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QUANTUM THEORY OF MAGNETISM

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QUANTUM THEORY OF MAGNETISM

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Preface

This is a supporting text for the undergraduate students interested in quantum theory of magnetism. The text represents an introduction to various theoretical approaches used in this field. It is an open material, in the sense that it will be supported by appropriate problems to be solved by student at seminars and also as a homework.

The text consists of four chapters that form closed themes of the introductory quantum theory of magnetism. In the first part we explain the quantum origin of the magnetism illustrating the appearance of the exchange interaction for the case of hydrogen molecule. The second chapter is devoted to the application of the Bogolyubov inequality to the Heisenberg model and it represents the part which is usually missing in the textbooks of magnetism. The third chapter deals with the standard spin wave-theory including the Bloch and Holstein-Primakoff a approach. Finally, we discuss the application of the Jordan-Wigner transformation to one-dimensional spin-1/2 XY model.

The primary ambition of this supportive text is to explain diverse mathematical methods and their applications in the quantum theory of magnetism. The text is written in the form which should be sufficient to develop the skills of the students up to the very high level. In fact, it is expected that students following this course will able to make their own original applications of the methods presented in this book.

The reading and understanding this text requires relevant knowledges from the mathematics, quantum and statistical mechanics, and also from the theory of phase transitions. It is also expected that students are familiar with computational physics, programming and numerical mathematics that are necessary to solve the problems that will be included in the MOODLE educational environment of the P.J. Šafárik University in Košice.

Finally one should note that the text is mathematically and physically rather advanced and its understanding assumes supplementary study of the

Preface

books listed in the list of references.

Košice, September 2013,

Michal Jaščur.

Chapter 1

Many-Body Systems

1.1 Systems of Identical Particles

Magnetism is a many-body phenomenon and its origin can only be explained within the quantum physics. In this part we will investigate some important properties of the wavefunctions of quantum systems consisting of many identical particles that are important to understand magnetic properties in the solid state. In general, the Hamiltonian of the many-body system depends on the time, coordinates and spin variables of all particles. However, in this part we will mainly investigate the symmetry properties of the wavefunction that are independent on the time and therefore we can exclude the time from our discussion. For simplicity we neglect also spin-degrees of freedom.

Let us consider a system of N identical particles described by the many-body Hamiltonian $\hat{\mathcal{H}}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N,)$ which remains unchanged with respect to the transposition of arbitrary two particles in the system. This fact can be mathematically expressed as

$$\hat{\mathcal{H}}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots, \mathbf{r}_k, \dots, \mathbf{r}_N) = \hat{\mathcal{H}}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k, \dots, \mathbf{r}_j, \dots, \mathbf{r}_N) \quad (1.1)$$

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or

$$\hat{\mathcal{P}}_{jk}\hat{\mathcal{H}}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots, \mathbf{r}_k, \dots, \mathbf{r}_N) = \hat{\mathcal{H}}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k, \dots, \mathbf{r}_j, \dots, \mathbf{r}_N)\hat{\mathcal{P}}_{jk}. \quad (1.2)$$

The previous equation defines the transposition operator $\hat{\mathcal{P}}_{jk}$ of the j th and k th particle. Since a mutual interchange of arbitrary particles in the system does not change its state, then the total wavefunction of the system obeys the following relation

$$\hat{\mathcal{P}}_{jk}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots, \mathbf{r}_k, \dots, \mathbf{r}_N) = e^{i\alpha}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k, \dots, \mathbf{r}_j, \dots, \mathbf{r}_N) \quad (1.3)$$

and

$$\hat{\mathcal{P}}_{jk}^2\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots, \mathbf{r}_k, \dots, \mathbf{r}_N, t) = e^{2i\alpha}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots, \mathbf{r}_k, \dots, \mathbf{r}_N), \quad (1.4)$$

where the real parameter α apparently satisfies equation

$$e^{2i\alpha} = 1 \quad \text{or} \quad e^{i\alpha} = \pm 1. \quad (1.5)$$

The last equation implies that the total wavefunction either remains the same, or changes its sign when two arbitrary particles are interchanged in the system. In the first case, the total wave function is called as a symmetric function and in the later one as an anti-symmetric function. The symmetry of the wavefunction of an ensemble of identical particles is exclusively given by the type of particles and does not depend on external conditions. In fact, it has been found that all particles obeying the Pauli exclusion principle have the antisymmetric wavefunction and all other particles have the symmetric wavefunction. Unfortunately, the direct theoretical proof of this statement is impossible for strongly interacting particles, since in real

1.1 Systems of Identical Particles

many-body systems is not possible to calculate exactly the total wavefunction. On the other hand, the situation becomes tractable for the case of non-interacting or weakly interacting particle. Therefore we at first will investigate the system of spinless non-interacting identical particles and then we clarify the role of the interaction and spin.

In the case of noninteracting particles the total Hamiltonian of the system can be expressed as a sum of single-particle Hamiltonians, i.e.

$$\hat{\mathcal{H}} = \sum_j^N \hat{\mathcal{H}}_j, \quad (1.6)$$

where N denotes the number of particles. It is also well known that the total wavefunction of non-interacting particles can be written as a product of the single-particle wavefunctions, namely,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots, \mathbf{r}_k, \dots, \mathbf{r}_N) = \prod_{j=1}^N \phi_{n_j}(\mathbf{r}_j), \quad (1.7)$$

where n_j represents the set of all quantum numbers characterizing the relevant quantum state of the j th particle. The single-particle functions $\phi_{n_j}(\mathbf{r}_j)$ are of course the solutions of the stationary Schrodinger equation

$$\hat{\mathcal{H}}_j \phi_{n_j}(\mathbf{r}_j) = \varepsilon_{n_j} \phi_{n_j}(\mathbf{r}_j). \quad (1.8)$$

Here ε_{n_j} denote the eigenvalues of the single-particle Hamiltonian $\hat{\mathcal{H}}_j$, so that the eigenvalue of the total Hamiltonian is given by $E_{n_1, n_2, \dots, n_N} = \sum_j \varepsilon_{n_j}$. The symmetric wavefunction describing whole system can be written in the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots, \mathbf{r}_k, \dots, \mathbf{r}_N) = A \sum_P \phi_{n_1}(\mathbf{r}_1) \phi_{n_2}(\mathbf{r}_2) \dots \phi_{n_N}(\mathbf{r}_N), \quad (1.9)$$

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where A denotes the normalization constant and summation is performed over all possible permutation of the particles. Similarly for the antisymmetric case we obtain the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots, \mathbf{r}_k, \dots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{n_1}(\mathbf{r}_1) & \phi_{n_1}(\mathbf{r}_2) & \dots & \phi_{n_1}(\mathbf{r}_N) \\ \phi_{n_2}(\mathbf{r}_1) & \phi_{n_2}(\mathbf{r}_2) & \dots & \phi_{n_2}(\mathbf{r}_N) \\ \vdots & \vdots & & \vdots \\ \phi_{n_N}(\mathbf{r}_1) & \phi_{n_N}(\mathbf{r}_2) & \dots & \phi_{n_N}(\mathbf{r}_N) \end{vmatrix} \quad (1.10)$$

which is usually called as the Slater determinant. It is clear, that interchanging of two particles in the system corresponds to the interchange of relevant rows in the determinant (1.10), which naturally leads to the sign change of the wavefunction. Moreover, if two or more particles occupy the same state, then two or more rows in the determinant (1.10) are equal and consequently, the resulting wavefunction is equal to zero in agreement with the Pauli exclusion principle.

Until now, we have considered a simplified system of non-interacting particles and we have completely neglected spin degrees of freedom. However, the situation in realistic experimental systems is much more complicated, since each particle has a spin and moreover, the interactions between particles often also substantially influence the behavior of the system. However, if we assume the case of weak interactions and if we neglect the spin-orbit interactions then the main findings discussed above remain valid and moreover, the existence of the exchange interaction can be clearly demonstrated. Instead of developing an abstract and general theory for such a case, it is much more useful to study a typical realistic example of the hydrogen molecule, which illustrates principal physical mechanisms leading to the appearance of magnetism.

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In the previous part, we have found that the total wavefunction of the many-electron system must be anti-symmetric. In this subsection, we will demonstrate that the use of anti-symmetric wave functions leads to the purely quantum contribution to the energy of the system, which is called the exchange energy. In fact, this energy initiates a certain ordering of the spins, i.e. it may lead to the magnetic order in the system. A similar effect we also obtain using the single-product wavefunctions, if we explicitly include the exchange-interaction term into Hamiltonian. This effect was independently found by Heisenberg and Dirac in 1926 and it represent the modern quantum-mechanical basis for understanding magnetic properties in many real systems.

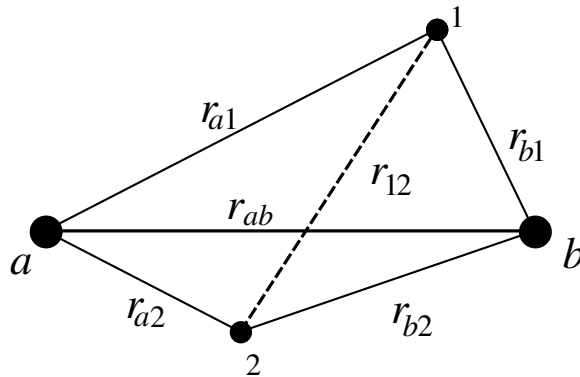


Figure 1.1: Schematic geometry of the H_2 molecule. The larger circles denote the protons and the smaller ones represent two electrons. The relevant distances between different pairs of particles are denoted as r_{ij} , where $i, j = a, b, 1, 2$

We start our analysis with one of the simplest possible system, namely,

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H₂ molecule. In the hydrogen molecule two electrons interact with each other and with the nuclei of the atoms. The situation is schematically depicted in Fig.1.1 and considering this geometry we can write the Hamiltonian of the H₂ molecule in the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2 + \hat{\mathcal{W}} + \hat{\mathcal{H}}_{LS} \quad (1.11)$$

where

$$\hat{\mathcal{H}}_1 = -\frac{\hbar^2}{2m}\Delta_1 - \frac{e_0^2}{r_{a1}} \quad (1.12)$$

$$\hat{\mathcal{H}}_2 = -\frac{\hbar^2}{2m}\Delta_2 - \frac{e_0^2}{r_{b2}} \quad (1.13)$$

$$\hat{\mathcal{W}} = \frac{e_0^2}{r_{ab}} + \frac{e_0^2}{r_{12}} - \frac{e_0^2}{r_{b1}} - \frac{e_0^2}{r_{a2}} \quad (1.14)$$

and we have used the abbreviation $e_0 = e/(4\pi\epsilon_0)$. The terms $\hat{\mathcal{H}}_1$ and $\hat{\mathcal{H}}_2$ in (1.11) describe the situation when the two hydrogen atoms are isolated. The operator $\hat{\mathcal{W}}$ describes the interaction between two cores, electrons, as well as between electrons and relevant nuclei. Finally, the last term represents the spin-orbit interaction, which is assumed to be small so that we can separate the orbital and spin degrees of freedom. To solve the problem of the hydrogen molecule, we apply the first-order perturbation theory neglecting the spin-orbit coupling and taking the term $\hat{\mathcal{W}}$ as a small perturbation. As it is usual in the perturbation theory, we at first solve the unperturbed problem, i.e. the system of two non-interacting hydrogen atoms. Thus, we have to solve the Schrodinger equation

$$(\hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2)\Psi = U_0\Psi \quad (1.15)$$

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As we already have noted above, we will assume that the total wave function can be written as a product of the orbital and spin functions, i.e. $\Psi = \varphi(\mathbf{r}_1, \mathbf{r}_2)\chi(s_1^z, s_2^z)$. Another very important point to be emphasized here is that our simplified Hamiltonian does not explicitly depend on the spin variables. Consequently, we can at first evaluate only the problem with orbital functions and at the end of the calculation we can multiply the result by an appropriate spin function to ensure the anti-symmetry of the total wavefunction. In order to express this situation mathematically, we introduce the following notations

- $\phi_\alpha(\mathbf{r}_i)$, where $\alpha = a, b$, $i = 1, 2$ represents the orbital wave function of the isolated hydrogen atom when the i th electron is localized closely to the α th nucleus
- $\xi_\gamma(i)$, where $\gamma = \uparrow, \downarrow$, $i = 1, 2$ is the spin function describing the spin up or spin down of the i th electron

Now, let us proceed with the discussion of the orbital functions of the system described by Eq.(1.15). Since the orbital functions $\phi_\alpha(\mathbf{r}_i)$ are eigenfunctions of the relevant one-atom Schrodinger equation with the same eigenvalue $E_0 = -13.55 eV$, it is clear that the ground state of the two noninteracting hydrogen atoms has the energy $U_0 = 2E_0$ and it is doubly degenerated. This is so-called exchange degeneracy and two wavefunctions corresponding to this U_0 can be expressed as $\varphi_1(\mathbf{r}_1, \mathbf{r}_2) = \phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2)$ and $\varphi_2(\mathbf{r}_1, \mathbf{r}_2) = \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)$.

