: Study a gas of N electrons with the reduced Hamiltonian in the superconducting regime.

10. Magnon-phonon interaction: Calculate the renormalized phonon spectrum taking into account the magnon-phonon interaction.

Chapter 4: Magnetism: Mean-Field Theory

1. Define the order parameter of an antiferromagnetic lattice of Ising spins.

2. Consider the q-state Potts model defined by the Hamiltonian (4.6) on a square lattice. Define the order parameter of the q-state Potts model. Describe the ground state and its degeneracy when J>0. If J<0, what is the ground state for q=2 and q=3? For q=3, find ways to construct some ground states and give comments. Show that the Potts model is equivalent to the Ising model when q=2.

3. Domain walls: In magnetic materials, due to several reasons, we may have magnetic domains schematically illustrated in Fig. 4.5. The spins at the interface between two neighboring domains should arrange themselves in a smooth configuration in order to make a gradual change from one domain to the other. An example of such a ``domain wall" is shown in that figure. Calculate the energy of a wall of thickness of N spins.

4. Bragg-Williams approximation: The mean-field theory can be demonstrated by the Bragg-Williams approximation described in this problem.

5. Binary alloys by spin language, mean-field theory

6. Critical temperature of ferrimagnet: Using the mean-field theory, calculate the critical temperature T_N of the simple model for a ferrimagnet.

7. Improvement of mean-field theory: In the first step, we treat exactly the interaction of two neighboring spins. In the second step, we use the mean-field theory to treat the interaction of the two-spin cluster embedded in the crystal. Show that the critical temperature T_C for S = 1/2 is given by

$$e^{-2J/k_BT_c} + 3 - 2(Z-1)J/k_BT = 0 \qquad (4.83)$$

8. Interaction between next-nearest neighbors in mean-field treatment

9. Improved mean-field theory - Bethe's approximation: Calculate the critical temperature and make a comparison with the result from the elementary mean-field theory.

10. Repeat Problem 7 in the case of an antiferromagnet.

11. Calculate the critical field H_C in the following cases: a simple cubic lattice of Ising spins with antiferromagnetic interaction between nearest neighbors, a square lattice of Ising spins with antiferromagnetic interaction J_1 between nearest neighbors and ferromagnetic interaction J_2 between next-nearest neighbors.

Chapter 5: Theory of Magnons

1. Prove (5.63)-(5.64).

2. Chain of Heisenberg spins with nearest neighbors and next-nearest neighbors: spectrum and instability

3. Heisenberg spin systems in two dimensions: spectrum, no ordering in 2D (thorem of Mermin-Wagner)

4. Prove Eqs. (5.143)-(5.145).

5. Consider the Ising spin model on a 'Union-Jack' lattice, namely the square lattice in which one square out of every two has a centered site. Define sublattice 1 containing the centered sites, and sublattice 2 containing the remaining sites (namely the cornered sites). Let J_1 be the interaction between a centered spin and its nearest neighbors, J_2 and J_3 the interactions between two nearest spins on the y and x axes of the sublattice 2, respectively. Determine the phase diagram of the ground state in the space (J_1,J_2,J_3)\$. Indicate the phases where the centered spins are undefined (partial disorder).

6. Using the method described in section 5.4, determine the ground-state spin configuration of a triangular lattice with XY spins interacting with each other via an antiferromagnetic exchange J_1 between nearest neighbors.

7. Uniaxial anisotropy: Calculate the magnon spectrum. Is it possible to have a long-range magnetic ordering at finite temperature in two dimensions? (cf. Problem 3).

8. Show that the operators a^+ and a defined in the Holstein-Primakoff approximation, Eqs. (5.35) and (5.36), respect rigorously the commutation relations between the spin operators.

9. Show that the operators defined in Eqs. (5.86)-(5.89) obey the commutation relations.

10. Show that the magnon spectrum (5.125) becomes unstable when the interaction between next-nearest neighbors defined in ε, Eq. (5.119), is larger than a critical constant.

Chapter 6: Green's Function Method in Magnetism

1. Give proofs of the formula (6.13).

2. Give the demonstration of Eq. (6.22).

3. Helimagnet by Green's function method: Calculate the magnon spectrum.

4. Apply the Green's function method to a system of Ising spins S=+/-1 in one dimension, supposing a ferromagnetic interaction between nearest neighbors under an applied magnetic field.

5. Apply the Green's function method to a system of Heisenberg spins on a simple cubic lattice, supposing ferromagnetic interactions between nearest neighbors and between next-nearest neighbors.

6. Calculate the magnon spectrum in Heisenberg triangular antiferromagnet: Green's function method.

7. Study the free electron gas by Green's function method.

Chapter 7: Phase Transition

1. Solution for an Ising chain: Calculate the partition function of a chain of N Ising spins using the periodic boundary condition. Calculate the free energy, the averaged energy and the heat capacity as functions of the temperature. Show that there is no phase transition at finite temperature.

2. Renormalization group applied to an Ising chain: Study by the renormalization group a chain of Ising spins with a ferromagnetic interaction between nearest neighbors. Show that there is no phase transition at finite temperature.

3. Transfer matrix method applied to an Ising chain: Study by the transfer matrix method the chain of Ising spins in the previous exercise using the periodic boundary condition.

4. Study the low- and high-temperature expansions of the Ising model on the square lattice. The low- and high-temperature expansions are useful not only for studying physical properties of a spin system in these temperature regions, but also for introducing a new concept called duality which allows to map a system of weak coupling into a system of strong coupling, as seen in this problem.