If we include into Hamiltonian also the interaction term $\hat{\mathcal{W}}$ then the situation becomes much more complex and the eigenfunctions and eigenvalues cannot be found exactly. In the spirit of the perturbation theory, we will assume that the wavefunction of the interacting system can be expressed in the form

$$\begin{aligned}\varphi(\mathbf{r}_1, \mathbf{r}_2) &= c_1\varphi_1(\mathbf{r}_1, \mathbf{r}_2) + c_2\varphi_2(\mathbf{r}_1, \mathbf{r}_2) \\ &= c_1\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) + c_2\phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)\end{aligned}\tag{1.16}$$

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where c_1 and c_2 are the constant that will be determined later. The system is now described by the following Schrodinger equation

$$(\hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2 + \hat{\mathcal{W}}) [c_1\varphi_1(\mathbf{r}_1, \mathbf{r}_2) + c_2\varphi_2(\mathbf{r}_1, \mathbf{r}_2)] = E [c_1\varphi_1(\mathbf{r}_1, \mathbf{r}_2) + c_2\varphi_2(\mathbf{r}_1, \mathbf{r}_2)] \quad (1.17)$$

Multiplying the previous equation by $\varphi_1^*(\mathbf{r}_1, \mathbf{r}_2)$ and integrating over the space one obtains

$$\begin{aligned} & 2c_1E_0 + 2c_2E_0 \iint \varphi_1^*(\mathbf{r}_1, \mathbf{r}_2)\varphi_2(\mathbf{r}_1, \mathbf{r}_2)dV_1dV_2 \\ & + 2c_1 \iint \varphi_1^*(\mathbf{r}_1, \mathbf{r}_2)\hat{\mathcal{W}}\varphi_1(\mathbf{r}_1, \mathbf{r}_2)dV_1dV_2 + c_2 \iint \varphi_1^*(\mathbf{r}_1, \mathbf{r}_2)\hat{\mathcal{W}}\varphi_2(\mathbf{r}_1, \mathbf{r}_2)dV_1dV_2 \\ & = c_1E + c_2E \iint \varphi_1^*(\mathbf{r}_1, \mathbf{r}_2)\varphi_2(\mathbf{r}_1, \mathbf{r}_2)dV_1dV_2. \end{aligned} \quad (1.18)$$

Similarly, by multiplying Eq.(1.17) by $\varphi_2^*(\mathbf{r}_1, \mathbf{r}_2)$ and integrating over the space one finds

$$\begin{aligned} & c_1E_0 \iint \varphi_2^*(\mathbf{r}_1, \mathbf{r}_2)\varphi_1(\mathbf{r}_1, \mathbf{r}_2)dV_1dV_2 + c_1 \iint \varphi_2^*(\mathbf{r}_1, \mathbf{r}_2)\hat{\mathcal{W}}\varphi_1(\mathbf{r}_1, \mathbf{r}_2)dV_1dV_2 \\ & + 2c_2E_0 + c_2 \iint \varphi_2^*(\mathbf{r}_1, \mathbf{r}_2)\hat{\mathcal{W}}\varphi_2(\mathbf{r}_1, \mathbf{r}_2)dV_1dV_2 \\ & = c_1E \iint \varphi_2^*(\mathbf{r}_1, \mathbf{r}_2)\varphi_1(\mathbf{r}_1, \mathbf{r}_2)dV_1dV_2 + c_2E. \end{aligned} \quad (1.19)$$

Here one should notice that in deriving Eqs.(1.18) and (1.19) we have used normalization conditions for φ_1 and φ_2 .

In order to express two previous equations in an abbreviated form one introduces the following quantities:

1. The overlap integral

$$S_0 = \int \phi_a^*(\mathbf{r}_i)\phi_b(\mathbf{r}_i)dV_i \quad i = 1, 2 \quad (1.20)$$

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2. The Coulomb integral

$$K = \iint \varphi_1^*(\mathbf{r}_1, \mathbf{r}_2) \hat{W} \varphi_1(\mathbf{r}_1, \mathbf{r}_2) dV_1 dV_2 = \iint \varphi_2^*(\mathbf{r}_1, \mathbf{r}_2) \hat{W} \varphi_2(\mathbf{r}_1, \mathbf{r}_2) dV_1 dV_2 \quad (1.21)$$

3. The exchange integral

$$A = \iint \varphi_1^*(\mathbf{r}_1, \mathbf{r}_2) \hat{W} \varphi_2(\mathbf{r}_1, \mathbf{r}_2) dV_1 dV_2 = \iint \varphi_2^*(\mathbf{r}_1, \mathbf{r}_2) \hat{W} \varphi_1(\mathbf{r}_1, \mathbf{r}_2) dV_1 dV_2 \quad (1.22)$$

Applying this notation we rewrite Eqs.(1.18) and (1.19) in the form

$$\begin{aligned} c_1(2E_0 + K - E) + c_2(2E_0 S_0^2 + A - ES_0^2) &= 0 \\ c_1(2E_0 S_0^2 + A - ES_0^2) + c_2(2E_0 + K - E) &= 0 \end{aligned} \quad (1.23)$$

This is a homogeneous set of equations which determines unknown coefficients c_1 and c_2 . Of course, we search for non-trivial solutions that can be naturally determined from the equation

$$\begin{vmatrix} 2E_0 + K - E & 2E_0 S_0^2 + A - ES_0^2 \\ 2E_0 S_0^2 + A - ES_0^2 & 2E_0 + K - E \end{vmatrix} = 0. \quad (1.24)$$

From this equation we easily find two possible solutions for the energy E and the coefficients c_i , namely,

$$E_a = 2E_0 + \frac{K - A}{1 - S_0^2}, \quad c_1 = -c_2 \quad (1.25)$$

and

$$E_s = 2E_0 + \frac{K + A}{1 + S_0^2}, \quad c_1 = c_2 \quad (1.26)$$

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Finally, from the normalization condition of the total wavefunction one obtains

$$\begin{aligned} 1 &= \int \int \varphi^*(\mathbf{r}_1, \mathbf{r}_2) \varphi(\mathbf{r}_1, \mathbf{r}_2) dV_1 dV_2 \\ &= 2|c_1|^2(1 \mp S^2) \end{aligned} \quad (1.27)$$

or

$$c_1 = \frac{1}{\sqrt{2(1 \mp S_0^2)}}, \quad (1.28)$$

where the $-$ and $+$ sign corresponds to E_a and E_s , respectively. Using (1.28) we can express the orbital part of the total wavefunctions as

$$\varphi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2(1 - S_0^2)}} [\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) - \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)] \quad (1.29)$$

which is clearly the anti-symmetric expression and it corresponds to E_a . Similarly, the symmetric orbital function which corresponds to E_s is given by

$$\varphi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2(1 + S_0^2)}} [\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) + \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)]. \quad (1.30)$$

Finally, we also can account for the spins of the electrons and to construct the following anti-symmetric wavefunctions:

$$\Psi = \frac{1}{\sqrt{2(1 - S_0^2)}} \begin{vmatrix} \phi_a(\mathbf{r}_1) & \phi_a(\mathbf{r}_2) \\ \phi_b(\mathbf{r}_1) & \phi_b(\mathbf{r}_2) \end{vmatrix} \xi_{\uparrow}(1)\xi_{\uparrow}(2), \quad S = 1, S^z = 1 \quad (1.31)$$

$$\Psi = \frac{1}{\sqrt{2(1 - S_0^2)}} \begin{vmatrix} \phi_a(\mathbf{r}_1) & \phi_a(\mathbf{r}_2) \\ \phi_b(\mathbf{r}_1) & \phi_b(\mathbf{r}_2) \end{vmatrix} \xi_{\downarrow}(1)\xi_{\downarrow}(2), \quad S = 1, S^z = 0 \quad (1.32)$$

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$$\Psi = \frac{1}{\sqrt{2(1 - S_0^2)}} \begin{vmatrix} \phi_a(\mathbf{r}_1) & \phi_a(\mathbf{r}_2) \\ \phi_b(\mathbf{r}_1) & \phi_b(\mathbf{r}_2) \end{vmatrix} \frac{1}{\sqrt{2}} [\xi_{\uparrow}(1)\xi_{\downarrow}(2) + \xi_{\downarrow}(1)\xi_{\uparrow}(2)]$$

$$S = 1, S^z = -1 \quad (1.33)$$

and

$$\Psi = \frac{1}{\sqrt{2(1 + S_0^2)}} [\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) + \phi_b(\mathbf{r}_1)\phi_a(\mathbf{r}_2)] \frac{1}{\sqrt{2}} \begin{vmatrix} \xi_{\uparrow}(1) & \xi_{\uparrow}(2) \\ \xi_{\downarrow}(1) & \xi_{\downarrow}(2) \end{vmatrix}$$

$$S = 0, S^z = 0 \quad (1.34)$$

Here the wavefunctions (1.31)-(1.33) form a triplet (threefold degenerate state) with the energy E_a , the total spin $S = 1$ and the total z th component $S^z = \pm 1, 0$. Similarly, the wavefunction (1.34) describes a singlet state with energy E_s , the total spin $S = 0$ and $S^z = 0$. Of course, both the triplet and singlet states can be the ground state of the system depending on the sign of the exchange integral. In order to prove this statement, we calculate the energy difference between E_a and E_s , i.e.,

$$\Delta E = E_a - E_s = \frac{2(KS_0^2 - A)}{1 - S_0^4} \approx -2A, \quad (1.35)$$

where we have neglected the overlap integral which very small in comparison with other terms in the expression. It is clear from the previous equation that for $A > 0$ the ground state of the system will be represented by the triplet state with parallel alignment of spins and for $A < 0$ the singlet state with anti-parallel orientation of the spins. Of course, the parallel (anti-parallel) spin orientation implies also parallel (anti-parallel) alignment of the magnetic moments, which is crucial for the observation of the ferromagnetic or antiferromagnetic ordering in the real systems.

The situation in the hydrogen molecule, of course, differs from the real situation in ionic crystal in many respects. For example, the electrons in

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the hydrogen molecule occupy $1s$ orbitals, while in the ionic crystals the unpaired localized electrons usually occupy d or f orbitals. In fact, the calculation of the exchange integral using $3d$ orbital functions leads to the positive value of the A . Therefore, the direct exchange interactions leads to the ferromagnetic ordering in such systems. Later it was discovered by Anderson, that the antiferromagnetic ordering is caused by so-called indirect exchange interaction via a non-magnetic bridging atom. The situation in real materials is usually much more complicated and other mechanism such as the Dzyaloshinskii-Moriya or Ruderman-Kittel-Kasuya-Yosida interactions can play an important role.

Although the calculation performed for the hydrogen molecule does not reflect the complex situation of the real magnetic systems, it is extremely important from the methodological point of view. In fact, it is clear from our calculation, that the parallel or anti-parallel alignment of the magnetic moments appears due to new contribution to the energy of the system which originates from the indistinguishability of quantum particles. The other mechanisms leading to the macroscopic magnetism have also quantum nature and cannot be included into the classical theory.

Thus we can conclude that the physical origin of magnetism can be correctly understood and described only within the quantum theory.

Chapter 2

Bogolyubov Inequality and Its Applications

2.1 General Remarks on Bogolyubov Inequality

The Bogolyubov inequality for the Gibbs free energy G of an interacting many-body system described by the Hamiltonian $\hat{\mathcal{H}}$ is usually written in the form

$$\mathcal{G} \leq \mathcal{G}_0 + \langle \hat{\mathcal{H}} - \hat{\mathcal{H}}_0 \rangle_0 = \phi(\lambda_x, \lambda_y, \lambda_z, \dots). \quad (2.1)$$

In this equation, the so-called trial Hamiltonian $\hat{\mathcal{H}}_0 = \hat{\mathcal{H}}_0(\lambda_x, \lambda_y, \lambda_z, \dots)$ depends on some variational parameters λ_i that are naturally determined in the process of calculation and the symbol $\langle \dots \rangle_0$ stands for the usual ensemble average calculated with the trial Hamiltonian. Finally, \mathcal{G}_0 denotes the Gibbs free energy of the trial system defined by

$$\mathcal{G}_0 = \mathcal{G}_0(\lambda_x, \lambda_y, \lambda_z, \dots) = -\frac{1}{\beta} \ln \mathcal{Z}_0. \quad (2.2)$$

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where $\beta = 1/k_B T$ and the the partition function \mathcal{Z}_0 is given by

$$\mathcal{Z}_0 = \text{Tr} e^{-\beta \hat{\mathcal{H}}_0} \quad (2.3)$$

In general, there is a remarkable freedom in defining the trial Hamiltonian. In fact, the only limitations to be taken into account follow from the two obvious requirements:

1. The trial Hamiltonian should naturally represent a simplified physical model of the real system.
2. The expression of \mathcal{G}_0 must be calculated exactly, in order to obtain a closed-form formula for the r.h.s of Eqs.(2.1).

2.2 Mean-Field Theory of the Spin-1/2 Anisotropic Heisenberg Model

2.2.1 General Formulation

The accurate theoretical analysis of the Heisenberg model is extremely hard due to interaction terms in the Hamiltonian including non-commutative spin operators. Probably the simplest analytic theory applicable to the model is the standard mean-field approach. Although, the mean-field theory can mathematically be formulated in many different ways, we will develop in this text an approach based on the Bogolyubov inequality for the free energy of the system. The main advantage of this formulation is its completeness (we can derive analytic formulas for all thermodynamic quantities of interest) and a possibility of further generalizations, for example, an extension to the Oguchi approximation.

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

In this part we will study the spin-1/2 anisotropic Heisenberg model on a crystal lattice described by the Hamiltonian

$$\hat{\mathcal{H}} = - \sum_{i,j} (J_x \hat{S}_i^x \hat{S}_j^x + J_y \hat{S}_i^y \hat{S}_j^y + J_z \hat{S}_i^z \hat{S}_j^z) - g\mu_B \sum_i (H_x \hat{S}_i^x + H_y \hat{S}_i^y + H_z \hat{S}_i^z) \quad (2.4)$$

where g is the Landé factor, μ_B is the Bohr magneton, J_α and H_α , $\alpha = x, y, z$ denote the spatial components of the exchange interaction and external magnetic field, respectively. One should note here that J_α is assumed to be positive for the ferromagnetic systems and negative for the antiferromagnetic ones. Moreover, it is well-known that the absolute value of exchange integrals very rapidly decreases with the distance, thus we can restrict the summation in the first term of (2.4) to the nearest-neighboring pairs of atoms on the lattice. Finally, the spatial components of the spin-1/2 operators are given by

$$\hat{S}_k^x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_k, \quad \hat{S}_k^y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_k, \quad \hat{S}_k^z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_k. \quad (2.5)$$

To proceed further we choose the trial Hamiltonian in the form

$$\hat{\mathcal{H}}_0 = - \sum_k^N (\lambda_x \hat{S}_k^x + \lambda_y \hat{S}_k^y + \lambda_z \hat{S}_k^z), \quad (2.6)$$

where N denotes the total number of the lattice sites and λ_i are variational parameters to be determined by minimizing of the r.h.s. of the Bogolyubov inequality. After substituting (2.5) into (2.6), we can apparently rewrite previous equation as follows

$$\hat{\mathcal{H}}_0 = \sum_{k=1}^N \hat{\mathcal{H}}_{0k}, \quad (2.7)$$

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

where the site Hamiltonian $\hat{\mathcal{H}}_{0k}$ is given by

$$\hat{\mathcal{H}}_{0k} = -\frac{1}{2} \begin{pmatrix} \lambda_z & \lambda_x - i\lambda_y \\ \lambda_x + i\lambda_y & -\lambda_z \end{pmatrix}_k. \quad (2.8)$$

In order to evaluate the terms entering the Bogolyubov inequality, we at first have to calculate the partition function \mathcal{Z}_0 . Taking into account the commutation relation $[\hat{\mathcal{H}}_{0k}, \hat{\mathcal{H}}_{0\ell}] = 0$ for $k \neq \ell$, we obtain the following expression

$$\mathcal{Z}_0 = \text{Tr} \exp\left(-\beta \sum_{k=1}^N \hat{\mathcal{H}}_{0k}\right) = \prod_{k=1}^N \text{Tr}_k \exp(-\beta \hat{\mathcal{H}}_{0k}), \quad (2.9)$$

where Tr_k denotes the trace of the relevant operator related to k th lattice site. Now, after setting Eq.(2.8) into (2.9) one obtains

$$\begin{aligned} \mathcal{Z}_0 &= \prod_{k=1}^N \text{Tr}_k \exp\left(\begin{pmatrix} \frac{\beta}{2}\lambda_z & \frac{\beta}{2}(\lambda_x - i\lambda_y) \\ \frac{\beta}{2}(\lambda_x + i\lambda_y) & -\frac{\beta}{2}\lambda_z \end{pmatrix}_k\right). \\ &= \left[\text{Tr}_k \exp\left(\begin{pmatrix} \frac{\beta}{2}\lambda_z & \frac{\beta}{2}(\lambda_x - i\lambda_y) \\ \frac{\beta}{2}(\lambda_x + i\lambda_y) & -\frac{\beta}{2}\lambda_z \end{pmatrix}_k\right) \right]^N. \end{aligned} \quad (2.10)$$

The crucial point for further calculation is the evaluation of exponential function in previous equation. Let us note that in performing this task, we will not follow the usual approach based on the diagonalization of modified matrix (2.8) entering the argument of exponential. Instead, we will perform all calculations in the real space by applying the following matrix form of the Cauchy integral formula

$$e^{-\beta \hat{\mathcal{H}}_{0k}} = \frac{1}{2\pi i} \oint_C \frac{e^z dz}{zI - (-\beta \hat{\mathcal{H}}_{0k})}. \quad (2.11)$$

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

After a straightforward calculation we obtain

$$e^{-\beta\hat{h}_{0k}} = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix} \quad (2.12)$$

with

$$h_{11} = \cosh\left(\frac{\beta}{2}\Lambda\right) + \frac{\lambda_z}{\Lambda} \sinh\left(\frac{\beta}{2}\Lambda\right) \quad (2.13)$$

$$h_{12} = \frac{\lambda_x - i\lambda_y}{\Lambda} \sinh\left(\frac{\beta}{2}\Lambda\right) \quad (2.14)$$

$$h_{21} = \frac{\lambda_x + i\lambda_y}{\Lambda} \sinh\left(\frac{\beta}{2}\Lambda\right) \quad (2.15)$$

$$h_{22} = \cosh\left(\frac{\beta}{2}\Lambda\right) - \frac{\lambda_z}{\Lambda} \sinh\left(\frac{\beta}{2}\Lambda\right), \quad (2.16)$$

where we have introduced the parameter

$$\Lambda = \sqrt{\lambda_x^2 + \lambda_y^2 + \lambda_z^2}. \quad (2.17)$$

Using previous equations we easily obtain the following expressions for \mathcal{Z}_0 and \mathcal{G}_0

$$\mathcal{Z}_0 = \left[2 \cosh\left(\frac{\beta}{2}\Lambda\right) \right]^N \quad (2.18)$$

$$\mathcal{G}_0 = -\frac{N}{\beta} \ln \left[2 \cosh\left(\frac{\beta}{2}\Lambda\right) \right]. \quad (2.19)$$

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

To obtain the complete expression for $\phi(\lambda_x, \lambda_y, \lambda_z, \dots)$, we have to evaluate the terms $\langle \hat{\mathcal{H}} \rangle_0$ and $\langle \hat{\mathcal{H}}_0 \rangle_0$ that can be expressed as

$$\begin{aligned} \langle \hat{\mathcal{H}} \rangle_0 &= -\frac{Nq}{2} \left(J_x \langle \hat{S}_i^x \hat{S}_j^x \rangle_0 + J_y \langle \hat{S}_i^y \hat{S}_j^y \rangle_0 + J_z \langle \hat{S}_i^z \hat{S}_j^z \rangle_0 \right) \\ &\quad - N \left(h_x \langle \hat{S}_j^x \rangle_0 + h_y \langle \hat{S}_j^y \rangle_0 + h_z \langle \hat{S}_j^z \rangle_0 \right), \end{aligned} \quad (2.20)$$

where q denotes the coordination number of the lattice and $h_\alpha = g\mu_B H_\alpha$, ($\alpha = x, y, z$). Similarly, we have

$$\langle \hat{\mathcal{H}}_0 \rangle_0 = -N \left(\lambda_x \langle \hat{S}_j^x \rangle_0 + \lambda_y \langle \hat{S}_j^y \rangle_0 + \lambda_z \langle \hat{S}_j^z \rangle_0 \right). \quad (2.21)$$

The ensemble averages of $\langle \hat{S}_j^\alpha \rangle_0$ entering two previous equations can be expressed in the form

$$\begin{aligned} \langle \hat{S}_j^\alpha \rangle_0 &= \frac{1}{\mathcal{Z}_0} \text{Tr} \hat{S}_j^\alpha e^{-\beta \hat{\mathcal{H}}_0} \\ &= \frac{\text{Tr}_j \hat{S}_j^\alpha \exp(-\beta \hat{\mathcal{H}}_{0j}) \prod_{k \neq j}^{N-1} \text{Tr}_k \exp(-\beta \hat{\mathcal{H}}_{0k})}{\text{Tr}_j \exp(-\beta \hat{\mathcal{H}}_{0j}) \prod_{k \neq j}^{N-1} \text{Tr}_k \exp(-\beta \hat{\mathcal{H}}_{0k})} \end{aligned} \quad (2.22)$$

which can be simplified as follows

$$\langle \hat{S}_j^\alpha \rangle_0 = \frac{\text{Tr}_j \hat{S}_j^\alpha \exp(-\beta \hat{\mathcal{H}}_{0j})}{\text{Tr}_j \exp(-\beta \hat{\mathcal{H}}_{0j})}. \quad (2.23)$$

Similarly, one easily finds that

$$\langle \hat{S}_i^\alpha \hat{S}_j^\alpha \rangle_0 = \frac{\text{Tr}_i \hat{S}_i^\alpha \exp(-\beta \hat{\mathcal{H}}_{0i})}{\text{Tr}_i \exp(-\beta \hat{\mathcal{H}}_{0i})} \frac{\text{Tr}_j \hat{S}_j^\alpha \exp(-\beta \hat{\mathcal{H}}_{0j})}{\text{Tr}_j \exp(-\beta \hat{\mathcal{H}}_{0j})} = \left(\langle \hat{S}_j^\alpha \rangle_0 \right)^2. \quad (2.24)$$

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

In order to complete our calculation, we substitute Eqs. (2.12)-(2.16) into Eq. (2.23) and then we evaluate the trace of relevant matrices. In this way we obtain the following equation

$$\langle \hat{S}_j^\alpha \rangle_0 = \frac{\lambda_\alpha}{2\Lambda} \tanh\left(\frac{\beta}{2}\Lambda\right). \quad (2.25)$$

and

$$\langle \hat{S}_i^\alpha \hat{S}_j^\alpha \rangle_0 = \left(\frac{\lambda_\alpha}{2\Lambda}\right)^2 \tanh^2\left(\frac{\beta}{2}\Lambda\right). \quad (2.26)$$

After introducing notation $\langle \hat{S}_j^\alpha \rangle_0 = m_\alpha$, $\alpha = x, y, z$, we can rewrite the r.h.s of the Bogolyubov inequality in the form:

$$\begin{aligned} \phi(\lambda_x, \lambda_y, \lambda_z) = & -\frac{N}{\beta} \ln\left(2 \cosh \frac{\beta}{2}\Lambda\right) - \frac{Nq}{2} \left(J_x m_x^2 + J_y m_y^2 + J_z m_z^2\right) \\ & + N\left[(\lambda_x - h_x)m_x + (\lambda_y - h_y)m_y + (\lambda_z - h_z)m_z\right]. \end{aligned} \quad (2.27)$$

Since the quantity ϕ represents an upper bound for the exact Gibbs free energy of the system, then the best possible approximation (with the trial Hamiltonian $\hat{\mathcal{H}}_0$) corresponds for those values of $\lambda_x, \lambda_y, \lambda_z$ that minimize $\phi(\lambda_x, \lambda_y, \lambda_z)$. Relevant values of $\lambda_x, \lambda_y, \lambda_z$ are obviously determined from the equations

$$\frac{\partial \phi}{\partial \lambda_x} = 0, \quad \frac{\partial \phi}{\partial \lambda_y} = 0, \quad \frac{\partial \phi}{\partial \lambda_z} = 0. \quad (2.28)$$

The above conditions lead to three independent equations that can be rewritten in the following simple matrix form:

$$\begin{pmatrix} \frac{\partial m_x}{\partial \lambda_x} & \frac{\partial m_y}{\partial \lambda_x} & \frac{\partial m_z}{\partial \lambda_x} \\ \frac{\partial m_x}{\partial \lambda_y} & \frac{\partial m_y}{\partial \lambda_y} & \frac{\partial m_z}{\partial \lambda_y} \\ \frac{\partial m_x}{\partial \lambda_z} & \frac{\partial m_y}{\partial \lambda_z} & \frac{\partial m_z}{\partial \lambda_z} \end{pmatrix} \begin{pmatrix} \lambda_x - qJ_x m_x - h_x \\ \lambda_y - qJ_y m_y - h_y \\ \lambda_z - qJ_z m_z - h_z \end{pmatrix} = \mathbf{0}. \quad (2.29)$$

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

Since the first matrix in (2.29) is in general non-zero, then the only possible solution of this equation is given by

$$\lambda_x = qJ_x m_x + h_x, \quad \lambda_y = qJ_y m_y + h_y, \quad \lambda_z = qJ_z m_z + h_z \quad (2.30)$$

and the cooresponding equilibrium Gibbs free energy can be after a small manipulation expressed in the form

$$\mathcal{G} = -\frac{N}{\beta} \ln \left\{ 2 \cosh \left(\frac{\beta h_{ef}}{2} \right) \right\} + \frac{Nq}{2} \left(J_x m_x^2 + J_y m_y^2 + J_z m_z^2 \right). \quad (2.31)$$

where we have denoted

$$h_{ef} = \sqrt{(qJ_x m_x + h_x)^2 + (qJ_y m_y + h_y)^2 + (qJ_z m_z + h_z)^2}. \quad (2.32)$$

Having obtained the last equation, we are able to identify the physical meaning of the parameters m_x, m_y, m_x and consequently also the meaning of variational parameters $\lambda_x, \lambda_y, \lambda_z$.