5. Critical temperatures of the triangular lattice and the honeycomb lattice by duality: Consider the triangular lattice with Ising spins with a ferromagnetic interaction between nearest neighbors. Construct its dual lattice. Calculate the partition functions of the two lattices. Deduce the critical temperature of each of them by following the method outlined in the previous problem.

6. Villain's model: We study the ground state spin configuration of the 2D Villain's model with XY spins defined in Fig. 7.7. Write the energy of the elementary plaquette. By minimizing this energy, determine the ground state as a function of the antiferromagnetic interaction $J_{AF}=-\eta J_F$ where η is a positive coefficient. Determine the angle between two neighboring spins as a function of η. Show that the critical value of η beyond which the spin configuration is not collinear is 1/3.

7. Give the proofs of Eq. (7.85).

8. Critical line of an antiferromagnet in an applied magnetic field: In chapter 4 we have seen that an antiferromagnet in a field can have a phase transition at a finite temperature T_C, in contrast to a ferromagnet. We calculate in this exercise T_C as a function of a weak field H.

Chapter 8: Methods of Monte Carlo Simulation

1. Write a program for Ising model using the model program shown in Appendix B by adding the calculation of the heat capacity and the magnetic susceptibility. Modify it for the case of a simple cubic lattice and a body-centered-cubic lattice.

2. Write a simple program for the classical Heisenberg spin model.

3. Write the instruction which realizes the energy histogram H(E) in the program for the Ising model shown in Appendix B.

4. Program to search for the ground state: We can determine in most cases the ground state of a spin system with Ising, XY, Heisenberg or Potts model by the steepest-descent method: at each spin, we minimize its energy by aligning it along its local field. Describe the necessary steps to make a program to this end. Write a program which realizes the above steps. Apply it to the Ising model on a square lattice with nearest-neighbor interaction J_1 and next-nearest neighbor interaction J_2. Determine the phase diagram at temperature T=0 in the space (J_1,J_2).

Chapter 9: Magnetic Properties of Thin Films

1. Surface magnon: Calculate the surface magnon modes in the case of a semi-infinite ferromagnetic crystal of body-centered cubic lattice for $k_x=k_y=0$, π/a in using the method presented in section 9.4.

2. Critical next-nearest-neighbor interaction: Calculate the critical value of ε defined in section 9.4 for an infinite crystal.

3. Uniform magnetization approximation: Show that with the hypothesis of uniform layer-magnetization [Eq. 9.50], the energy eigenvalue E_i is proportional to M.

4. Multilayers - critical magnetic field: One considers a system composed of three films A, B and C, of Ising spins with respective thicknesses N_1, N_2 and N_3. The lattice sites are occupied by Ising spins pointing in the +\- z direction perpendicular to the films. The interaction between two spins of the same film is ferromagnetic. Let J_1, J_2 and J_3 the magnitudes of these interactions in the three films. One supposes that the interactions at the interfaces A-B and B-C are antiferromagnetic and both equal to J_s. One applies a magnetic field along the z direction. Determine the critical field above which all spins are turned into the field direction. For simplicity, consider the case $J_1=J_2 = J_3$.

5. Mean-field theory of thin films: Calculate the layer magnetizations of a 3-layer film by the mean-field theory (cf. chapter 4). One supposes the Ising spin model with values +\- 1/2 and a ferromagnetic interaction J for all pairs of nearest neighbors.

6. Holstein-Primakoff method: Using the Holstein-Primakoff method of chapter 5 for a semi-infinite crystal with the Heisenberg spin model, write the expression which allows us to calculate the surface magnetization as a function of temperature. Show that a surface mode of low energy (acoustic surface mode) diminishes the surface magnetization.

7. Frustrated surface - surface spin rearrangement: Consider a semi-infinite system of Heisenberg spins composed of stacked triangular lattices. Suppose that the interaction between nearest neighbors J is everywhere ferromagnetic except for the spins on the surface: they interact with each other via n antiferromagnetic interaction J_S. Determine the ground state of the system as a function of J_S/J.

8. Ferrimagnetic film: Write the equations of motion for a five-layer ferrimagnetic film of body-centered cubic lattice, using the model and the method presented in section 9.4. Consider the cases $k_x=k_y=0, \pi/a$. Solve numerically these equations to find surface and bulk magnons.

Chapter 10: Monte Carlo Simulation of Spin Transport

1. Effect of magnetic field: demonstrate Eq. (10.24).

2. Ohm's law: demonstrate Eq. (10.29).

3. Hall effect - Magneto-resistance: The general expression of the current density in a system under an applied electric field $\boldsymbol{\varepsilon}$ and an external magnetic field **B** can be written as a series of $\boldsymbol{\varepsilon}$ and **B**:

$$j_i = \sum_j \sigma_{ij}\epsilon_j + \sum_{j,l} \sigma_{ijl}\epsilon_j B_l + \sum_{j,l,m} \sigma_{ijlm}\epsilon_j B_l B_m$$

where σ_{ij} is the ``normal" or ``ordinary" electric conductivity tensor, and σ_{ijl} denotes the conductivity tensor due to the interaction between ε and B. When $\boldsymbol{\varepsilon}$. **B**=0, we have the geometry of the Hall effect. σ_{ijlm} is the conductivity tensor due to the interaction between $\boldsymbol{\varepsilon}$ and **B** at the second order. This is at the origin of the magneto-resistance. In this problem, we study the cases of weak, moderate and strong fields.

4. Using the Boltzmann's equation study the case of a strong field.