For this purpose, we at first recall that the spatial component of the total magnetization M_α is defined as

$$M_\alpha = - \left(\frac{\partial \mathcal{G}}{\partial H_\alpha} \right)_\beta = -g\mu_B \left(\frac{\partial \mathcal{G}}{\partial h_\alpha} \right)_\beta. \quad (2.33)$$

After a straightforward calculation we obtain the following very simple expressions

$$\frac{M_x}{Ng\mu_B} = m_x = \langle \hat{S}_j^x \rangle_0, \quad \frac{M_y}{Ng\mu_B} = m_y = \langle \hat{S}_j^y \rangle_0, \quad \frac{M_z}{Ng\mu_B} = m_z = \langle \hat{S}_j^z \rangle_0, \quad (2.34)$$

which clearly indicate that m_α represents the spatial components of the magnetization. Consequently, the parameters λ_α have the meaning of of the molecular-field components acting on one atom in the lattice. Thus our formulation is nothing but the standard mean-field theory. The main advantage of our approach is that this formulation provides a close-form analytical expression for the Gibbs free energy which is of principal importance for finding stability conditions of various physical quantities.

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

2.2.2 Thermodynamic Properties of the Heisenberg Model

Now let us proceed with the calculation of several interesting physical quantities for the system under investigation. Using Eqs. (2.22), (2.30) and (2.34) one simply obtains for the components of reduced magnetization a set of three coupled equations, namely,

$$m_x = \frac{qJ_x m_x + h_x}{2h_{ef}} \tanh\left(\frac{\beta}{2} h_{ef}\right), \quad (2.35)$$

$$m_y = \frac{qJ_y m_y + h_y}{2h_{ef}} \tanh\left(\frac{\beta}{2} h_{ef}\right), \quad (2.36)$$

$$m_z = \frac{qJ_z m_z + h_z}{2h_{ef}} \tanh\left(\frac{\beta}{2} h_{ef}\right), \quad (2.37)$$

where we have denoted

In order to investigate the long-range ordering the systems, we set $h_x = h_y = h_z = 0$ and obtain

$$m_x = \frac{J_x m_x}{2h_0} \tanh\left(\frac{\beta q}{2} h_0\right), \quad (2.38)$$

$$m_y = \frac{J_y m_y}{2h_0} \tanh\left(\frac{\beta q}{2} h_0\right), \quad (2.39)$$

$$m_z = \frac{J_z m_z}{2h_0} \tanh\left(\frac{\beta q}{2} h_0\right), \quad (2.40)$$

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

with

$$h_0 = \sqrt{(J_x m_x)^2 + (J_y m_y)^2 + (J_z m_z)^2}. \quad (2.41)$$

These three nonlinear equations have always the trivial solution $m_x = m_y = m_z = 0$ corresponding to the disordered paramagnetic phase (DP). Moreover, depending on the temperature and the values of exchange parameters there also exist non-trivial solutions corresponding to ordered ferromagnetic phase (OP). The stability of the relevant solutions is then determined by the minimum of the Gibbs free energy given by Eq.(2.31). Now we briefly analyze possible trivial and non-trivial solutions of (2.38)-(2.40) for some particular cases of the exchange interactions:

1. Ising model $J_x = J_y = 0, J_z = J \neq 0$

$$m_x = m_y = 0 \quad \text{and} \quad m_z = \frac{1}{2} \tanh\left(\frac{q\beta J}{2} m_z\right) \quad \text{for } T < T_c$$

$$m_x = m_y = m_z = 0 \quad \text{for } T > T_c \quad (2.42)$$

2. Isotropic XY model $J_x = J_y = J \neq 0, J_z = 0$

$$m_z = 0, m_y = m_x \quad \text{and} \quad m_x = \frac{1}{2\sqrt{2}} \tanh\left(\frac{\sqrt{2}q\beta J}{2} m_x\right) \quad \text{for } T < T_c$$

$$m_x = m_y = m_z = 0 \quad \text{for } T > T_c \quad (2.43)$$

3. Isotropic Heisenberg model $J_x = J_y = J_z \neq 0$

$$m_y = m_x = m_z \quad \text{and} \quad m_z = \frac{1}{2\sqrt{3}} \tanh\left(\frac{\sqrt{3}q\beta J_x}{2} m_x\right) \quad \text{for } T < T_c$$

$$m_x = m_y = m_z = 0 \quad \text{for } T > T_c \quad (2.44)$$

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

Here one should note that non-trivial results for isotropic XY and Heisenberg model model represents valid solution for the models when the axis of quantization is given by the equation $y = x = t$, $t \in \mathcal{R}$ for the XY model and $y = x = z = t$, $t \in \mathcal{R}$ for the Heisenberg model. On the other hand, if choose as a quantization axis for example the x axis, then we obtain for both models identical result as that for the Ising one. Thus one can conclude that mean-field theory is not able to describe correctly quantum features of localized spin models. In order to illustrate the numerical accuracy of the method, we have compared in Fig. 2.3 the temperature variation of the mean-field magnetization with exact result on the square lattice with $q = 4$.

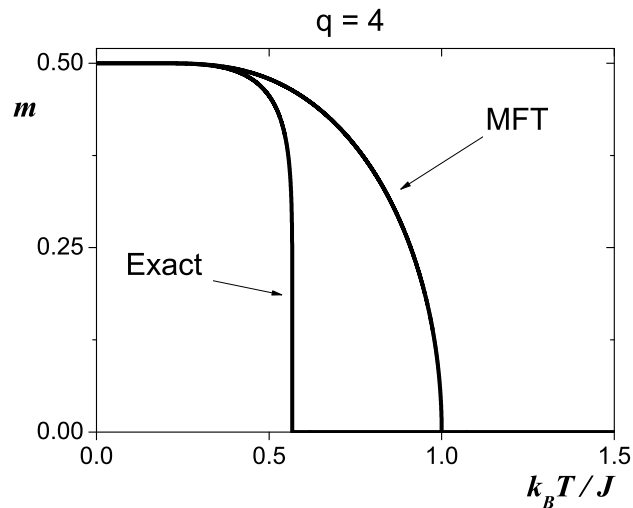


Figure 2.1: Comparison of the temperature dependence of magnetization for the Ising model on a square lattice.

The critical (or Curie) temperature is defined as a temperature at which the long-range order (or magnetization) vanishes. In order to determine the

2.2 Mean-Field Theory of Anisotropic Heisenberg Model

Curie temperature, we take into account that $\tanh(x) \approx x$ for $x \ll 1$ and obtain an universal solution

$$T_c = \frac{qJ_\alpha}{4k_B}, \quad \alpha = x, y, z \quad (2.45)$$

which valid for all three cases mentioned above. Of course, the critical temperature should be different depending on the model considered. Thus the present method is not able to distinguish specific features of the models as long as concerns the critical behavior. Moreover, it is also clear that the topology of the lattice is taken into account only through its coordination number, that is also weak point of the present method. It is well known that this approach significantly fails for the low-dimensional systems, nevertheless it gives rather good qualitative picture for the three-dimensional systems and therefore it is frequently used to obtain analytical results, particularly, for complex systems.

Finally, one should note that calculations of other thermodynamic quantities is easy and straightforward, since we have analytical solution for the Gibbs free energy of the system from which other quantities are easily obtained.

This calculation including numerical analysis and discussion is left for the readers as an appropriate exercise.

Let us conclude this part by noticing that the present approach can be extended to case of the the so-called Oguchi approximation which already account much better for the quantum effects as well as for the spin-spin correlations. Possible extensions are rather involved and require lengthy calculations that are beyond the scope of the present book.

Chapter 3

Spin-Wave Theory

3.1 Bloch Spin-Wave Theory of Ferromagnets

In this part we will discuss the concept of spin waves which enables to study the some physical properties of magnetic systems at low temperatures. This theory was originally introduced by F. Bloch [1] and its main assumption is that the ground state of the system is ordered and the excited states are described as a collection of spin waves. At low temperatures it is reasonable to expect the small amplitudes of the spin waves, thus the interaction among spin waves can be neglected. We will consider in this part an isotropic Heisenberg model defined by the Hamiltonian

$$\hat{\mathcal{H}} = -J \sum_{i,j} \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j - g\mu_B H \sum_i \hat{S}_i^z. \quad (3.1)$$

Here $\hat{\mathbf{S}}_i$ represents a vector spin-operator at the i th site of the lattice. This operator is naturally defined as $\hat{\mathbf{S}}_i = (\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z)$ where \hat{S}_i^α ($\alpha = x, y, z$) represent spatial components of the standard spin operators, g is the Landé

3.1 Bloch Spin-Wave Theory of Ferromagnets

factor, μ_B is the Bohr magneton and H denotes the external magnetic field which is applied along z axis. J is the exchange integral which is assumed to be positive since we are going to investigate the ferromagnetic systems.

Adopting the basic concept of lattice vibrations, we can write the following equation of motion of the spin $\hat{\mathbf{S}}_\ell$ on the j th lattice point

$$\frac{d\hat{\mathbf{S}}_\ell}{dt} = \frac{i}{\hbar}[\mathcal{H}, \hat{\mathbf{S}}_\ell]. \quad (3.2)$$

In what follows, we will use the following commutation relations for spin operators

$$[\hat{S}_i^a, \hat{S}_j^b] = i\varepsilon^{abc}\delta_{ij}\hat{S}_j^c, \quad a, b, c = x, y, \text{ or } z \quad (3.3)$$

where ε^{abc} represents Levi-Civita tensor and δ_{ij} is the Kronecker symbol. Now, substituting the Hamiltonian (3.1) into (3.2) and employing relations (3.3) one obtains

$$\frac{d\hat{\mathbf{S}}_\ell}{dt} = -\frac{1}{\hbar}(\mathbf{H}_\ell \times \hat{\mathbf{S}}_\ell), \quad (3.4)$$

where the local magnetic field \mathbf{H}_ℓ acting on the j th spin is given by

$$\mathbf{H}_\ell = \sum_j J_{j\ell} \hat{\mathbf{S}}_j + g\mu_B H \mathbf{e}_3 \quad (3.5)$$

with $\mathbf{e}_3 = (0, 0, 1)$. Using two previous equations one easily obtains the following equations of motion of the x, y and z components of the spin operator

$$\hbar \frac{d\hat{S}_\ell^x}{dt} = - \sum_j J_{j\ell} (\hat{S}_j^y \hat{S}_\ell^z - \hat{S}_j^z \hat{S}_\ell^y) + g\mu_B H \hat{S}_\ell^y \quad (3.6)$$

$$\hbar \frac{d\hat{S}_\ell^y}{dt} = - \sum_j J_{j\ell} (\hat{S}_j^z \hat{S}_\ell^x - \hat{S}_j^x \hat{S}_\ell^z) - g\mu_B H \hat{S}_\ell^x \quad (3.7)$$

3.1 Bloch Spin-Wave Theory of Ferromagnets

$$\hbar \frac{d\hat{S}_\ell^z}{dt} = - \sum_j J_{j\ell} (\hat{S}_j^x \hat{S}_\ell^y - \hat{S}_j^y \hat{S}_\ell^x) \quad (3.8)$$

If we restrict ourselves to the case of low-energy excitation, then the components $\hat{S}_\ell^x, \hat{S}_\ell^y$ can be regarded as small quantities of first order. Consequently, the right-hand side of (3.8) is a small quantity of the second order, which can be neglected and it follows from Eq. (3.8) that the z th component becomes a constant. Moreover, it is reasonable to put explicitly $\hat{S}_\ell^z = S$, since the external magnetic field is assumed to be applied parallel to the z th axis. Under these assumptions Eqs. (3.6) and (3.7) can be rewritten in the form

$$\hbar \frac{d\hat{S}_\ell^x}{dt} = -S \sum_j J_{j\ell} (\hat{S}_j^y - \hat{S}_\ell^y) + g\mu_B H \hat{S}_\ell^y \quad (3.9)$$

$$\hbar \frac{d\hat{S}_\ell^y}{dt} = -S \sum_j J_{j\ell} (\hat{S}_\ell^x - \hat{S}_j^x) - g\mu_B H \hat{S}_\ell^x, \quad (3.10)$$

or alternatively

$$\hbar \frac{d\hat{S}_\ell^+}{dt} = -iS \sum_j J_{j\ell} (\hat{S}_\ell^+ - \hat{S}_j^+) - g\mu_B H \hat{S}_\ell^+ \quad (3.11)$$

$$\hbar \frac{d\hat{S}_\ell^-}{dt} = -iS \sum_j J_{j\ell} (\hat{S}_\ell^- - \hat{S}_j^-) - g\mu_B H \hat{S}_\ell^- \quad (3.12)$$

where we have introduced the spin-raising and spin-lowering operators

$$\hat{S}_\ell^+ = \hat{S}_\ell^x + i\hat{S}_\ell^y \quad \hat{S}_\ell^- = \hat{S}_\ell^x - i\hat{S}_\ell^y, \quad (3.13)$$

that obey the following commutation rules

$$[\hat{S}_k^z, \hat{S}_\ell^+] = \hat{S}_k^+ \delta_{k\ell}, \quad [\hat{S}_k^z, \hat{S}_\ell^-] = -\hat{S}_k^- \delta_{k\ell}, \quad [\hat{S}_k^+, \hat{S}_\ell^+] = 2\hat{S}_k^z \delta_{k\ell}. \quad (3.14)$$

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The above relations are directly obtained with the help of well-known commutation relations of the spin operators (3.3).

To proceed further, we now express the spin-raising and spin-lowering operators with the help of the Fourier transform, i.e.,

$$\hat{S}_{\mathbf{q}}^+ = \frac{1}{\sqrt{N}} \sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j} \hat{S}_j^+, \quad \hat{S}_{\mathbf{q}}^- = \frac{1}{\sqrt{N}} \sum_j e^{-i\mathbf{q}\cdot\mathbf{R}_j} \hat{S}_j^- \quad (3.15)$$

$$\hat{S}_j^+ = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{R}_j} \hat{S}_{\mathbf{q}}^+, \quad \hat{S}_j^- = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}_j} \hat{S}_{\mathbf{q}}^- \quad (3.16)$$

Substituting Eq.(3.16) into Eq.(3.12) and applying the following relation

$$\sum_{\ell} e^{-i(\mathbf{q}_1 - \mathbf{q}_2)\cdot\mathbf{R}_{\ell}} = N\delta_{\mathbf{q}_1, \mathbf{q}_2} \quad (3.17)$$

one gets equation

$$-i\hbar \frac{d\hat{S}_{\mathbf{q}}^-}{dt} = \left[S \sum_{\ell} J_{j\ell} (1 - e^{-i\mathbf{q}\cdot(\mathbf{R}_j - \mathbf{R}_{\ell})}) + g\mu_B H \right] \hat{S}_{\mathbf{q}}^-. \quad (3.18)$$

If we now introduce a real quantity

$$J(\mathbf{q}) = \sum_j J(\mathbf{R}_j) e^{-i\mathbf{q}\cdot\mathbf{R}_j} \quad (3.19)$$

then we rewrite (3.18) as

$$-i\hbar \frac{d\hat{S}_{\mathbf{q}}^-}{dt} = \left\{ S[J(0) - J(\mathbf{q})] + g\mu_B H \right\} \hat{S}_{\mathbf{q}}^-. \quad (3.20)$$

It is straightforward to obtain the solution of this equation in the form

$$\hat{S}_{\mathbf{q}} = \delta \hat{S}_{\mathbf{q}} e^{i(\omega_{\mathbf{q}} t + \alpha)} \quad (3.21)$$

3.1 Bloch Spin-Wave Theory of Ferromagnets

where the eigenfrequencies of the spin waves are given by

$$\hbar\omega_{\mathbf{q}} = S[J(0) - J(\mathbf{q})] + g\mu_B H. \quad (3.22)$$

One should notice here that in the limit of small \mathbf{q} we obtain $\hbar\omega_{\mathbf{q}} \approx q^2$.

Now, using Eq.(3.21) we can express the spin operators in the real space as follows

$$\hat{S}_j^- = \frac{1}{\sqrt{N}} \delta\hat{S}_{\mathbf{q}} e^{i(\mathbf{q}\cdot\mathbf{R}_j + \omega_{\mathbf{q}}t + \alpha)} \quad (3.23)$$

$$\hat{S}_j^x = \frac{1}{\sqrt{N}} \delta\hat{S}_{\mathbf{q}} \cos[i(\mathbf{q}\cdot\mathbf{R}_j + \omega_{\mathbf{q}}t + \alpha)] \quad (3.24)$$

and

$$\hat{S}_j^y = -\frac{1}{\sqrt{N}} \delta\hat{S}_{\mathbf{q}} \sin[i(\mathbf{q}\cdot\mathbf{R}_j + \omega_{\mathbf{q}}t + \alpha)]. \quad (3.25)$$

Finally, it is straightforward to prove that the energy difference between an excited state and ground state is given by

$$E_{\mathbf{q}} - E_0 = \hbar\omega_{\mathbf{q}}, \quad (3.26)$$

where $\hbar\omega_{\mathbf{q}}$ represents the excitation energy of the spin wave with the wavevector \mathbf{q} . The proof of the last statement is left as an appropriate exercise for readers.

3.2 Holstein-Primakoff theory of ferromagnets

The Bloch's spin-wave theory discussed in previous chapter represents a very simple approach in which we completely neglect the interaction among spin waves. This deficiency can be eliminated using an alternative formulation based on magnon variables (or creation-annihilation operators) developed by Holstein and Primakoff [2]. In this part we apply The Holstein-Primakoff theory to case of an anisotropic quantum Heisenberg model described by the Hamiltonian

$$\hat{\mathcal{H}} = -J \sum_{i,j} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_j^z) - g\mu_B H \sum_i \hat{S}_i^z. \quad (3.27)$$

The meaning of all symbols in previous Eq. (3.27) is the same as in previous text.

In order to apply a spin-wave picture to analyze magnetic properties of the model under investigation, one has to perform three subsequent mathematical transformation. At first, we express the components of the spin operators through spin-lowering and spin raising operators, then we introduce so-called creation and annihilation operators and finally, we perform a Fourier transform of the relevant all creation and annihilation operators entering the Hamiltonian. The eigenvalues of the final Hamiltonian then enable to determine relevant physical quantities applying standard relations of statistical mechanics. For further manipulations it is more convenient to rewrite (3.27) as follows

$$\hat{\mathcal{H}} = -J \sum_{\ell,\delta} (\hat{S}_\ell^x \hat{S}_{\ell+\delta}^x + \hat{S}_\ell^y \hat{S}_{\ell+\delta}^y + \hat{S}_\ell^z \hat{S}_{\ell+\delta}^z) - g\mu_B H \sum_\ell \hat{S}_\ell^z \quad (3.28)$$

where ℓ labels the lattice sites and δ denotes nearest neighbors of the relevant site and we assume that $J > 0$. The integrals of motion for Hamiltonian

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(3.28) are the total z th component $\hat{S}^z = \sum_k \hat{S}_k^z$ and the total spin of the system.

The ground state of the system is ordered and for $H > 0$ the magnetic moment is parallel to the z axis. If we consider the lattice consisting of N atoms with spin S , then the ground-state vector in the spin basis reads $|0\rangle = |NS, NS\rangle$. Of course, we work in a real space basis in which the spin operators \hat{S}_ℓ^z are diagonal. We recall that the eigenvalues $M_S = -S, -S + 1, \dots, S$ and eigenvectors $|M_S\rangle_\ell$ of the operator \hat{S}_ℓ^z satisfy the following equation

$$\hat{S}_\ell^z |M_S\rangle_\ell = M_S |M_S\rangle_\ell. \quad (3.29)$$

Now, applying operators (3.13) to the eigenvectors $|M_S\rangle_\ell$ one obtains

$$\hat{S}_\ell^+ |M_S\rangle_\ell = \sqrt{(S - M_S)(S - M_S - 1)} |M_S + 1\rangle_\ell \quad (3.30)$$

and

$$\hat{S}_\ell^- |M_S\rangle_\ell = \sqrt{(S + M_S)(S - M_S - 1)} |M_S - 1\rangle_\ell. \quad (3.31)$$

In addition to the spin-raising and spin-lowering operators, we will also use in our analysis the operator describing a deviation of the z th spin-component from its maximum value, namely,

$$\hat{n}_\ell = S - \hat{S}_\ell^z. \quad (3.32)$$

The eigenvalues of this operator are integers $n_\ell = 0, 1, 2, \dots, 2S$, (or $n_\ell = S - M_S$), thus we can rewrite Eqs.(3.30) in the form

$$\hat{S}_\ell^+ |n_\ell\rangle_\ell = \sqrt{2S} \sqrt{1 - \frac{(n_\ell - 1)}{2S}} \sqrt{n_\ell} |n_\ell - 1\rangle_\ell. \quad (3.33)$$

Let us note that performing a similar procedure is also possible for Eq.(3.31) and it will be used later.

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Now, with the help of (3.13), we can rewrite the Hamiltonian (3.28) in the form

$$\hat{\mathcal{H}} = -J \sum_{\ell, \delta} \left[\frac{1}{2} (\hat{S}_\ell^+ \hat{S}_{\ell+\delta}^- + \hat{S}_\ell^- \hat{S}_{\ell+\delta}^+) + \hat{S}_\ell^z \hat{S}_{\ell+\delta}^z \right] - g\mu_B H \sum_{\ell} \hat{S}_\ell^z. \quad (3.34)$$

which is suitable for introducing the Holstein-Primakoff magnon representation. In order to define the relevant transformation, we at first introduce the standard creation and annihilation operators that are defined as

$$a_\ell^\dagger \Psi_{n_\ell} = \sqrt{n_\ell + 1} \Psi_{n_\ell+1}, \quad a_\ell \Psi_{n_\ell} = \sqrt{n_\ell} \Psi_{n_\ell-1}. \quad (3.35)$$

The central idea of the Holstein-Primakoff approach is based on the introduction of the following transformation

$$\hat{S}_\ell^+ = (2S)^{1/2} \left(1 - \frac{a_\ell^\dagger a_\ell}{2S} \right)^{1/2} a_\ell \quad (3.36)$$

$$\hat{S}_\ell^- = (2S)^{1/2} a_\ell^\dagger \left(1 - \frac{a_\ell^\dagger a_\ell}{2S} \right)^{1/2} \quad (3.37)$$

$$\hat{S}_\ell^z = S - a_\ell^\dagger a_\ell. \quad (3.38)$$

As already noted above, the eigenvalues of $a_\ell^\dagger a_\ell$ are arbitrary integers, while that of \hat{n}_ℓ are limited to the range $0 \leq n_\ell \leq 2S$. Fortunately, this discrepancy does not play any important role in the calculation, since the transition from the state with $n_\ell \leq 2S$ to states with $n_\ell > 2S$ never occur, e.g.

$$\hat{S}_\ell^- \Psi_{2S} = (2S)^{1/2} (2S + 1)^{1/2} \left(1 - \frac{2S}{2S} \right)^{1/2} \Psi_{2S+1} = 0. \quad (3.39)$$

Now we transform the operators a_ℓ, a_ℓ^\dagger from the real space to the reciprocal space by the following Fourier transform

$$a_\ell = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{-i\mathbf{q} \cdot \mathbf{R}_\ell} b_{\mathbf{q}} \quad (3.40)$$

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$$a_\ell^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}_\ell} b_{\mathbf{q}}^\dagger \quad (3.41)$$

where N denotes the total number of atoms, \mathbf{q} represents a vector of the reciprocal space, and \mathbf{R}_ℓ represents a vector specifying the position of ℓ th atom in the lattice.

The magnon-annihilation and magnon-creation operators are given by

$$b_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\ell} e^{i\mathbf{q}\cdot\mathbf{R}_\ell} a_{\ell} \quad (3.42)$$

$$b_{\mathbf{q}}^\dagger = \frac{1}{\sqrt{N}} \sum_{\ell} e^{-i\mathbf{q}\cdot\mathbf{R}_\ell} a_{\ell}^\dagger \quad (3.43)$$

and they obey the usual magnon commutation relations

$$[b_{\mathbf{q}_1}, b_{\mathbf{q}_2}^\dagger] = \delta_{\mathbf{q}_1, \mathbf{q}_2}, \quad [b_{\mathbf{q}_1}, b_{\mathbf{q}_2}] = [b_{\mathbf{q}_1}^\dagger, b_{\mathbf{q}_2}^\dagger] = 0. \quad (3.44)$$

It is useful to note here that the operator $b_{\mathbf{q}}^\dagger$ creates a magnon with the wave vector \mathbf{q} and the operator $b_{\mathbf{q}}$ annihilates it. Moreover, it follows from the transformation (3.40) and (3.41) that any change of the spin state at arbitrary lattice site is described as a superposition of an infinite number of the spin waves.

At this stage it is clear that further exact treatment of the problem is impossible due to the complexity of applied transformations. The progress is, however, still possible if we restrict ourselves to the case when the number of excited states is small in comparison with $2S$. Under this assumption, we can neglect the higher order terms in expansion of the square root and rewrite Eqs. (3.36) and (3.37) in the form

$$\hat{S}_\ell^+ = (2S)^{1/2} \left(1 - \frac{a_\ell^\dagger a_\ell}{4S} \right) a_\ell + \dots \quad (3.45)$$

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$$\hat{S}_\ell^- = (2S)^{1/2} a_\ell^\dagger \left(1 - \frac{a_\ell^\dagger a_\ell}{4S}\right) + \dots \quad (3.46)$$

Finally, substituting (3.40) and (3.41) into previous equation one obtains

$$\hat{S}_\ell^+ = \left(\frac{2S}{N}\right)^{1/2} \left[\sum_{\mathbf{q}_1} e^{-i\mathbf{q}_1 \cdot \mathbf{R}_\ell} b_{\mathbf{q}_1} - \frac{1}{4SN} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} e^{i(\mathbf{q}_1 - \mathbf{q}_2 - \mathbf{q}_3) \cdot \mathbf{R}_\ell} b_{\mathbf{q}_1}^\dagger b_{\mathbf{q}_2} b_{\mathbf{q}_3} + \dots \right] \quad (3.47)$$

$$\hat{S}_\ell^- = \left(\frac{2S}{N}\right)^{1/2} \left[\sum_{\mathbf{q}_1} e^{i\mathbf{q}_1 \cdot \mathbf{R}_\ell} b_{\mathbf{q}_1}^\dagger - \frac{1}{4SN} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} e^{i(\mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_3) \cdot \mathbf{R}_\ell} b_{\mathbf{q}_1}^\dagger b_{\mathbf{q}_2}^\dagger b_{\mathbf{q}_3} + \dots \right] \quad (3.48)$$

Similarly, the operator \hat{S}_ℓ^z is given by

$$\hat{S}_\ell^z = S - \frac{1}{N} \sum_{\mathbf{q}_1 \mathbf{q}_2} e^{i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}_\ell} b_{\mathbf{q}_1}^\dagger b_{\mathbf{q}_2}. \quad (3.49)$$

If we assume that each lattice site has z nearest neighbors, then we can specify their positions on the lattice by introducing the vector

$$\boldsymbol{\delta} = \mathbf{R}_{\ell+\delta} - \mathbf{R}_\ell. \quad (3.50)$$

Substituting (3.47)-(3.50) into Eq.(3.34) and performing a rearrangement of the terms one can rewrite the Hamiltonian as

$$\hat{\mathcal{H}} = -JNzS^2 - g\mu_B N H S + \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_1, \quad (3.51)$$

where \mathcal{H}_0 is a bilinear form in the magnon variables and it is given by

$$\begin{aligned} \hat{\mathcal{H}}_0 = & - \frac{JS}{N} \sum_{\ell, \delta} \sum_{\mathbf{q}_1 \mathbf{q}_2} \left[e^{-i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}_\ell} e^{i\mathbf{q}_2 \cdot \boldsymbol{\delta}} b_{\mathbf{q}_1} b_{\mathbf{q}_2}^\dagger + e^{i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}_\ell} e^{-i\mathbf{q}_2 \cdot \boldsymbol{\delta}} b_{\mathbf{q}_1}^\dagger b_{\mathbf{q}_2} \right] \\ & + \frac{JS}{N} \sum_{\ell, \delta} \sum_{\mathbf{q}_1 \mathbf{q}_2} \left[e^{i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}_\ell} b_{\mathbf{q}_1} b_{\mathbf{q}_2}^\dagger + e^{-i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}_\ell} e^{i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \boldsymbol{\delta}} b_{\mathbf{q}_1}^\dagger b_{\mathbf{q}_2} \right] \\ & + \frac{g\mu_B H}{N} \sum_{\ell, \mathbf{q}_1 \mathbf{q}_2} e^{i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}_\ell} b_{\mathbf{q}_1}^\dagger b_{\mathbf{q}_2}. \end{aligned} \quad (3.52)$$

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The term \mathcal{H}_1 includes higher-order terms and for the sake of simplicity will be neglected. Now, taking into account the relation (3.17) and performing the summation over ℓ and \mathbf{q}_2 , we can simplify Eq.(3.52) as follows

$$\hat{\mathcal{H}}_0 = -JzS \sum_{\mathbf{q}} (\gamma_{\mathbf{q}} b_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} + \gamma_{-\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} - 2b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}}) + g\mu_B H \sum_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}}, \quad (3.53)$$

where

$$\gamma_{\mathbf{q}} = \frac{1}{z} \sum_{\delta} e^{i\mathbf{q}\cdot\delta} \quad (3.54)$$

and the summation in (3.54) runs over all nearest neighbors. For further manipulation it is useful to notice that $\sum_{\mathbf{q}} \gamma_{\mathbf{q}} = 0$ and moreover, for the crystals with the symmetry center we have $\gamma_{\mathbf{q}} = \gamma_{-\mathbf{q}}$. Employing the magnon commutation rules $[b_{\mathbf{q}}^{\dagger}, b_{\mathbf{q}}] = \mathbf{1}$, one obtains

$$\hat{\mathcal{H}}_0 = \sum_{\mathbf{q}} [2JzS(1 - \gamma_{\mathbf{q}}) + g\mu_B H] b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}}. \quad (3.55)$$

The last equation can be rewritten in the following very simple form

$$\hat{\mathcal{H}}_0 = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \hat{n}_{\mathbf{q}}, \quad (3.56)$$

where $\hat{n}_{\mathbf{q}}$ is the magnon occupation operator and

$$\hbar\omega_{\mathbf{q}} = 2JzS(1 - \gamma_{\mathbf{q}}) + g\mu_B H. \quad (3.57)$$

Since the quantity $\gamma_{\mathbf{q}}$ can be expressed as follows

$$\gamma_{\mathbf{q}} = \frac{1}{z} \sum_{\delta} e^{i\mathbf{q}\cdot\delta} = \frac{1}{2z} \sum_{\delta} (e^{i\mathbf{q}\cdot\delta} + e^{-i\mathbf{q}\cdot\delta}) = \frac{1}{2z} \sum_{\delta} \cos(\mathbf{q}\cdot\delta), \quad (3.58)$$

then the dispersion relation becomes

$$\hbar\omega_{\mathbf{q}} = 2JzS \left[1 - \frac{1}{2z} \sum_{\delta} \cos(\mathbf{q}\cdot\delta) \right] + g\mu_B H. \quad (3.59)$$

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3.2.1 Internal Energy and Specific heat

In this subsection we will show how one can calculate the internal energy and specific heat of Heisenberg model within the Holstein-Primakoff theory. Before performing any calculation, it is useful noticing that due to neglecting higher order terms in Eq. (3.45) and (3.46), we treat the ensemble of non-interacting magnons. In further calculation, we also will assume $H = 0$ and $|\mathbf{q} \cdot \boldsymbol{\delta}| \ll 1$.

Under these assumptions, the internal energy of the magnon gas in thermodynamic equilibrium at temperature T can be expressed as

$$U = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \langle n_{\mathbf{q}} \rangle, \quad (3.60)$$

where $\langle n_{\mathbf{q}} \rangle$ is given by the well-known Bose-Einstein relation

$$\langle n_{\mathbf{q}} \rangle = \left[\exp\left(\frac{\hbar \omega_{\mathbf{q}}}{k_B T}\right) - 1 \right]^{-1}. \quad (3.61)$$

Substituting (3.61) into (3.60) one gets

$$\begin{aligned} U &= \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \left[\exp\left(\frac{\hbar \omega_{\mathbf{q}}}{k_B T}\right) - 1 \right]^{-1} \\ &= \frac{1}{(2\pi)^3} \int Dq^2 \left[\exp\left(\frac{Dq^2}{k_B T}\right) - 1 \right]^{-1} d^3q \\ &= \frac{1}{2\pi^2} \int Dq^4 \left[\exp\left(\frac{Dq^2}{k_B T}\right) - 1 \right]^{-1} dq \end{aligned} \quad (3.62)$$

where we have introduced the lattice stiffness as $D = 2SJa^2$. If we denote $x = Dq^2/k_B T$, then we can rewrite (3.62) as

$$U = \frac{(k_B T)^{5/2}}{4\pi^2 D^{3/2}} \int_0^{x_m} \frac{x^{3/2}}{\exp(x) - 1} dx. \quad (3.63)$$

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The last expression can be further simplified by considering the region $k_B T \ll \omega_{max}$. Then the upper limit in the integral (3.63) can be approximated by infinity and one obtains for internal energy the following analytical expression for internal energy of the system

$$U = \frac{(k_B T)^{5/2}}{4\pi^2 D^{3/2}} \Gamma\left(\frac{5}{2}\right) \zeta\left(\frac{5}{2}, 1\right). \quad (3.64)$$

Here Γ and ζ denote the Gamma- and Riemann zeta-functions, respectively and their numerical values of relevant arguments are known to be $\Gamma\left(\frac{5}{2}\right) = \frac{3\sqrt{\pi}}{4}$ and $\zeta\left(\frac{5}{2}, 1\right) = 1.341$.

Thus, we finally obtain

$$U \simeq \frac{0.45(k_B T)^{5/2}}{\pi^2 D^{3/2}}. \quad (3.65)$$

Consequently for the magnetic part of specific heat at constant volume is given by

$$C_V = 0.113 k_B \left(\frac{k_B T}{D}\right)^{\frac{3}{2}}. \quad (3.66)$$

In this work we consider strictly insulating materials, thus there is no electron contribution to the total specific heat. Consequently, taking into account the phonon and magnon contribution we can express the total specific heat at low temperatures by the formula

$$C = aT^3 + bT^{3/2}. \quad (3.67)$$

It is clear from this equation that the magnon contribution can experimentally easily determined if we plot the dependence of reduced specific heat $CT^{3/2}$ versus $T^{3/2}$. The situation is schematically illustrated in Fig. 3.1

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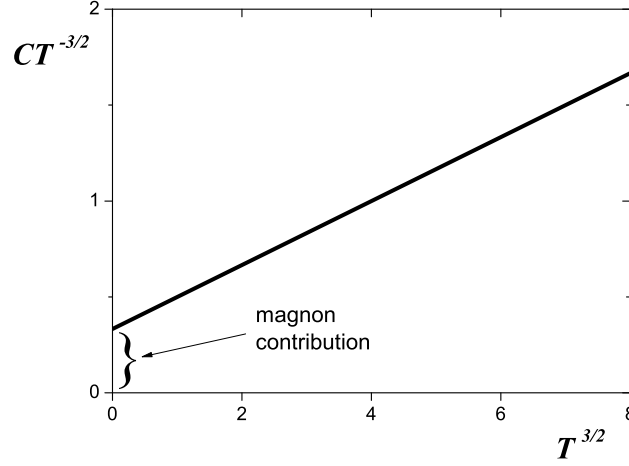


Figure 3.1: *The re-scaled specific heat vs. $T^{3/2}$*

3.2.2 Magnetization and Critical Temperature

The magnetic moment of the system can be calculated from the equation

$$M_S = g\mu_B \left\langle \left(NS - \sum_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} \right) \right\rangle. \quad (3.68)$$

The deviation of the magnetization from its saturation value can be expressed as

$$\begin{aligned} \Delta M &= M(0) - M(T) = g\mu_B \sum_{\mathbf{q}} \langle n_{\mathbf{q}} \rangle \\ &= \frac{g\mu_B}{(2\pi)^3} \int_0^{q_m} \left[\exp\left(\frac{Dq^2}{k_B T}\right) - 1 \right]^{-1} d^3q \end{aligned} \quad (3.69)$$

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At low temperatures ($Dq^2 \gg k_B T/J$) we obtain

$$\begin{aligned}
 \Delta M &= \frac{g\mu_B}{2\pi^2} \left(\frac{k_B T}{JD}\right)^{3/2} \int_0^\infty \frac{x^{1/2}}{\exp(x) - 1} dx. \\
 &= \frac{g\mu_B}{2\pi^2} \left(\frac{k_B T}{JD}\right)^{3/2} \Gamma\left(\frac{5}{2}\right) \zeta\left(\frac{3}{2}, 1\right) \\
 &= 0.117 g\mu_B \left(\frac{k_B T}{D}\right)^{3/2}. \tag{3.70}
 \end{aligned}$$

The finite-temperature magnetization can be then expressed as

$$M(T) = M(0) \left[1 - \left(\frac{T}{T_c}\right)^{\frac{3}{2}}\right] \tag{3.71}$$

where the critical temperature T_c is given by

$$T_c = \left(\frac{M(0)}{0.117 g\mu_B}\right)^{\frac{2}{3}} \frac{D}{k_B}. \tag{3.72}$$

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The Holstein-Primakoff theory can be extended also to the case of antiferromagnetic Heisenberg model which can describe many real materials [7]. On the other hand, the generalization of the Holstein-Primakoff for quantum antiferromagnets is very interesting because such systems exhibit very interesting magnetic properties that differ from quantum ferromagnets in many respects. Our aim in this subsection is to investigate the antiferromagnetic Heisenberg model spin system consisting of two interpenetrating sublattices a and b , which is described by the Hamiltonian

$$\hat{\mathcal{H}} = -J \sum_{i,j} \hat{\mathbf{S}}_{ai} \hat{\mathbf{S}}_{bj} - g\mu_B H_a \sum_i \hat{S}_{ai}^z + g\mu_B H_b \sum_j \hat{S}_{bj}^z, \tag{3.73}$$

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where $J < 0$ is the exchange interaction which couples the nearest neighbors on lattice and the quantity $H_a > 0$ represents an external magnetic field which is parallel to the z axis. In what follows, we will treat the problem applying the Holstein-Primakoff transformation for each sublattice separately. At first we express the spin rising and lowering sublattice operators with the help of creation-annihilation operators as follows

$$\hat{S}_{aj}^+ = (2S)^{1/2} \left(1 - \frac{a_j^\dagger a_j}{2S}\right)^{1/2} a_j, \quad \hat{S}_{aj}^- = (2S)^{1/2} a_j^\dagger \left(1 - \frac{a_j^\dagger a_j}{2S}\right)^{1/2} \quad (3.74)$$

$$\hat{S}_{b\ell}^+ = (2S)^{1/2} \left(1 - \frac{b_\ell^\dagger b_\ell}{2S}\right)^{1/2} b_\ell, \quad \hat{S}_{b\ell}^- = (2S)^{1/2} b_\ell^\dagger \left(1 - \frac{b_\ell^\dagger b_\ell}{2S}\right)^{1/2} \quad (3.75)$$

$$\hat{S}_{aj}^z = S - a_j^\dagger a_j, \quad -\hat{S}_{b\ell}^z = S - b_\ell^\dagger b_\ell. \quad (3.76)$$

Next, we introduce the sublattice spin-wave variables

$$c_{\mathbf{q}} = \frac{2}{\sqrt{N}} \sum_j e^{-i\mathbf{q}\cdot\mathbf{R}_j} a_j, \quad c_{\mathbf{q}}^\dagger = \frac{2}{\sqrt{N}} \sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j} a_j^\dagger \quad (3.77)$$

$$d_{\mathbf{q}} = \frac{2}{\sqrt{N}} \sum_\ell e^{i\mathbf{q}\cdot\mathbf{R}_\ell} b_\ell, \quad d_{\mathbf{q}}^\dagger = \frac{2}{\sqrt{N}} \sum_\ell e^{-i\mathbf{q}\cdot\mathbf{R}_\ell} b_\ell^\dagger. \quad (3.78)$$

In previous equations summations run over all N atoms of the a and b sublattice, respectively. Moreover, the following magnon commutation relations hold

$$\begin{aligned} [c_{\mathbf{q}_1}, c_{\mathbf{q}_2}^\dagger] &= [d_{\mathbf{q}_1}, d_{\mathbf{q}_2}^\dagger] = \delta_{\mathbf{q}_1 \mathbf{q}_2}, \\ [c_{\mathbf{q}_1}, c_{\mathbf{q}_2}] &= [c_{\mathbf{q}_1}^\dagger, c_{\mathbf{q}_2}^\dagger] = 0. \quad [d_{\mathbf{q}_1}, d_{\mathbf{q}_2}] = [d_{\mathbf{q}_1}^\dagger, d_{\mathbf{q}_2}^\dagger] = 0. \end{aligned} \quad (3.79)$$

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Now, we expand (3.74)-(3.75) as

$$\hat{S}_{aj}^+ = \left(\frac{4S}{N}\right)^{1/2} \left[\sum_{\mathbf{q}_1} e^{-i\mathbf{q}_1 \cdot \mathbf{R}_j} c_{\mathbf{q}_1} - \frac{1}{8SN} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} e^{i(\mathbf{q}_1 - \mathbf{q}_2 - \mathbf{q}_3) \cdot \mathbf{R}_j} c_{\mathbf{q}_1}^\dagger c_{\mathbf{q}_2} c_{\mathbf{q}_3} + \dots \right] \quad (3.80)$$

$$\hat{S}_{aj}^- = \left(\frac{4S}{N}\right)^{1/2} \left[\sum_{\mathbf{q}_1} e^{i\mathbf{q}_1 \cdot \mathbf{R}_j} c_{\mathbf{q}_1}^\dagger - \frac{1}{8SN} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} e^{i(\mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_3) \cdot \mathbf{R}_j} c_{\mathbf{q}_1}^\dagger c_{\mathbf{q}_2}^\dagger c_{\mathbf{q}_3} + \dots \right] \quad (3.81)$$

$$\hat{S}_{bl}^+ = \left(\frac{4S}{N}\right)^{1/2} \left[\sum_{\mathbf{q}_1} e^{-i\mathbf{q}_1 \cdot \mathbf{R}_\ell} d_{\mathbf{q}_1} - \frac{1}{8SN} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} e^{i(\mathbf{q}_1 - \mathbf{q}_2 - \mathbf{q}_3) \cdot \mathbf{R}_\ell} d_{\mathbf{q}_1}^\dagger d_{\mathbf{q}_2} d_{\mathbf{q}_3} + \dots \right] \quad (3.82)$$

$$\hat{S}_{bl}^- = \left(\frac{4S}{N}\right)^{1/2} \left[\sum_{\mathbf{q}_1} e^{i\mathbf{q}_1 \cdot \mathbf{R}_\ell} d_{\mathbf{q}_1}^\dagger - \frac{1}{8SN} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} e^{i(\mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_3) \cdot \mathbf{R}_\ell} d_{\mathbf{q}_1}^\dagger d_{\mathbf{q}_2}^\dagger d_{\mathbf{q}_3} + \dots \right] \quad (3.83)$$

$$\hat{S}_{aj}^z = S - \frac{1}{N} \sum_{\mathbf{q}_1 \mathbf{q}_2} e^{i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}_j} c_{\mathbf{q}_1}^\dagger c_{\mathbf{q}_2}. \quad (3.84)$$

$$\hat{S}_{bl}^z = -S + \frac{1}{N} \sum_{\mathbf{q}_1 \mathbf{q}_2} e^{-i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}_\ell} d_{\mathbf{q}_1}^\dagger d_{\mathbf{q}_2}. \quad (3.85)$$

Substituting these expansions into (3.73) and using (3.17) we obtain

$$\hat{\mathcal{H}} = NzJS^2 + \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_1 \quad (3.86)$$

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where $\hat{\mathcal{H}}_0$ is a part of the Hamiltonian which is bilinear in magnon variables, i.e.,

$$\begin{aligned}\hat{\mathcal{H}}_0 &= -2JzS \sum_{\mathbf{q}} \left[\gamma_{\mathbf{q}} (c_{\mathbf{q}}^\dagger d_{\mathbf{q}}^\dagger + c_{\mathbf{q}} d_{\mathbf{q}}) + (c_{\mathbf{q}}^\dagger c_{\mathbf{q}} + d_{\mathbf{q}}^\dagger d_{\mathbf{q}}) \right] \\ &+ g\mu_B H \sum_{\mathbf{q}} (c_{\mathbf{q}}^\dagger c_{\mathbf{q}} - d_{\mathbf{q}}^\dagger d_{\mathbf{q}})\end{aligned}\quad (3.87)$$

where $\gamma_{\mathbf{q}}$ is given by (3.54) and the existence of symmetry center of the lattice has been assumed. The quantity $\hat{\mathcal{H}}_1$ includes higher-order terms and will be for the simplicity neglected. However, even after neglecting $\hat{\mathcal{H}}_1$, the energy spectrum of system cannot be simply obtained, since the Hamiltonian is not yet diagonal. Thus the main problem to be solved is the diagonalization of $\hat{\mathcal{H}}_0$. In order to make a progress, we introduce here new set of the creation and annihilation operators $\alpha_{\mathbf{q}}^\dagger, \alpha_{\mathbf{q}}, \beta_{\mathbf{q}}^\dagger, \beta_{\mathbf{q}}$

$$\alpha_{\mathbf{q}} = u_{\mathbf{q}} c_{\mathbf{q}} - v_{\mathbf{q}} d_{\mathbf{q}}^\dagger, \quad \alpha_{\mathbf{q}}^\dagger = u_{\mathbf{q}} c_{\mathbf{q}}^\dagger - v_{\mathbf{q}} d_{\mathbf{q}}, \quad (3.88)$$

$$\beta_{\mathbf{q}} = u_{\mathbf{q}} d_{\mathbf{q}} - v_{\mathbf{q}} c_{\mathbf{q}}^\dagger, \quad \beta_{\mathbf{q}}^\dagger = u_{\mathbf{q}} d_{\mathbf{q}}^\dagger - v_{\mathbf{q}} c_{\mathbf{q}}, \quad (3.89)$$

obeying the following commutation rules

$$[\alpha_{\mathbf{q}}, \alpha_{\mathbf{q}}^\dagger] = 1, \quad [\beta_{\mathbf{q}}, \beta_{\mathbf{q}}^\dagger] = 1, \quad [\alpha_{\mathbf{q}}, \beta_{\mathbf{q}}] = 0. \quad (3.90)$$

The real quantities entering previous equations satisfy relation

$$u_{\mathbf{q}}^2 - v_{\mathbf{q}}^2 = 1, \quad (3.91)$$

and the inverse transformation are given by

$$c_{\mathbf{q}} = u_{\mathbf{q}} \alpha_{\mathbf{q}} - v_{\mathbf{q}} \beta_{\mathbf{q}}^\dagger, \quad c_{\mathbf{q}}^\dagger = u_{\mathbf{q}} \alpha_{\mathbf{q}}^\dagger - v_{\mathbf{q}} \beta_{\mathbf{q}}, \quad (3.92)$$

$$d_{\mathbf{q}} = u_{\mathbf{q}} \beta_{\mathbf{q}} - v_{\mathbf{q}} \alpha_{\mathbf{q}}^\dagger, \quad d_{\mathbf{q}}^\dagger = u_{\mathbf{q}} \beta_{\mathbf{q}}^\dagger - v_{\mathbf{q}} \alpha_{\mathbf{q}}, \quad (3.93)$$

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The parameters $u_{\mathbf{q}}$ and $v_{\mathbf{q}}$ in transformations (3.92) and (3.93) can be determined explicitly in the form

$$u_{\mathbf{q}} = \cosh \theta_{\mathbf{q}}, \quad v_{\mathbf{q}} = \sinh \theta_{\mathbf{q}}, \quad (3.94)$$

where $\theta_{\mathbf{q}}$ is given by

$$\tanh(2\theta_{\mathbf{q}}) = \gamma_{\mathbf{q}}. \quad (3.95)$$

The explicit forms of the transformation given by (3.94) and (3.95) is usually called in the literature as Bogolyubov transformation. Substituting (3.92) and (3.93) into (3.87) one finally obtains for $\hat{\mathcal{H}}$ the following simple relation

$$\hat{\mathcal{H}} = NJzS(S+1) + \sum_{\mathbf{q}} \left[\hbar\omega_{\mathbf{q}}^+ \left(\alpha_{\mathbf{q}}^\dagger \alpha_{\mathbf{q}} + \frac{1}{2} \right) + \hbar\omega_{\mathbf{q}}^- \left(\beta_{\mathbf{q}}^\dagger \beta_{\mathbf{q}} + \frac{1}{2} \right) \right] \quad (3.96)$$

where we have defined the eigenfrequencies of the system as

$$\hbar\omega_{\mathbf{q}}^\pm = -2JzS \sqrt{1 - \gamma_{\mathbf{q}}^2} \pm g\mu_B H. \quad (3.97)$$

3.3.1 Ground-State Energy

In this part we investigate the ground-state energy of the two sublattice antiferromagnetic Heisenberg system.

The lowest possible energy (i.e., the ground-state energy) can be straightforwardly obtained after setting $H = 0$ and averaging Eq.(3.96)

$$E_g \equiv \langle \hat{\mathcal{H}} \rangle = NJzS(S+1) + \sum_{\mathbf{q}} \left[\hbar\omega_{\mathbf{q}}^+ \left(\langle \alpha_{\mathbf{q}}^\dagger \alpha_{\mathbf{q}} \rangle + \frac{1}{2} \right) + \hbar\omega_{\mathbf{q}}^- \left(\langle \beta_{\mathbf{q}}^\dagger \beta_{\mathbf{q}} \rangle + \frac{1}{2} \right) \right]. \quad (3.98)$$

Of course, the ground state corresponds to the vacuum state in which no excited magnons are present in the system and therefore the previous equation

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reduces to

$$\begin{aligned}
 E_g &= NJzS(S+1) - 2JzS \sum_{\mathbf{q}} (1 - \gamma_{\mathbf{q}}^2)^{1/2} \\
 &= NJzS^2 \left[1 + \frac{1}{S} \left(1 - \frac{2}{N} \sum_{\mathbf{q}} \sqrt{1 - \gamma_{\mathbf{q}}^2} \right) \right]. \quad (3.99)
 \end{aligned}$$

The parameter $\gamma_{\mathbf{q}}$ depends on the lattice structure and it is given by

$$\gamma_{\mathbf{q}} = \frac{1}{d} \sum_{i=1}^d \cos q_i, \quad (3.100)$$

where $d = 1$ for the one-dimensional chain, $d = 2$ for two-dimensional square, and $d = 3$ for three-dimensional simple-cubic lattice, respectively. In order to find numerical values of E_g we have to evaluate the sum over \mathbf{q} in Eq. (3.99) which must be taken over all $N/2$ points in the first Brillouin zone of the sublattice. The relevant sum can be expressed as

$$\begin{aligned}
 I_d &= \frac{2}{N} \sqrt{1 - \gamma_{\mathbf{q}}^2} \\
 &= \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} \dots \int_{-\pi}^{\pi} dq_1 \dots dq_d \left[1 - \left(\frac{1}{d} \sum_{i=1}^d \cos q_i \right)^2 \right]^{1/2}. \quad (3.101)
 \end{aligned}$$

Evaluating the above expression one gets

$$I_1 \doteq 0.637, \quad I_2 \doteq 0.842, \quad I_3 \doteq 0.903, \quad (3.102)$$

and using these numerical values, we obtain the ground-state energy in the

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form

$$\begin{aligned}
 E_g &= 2NJS^2\left(1 + \frac{0.363}{S}\right) && \text{for the linear chain} \\
 E_g &= 4NJS^2\left(1 + \frac{0.158}{S}\right) && \text{for the square lattice} \quad (3.103) \\
 E_g &= 6NJS^2\left(1 + \frac{0.097}{S}\right) && \text{for the cubic lattice.}
 \end{aligned}$$

One should note here that all numerical values of the ground-state energy satisfy the Anderson inequality

$$\frac{1}{2}NJzS^2\left(1 + \frac{1}{zS}\right) < E_g < \frac{1}{2}NJzS^2. \quad (3.104)$$

It is also useful to note that for the spin-1/2 linear chain Eq.(3.104) gives the value $E_g/(NJ) = 0.863$ which is in agreement with the exact Bethe-Hulten [3, 4] value $E_g/(NJ) = 0.5(4 \ln 2 - 1) = 0.886$. On the basis of this excellent agreement one should assume that the spin-wave theory gives acceptable quantitative results also for other lattices and spin values.

The most important qualitative finding in this part is the fact that the energy corresponding to the saturated antiparallel ordering is not the ground state energy of the two-sublattice antiferromagnetic system. This finding is a direct consequence of the fact that the total sublattice magnetization are not the constants of motion.

3.3.2 Sublattice Magnetization

At first let us examine in this part the ground-state sublattice magnetization which is defined as

$$M_a = g\mu_B \left\langle \sum_j \hat{S}_{aj}^z \right\rangle = \frac{1}{2}NS - \sum_{\mathbf{q}} \langle c_{\mathbf{q}}^\dagger c_{\mathbf{q}} \rangle \quad (3.105)$$

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Using the Bogolyubov transformation (3.94) we obtain

$$M_a = \frac{1}{2}NS - \sum_{\mathbf{q}} \left\{ \cosh^2(\theta_{\mathbf{q}}) \langle \alpha_{\mathbf{q}}^\dagger \alpha_{\mathbf{q}} \rangle + \sinh^2(\theta_{\mathbf{q}}) \langle \beta_{\mathbf{q}} \beta_{\mathbf{q}}^\dagger \rangle \right. \\ \left. - \sinh(\theta_{\mathbf{q}}) \cosh(\theta_{\mathbf{q}}) (\langle \alpha_{\mathbf{q}}^\dagger \beta_{\mathbf{q}}^\dagger \rangle + \langle \alpha_{\mathbf{q}} \beta_{\mathbf{q}} \rangle) \right\} \quad (3.106)$$

At zero temperature there are no excited states and therefore Eq.(3.106) simplifies as follows

$$M_a = \frac{1}{2}NS - \sum_{\mathbf{q}} \sinh^2(\theta_{\mathbf{q}}). \quad (3.107)$$

After substituting the relevant expression for $\sinh(\theta_{\mathbf{q}})$ one obtains expression

$$M_a = \frac{1}{2}NS - \frac{1}{4} \sum_{\mathbf{q}} \left[\left(\frac{1 - \gamma_{\mathbf{q}}}{1 + \gamma_{\mathbf{q}}} \right)^{1/2} + \left(\frac{1 + \gamma_{\mathbf{q}}}{1 - \gamma_{\mathbf{q}}} \right)^{1/2} - 2 \right], \quad (3.108)$$

which can finally be rewritten as

$$M_a = \frac{NS}{2} \left[1 - \frac{1}{2S} \left(\frac{2}{N} \sum_{\mathbf{q}} \frac{1}{\sqrt{1 - \gamma_{\mathbf{q}}^2}} - 1 \right) \right]. \quad (3.109)$$

In order to proceed further, we express the sum $S_d = \frac{2}{N} \sum_{\mathbf{q}} \frac{1}{\sqrt{1 - \gamma_{\mathbf{q}}^2}}$ appearing in (3.109) in the following integral form

$$S_d = \frac{2}{N} \sum_{\mathbf{q}} \frac{1}{\sqrt{1 - \gamma_{\mathbf{q}}^2}} \\ = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d\lambda_1 \cdots d\lambda_d \left[1 - \left(\frac{1}{d} \sum_{j=1}^d \cos \lambda_j \right)^2 \right]^{-1/2} \quad (3.110)$$

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Evaluating this integral for the simple cubic lattice ($d = 3$) and plane square lattice ($d = 2$) one obtains values $S_3 = 1.156$ and $S_2 = 1.393$ from which the sublattice magnetization are given by

$$M_a = \frac{NS}{2} \left(1 - \frac{0.078}{S} \right) \quad \text{for } d = 3 \quad (3.111)$$

$$M_a = \frac{NS}{2} \left(1 - \frac{0.197}{S} \right) \quad \text{for } d = 2. \quad (3.112)$$

Thus we can conclude that the spin-wave theory predicts a long-range order in three- and two dimensional antiferromagnetic Heisenberg systems, however, as it is clear from (3.110)-(3.112), the sublattice magnetizations do not take their saturation values at zero temperature. This behavior appears due to quantum fluctuations at the ground state that are stronger in lower dimensions.

In the case of linear chain ($d = 1$), the integral S_1 diverges logarithmically indicating that the sublattice magnetization has zero expectation value. This result is in agreement with exact calculations and represents a significant improvement over the standard mean-field theory which predicts the existence of long-range order also for one dimensional Heisenberg model.

Finally, let us comment on the calculation of the temperature dependence of the sublattice magnetization for the antiferromagnetic Heisenberg model. The deviation of the sublattice magnetization from its ground-state value is calculated from

$$\begin{aligned} M_a(0) - M_a(T) &= \sum_{\mathbf{q}} \langle n_{\mathbf{q}} \rangle \cosh(2\theta_{\mathbf{q}}) \\ &= \sum_{\mathbf{q}} \langle n_{\mathbf{q}} \rangle (1 - \gamma_{\mathbf{q}}^2)^{-1/2} \end{aligned} \quad (3.113)$$

where the mean number of bosons is obviously given by

$$\langle n_{\mathbf{q}} \rangle = \frac{1}{\exp\left(\frac{\hbar\omega_{\mathbf{q}}}{k_B T}\right) - 1} \quad (3.114)$$

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with

$$\hbar\omega_{\mathbf{q}} = (2JSz)^2(1 - \gamma_{\mathbf{q}}^2) \quad (3.115)$$

However, the explicit calculation of sublattice magnetizations at arbitrary temperature represents hard and non-trivial mathematical task. Nevertheless, at the temperatures that are significantly lower than the Neel transition temperature T_N , one finds that the sublattice magnetization is proportional to $(T/T_N)^2$. The proof of this behavior is left for the reader.

Chapter 4

Jordan-Wigner Transformation for the XY Model

In previous parts of this text we have discussed how to apply the bosonization technique within the Holstein-Primakoff approach to the ferromagnetic and antiferromagnetic spin systems. In the present chapter we will investigate a similar approach, which is known as a method of fermionization. In particular, we will discuss application of the Wigner-Jordan transformation to the isotropic quantum XY model in order to clarify important points of this method.

The main idea of this approach is to transform the Hamiltonian describing a spin system by the use of new operators obeying the fermion anticommutation rules.

Before we start our analysis, it is useful to note that the spectrum of the XY model was exactly found by H.Bethe [3] in 1931. The Bethe's approach is of great importance, however, it is quite involved and rather abstract, thus it is difficult to understand even such basic properties as long-range order. A much more natural approach to the problem of interacting spin-1/2 systems was originally introduced in 1928 by Jordan and Wigner [5],

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who invented simple mathematical transformations converting spin-1/2 systems into problems of interacting (and in some cases even non-interacting) spinless fermions. In fact, the XY model which is a special case of the Heisenberg Hamiltonian, reduces to a free theory of spinless fermions under the Jordan-Wigner transformations. Another reason for choosing the XY model, is that the low-energy properties of the full anti-ferromagnetic Heisenberg chain, such as the presence of gapless excitations and absence of a long range order are very similar to those of the XY model (see [6] and references therein).

We will study a linear chain of N spin-1/2 atoms interacting antiferromagnetically with their nearest neighbors. This system is described by the Hamiltonian

$$\hat{\mathcal{H}} = J \sum_{j=1}^N (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y), \quad (4.1)$$

where $J > 0$ represents the exchange interaction and \hat{S}_i^α are spin-1/2 operators obeying the usual commutation relations (3.3). As usually, we assume cyclic boundary conditions, with $\hat{S}_{N+1}^\alpha = \hat{S}_1^\alpha$, $\alpha = x, y$. Of course, for $J < 0$ the ferromagnetic case of (4.1) is obtained. Thus, if we solve the antiferromagnetic problem exactly, then we can immediately obtain also the solution of the ferromagnetic XY chain. Similarly as in the case of bozonization, we at first introduce spin-raising and spin-lowering operators (3.13) and rewrite the Hamiltonian as a bilinear form in these operators, i.e.

$$\hat{\mathcal{H}} = \frac{J}{2} \sum_{j=1}^N (\hat{S}_j^- \hat{S}_{j+1}^+ + \hat{S}_{j+1}^- \hat{S}_j^+). \quad (4.2)$$

It clear that without loss of generality we can set $J = 1$ in all subsequent calculations. We know that the \hat{S}^\pm operators belonging to the same site obey anticommutation relations, while that ones on different sites satisfy

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usual commutation relations and this mathematical property disables a direct diagonalization of (4.2). The key to the solution of this problem is the Jordan-Wigner transformation which enables to obtain the Hamiltonian in terms of pure fermion operators.

The Jordan-Wigner transformation explicitly reads

$$c_n^\dagger = \hat{S}_n^+ \exp\left(-i\pi \sum_{j=1}^{n-1} \hat{S}_j^+ \hat{S}_j^-\right), \quad c_n = \hat{S}_n^- \exp\left(i\pi \sum_{j=1}^{n-1} \hat{S}_j^+ \hat{S}_j^-\right), \quad (4.3)$$

and the inverse transformation is given by

$$\hat{S}_n^+ = c_n^\dagger \exp\left(i\pi \sum_{j=1}^{n-1} c_j^\dagger c_j\right), \quad \hat{S}_n^- = c_n \exp\left(i\pi \sum_{j=1}^{n-1} c_n^\dagger c_n\right). \quad (4.4)$$

Here it is worth noticing that the signs in the exponents and the order of the multipliers in (4.3) and (4.4) are not important.

The operators c_j^\dagger, c_k obey the canonical fermion algebra, i.e.

$$\{c_j, c_k^\dagger\} = \delta_{jk}, \quad \{c_j^\dagger, c_k^\dagger\} = 0, \quad \{c_j, c_k\} = 0. \quad (4.5)$$

To illustrate the mathematics behind, we will explicitly prove the first relation, while the other anti-commutators in (4.5) can be computed in a similar fashion.

At first we recall the validity of the following relations $[\hat{S}_j^+ \hat{S}_j, \hat{S}_k^+ \hat{S}_k] = 0$, $[\hat{S}_j^+ \hat{S}_j, \hat{S}_k] = -\delta_{jk} \hat{S}_k$, $[\hat{S}_j^+ \hat{S}_j, \hat{S}_k^+] = \delta_{jk} \hat{S}_k^+$, $(\hat{S}_j^+ \hat{S}_j)^2 = \hat{S}_j^+ \hat{S}_j$, since the spin-raising and spin-lowering operators on different sites commute and on the same site behave like fermions. Therefore,

$$\exp\left(\pm i\pi \sum_{j=n}^m \hat{S}_j^+ \hat{S}_j^-\right) = \prod_{j=n}^m \exp(\pm i\pi \hat{S}_j^+ \hat{S}_j^-) \quad (4.6)$$

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and the exponential function on the r.h.s of previous equation can be easily evaluated as follows

$$\begin{aligned}
 \exp(\pm i\pi \hat{S}_j^+ \hat{S}_j^-) &= \sum_{k=0}^{\infty} \frac{1}{k!} (\pm i\pi)^k (\hat{S}_j^+ \hat{S}_j^-)^k \\
 &= 1 + \sum_{k=1}^{\infty} \frac{1}{k!} (\pm i\pi)^k \hat{S}_j^+ \hat{S}_j^- \\
 &= 1 + (e^{\pm i\pi} - 1) \hat{S}_j^+ \hat{S}_j^- = 1 - 2\hat{S}_j^+ \hat{S}_j^-. \quad (4.7)
 \end{aligned}$$

Similarly, using the following anticommutators

$$\{\hat{S}_j^-, 1 - 2\hat{S}_j^+ \hat{S}_j^-\} = 0, \quad \{\hat{S}_j^+, 1 - 2\hat{S}_j^+ \hat{S}_j^-\} = 0, \quad (4.8)$$

one obtains relations

$$\left[\exp\left(\pm i\pi \sum_{j=n}^m \hat{S}_j^+ \hat{S}_j^-\right), \hat{S}_k^- \right] = \left[\exp\left(\pm i\pi \sum_{j=n}^m \hat{S}_j^+ \hat{S}_j^-\right), \hat{S}_k^+ \right] = 0, \quad k \notin [n, m] \quad (4.9)$$

$$\left\{ \exp\left(\pm i\pi \sum_{j=n}^m \hat{S}_j^+ \hat{S}_j^-\right), \hat{S}_k^- \right\} = \left\{ \exp\left(\pm i\pi \sum_{j=n}^m \hat{S}_j^+ \hat{S}_j^-\right), \hat{S}_k^+ \right\} = 0, \quad k \in [n, m]. \quad (4.10)$$

Although all the above calculations have a preparatory character, they are of crucial importance to demonstrate the fermionic nature of c_j and c_k^\dagger . Really, using (4.6)- (4.10), we can now straightforwardly calculate the following

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anti-commutators:

$$\begin{aligned}
\{c_j, c_k^\dagger\} &= \hat{S}_j^- \exp\left(i\pi \sum_{\ell=1}^{j-1} \hat{S}_\ell^+ \hat{S}_\ell^-\right) \exp\left(-i\pi \sum_{\ell=1}^{k-1} \hat{S}_\ell^+ \hat{S}_\ell^-\right) \hat{S}_k^+ \\
&+ \hat{S}_k^+ \exp\left(-i\pi \sum_{\ell=1}^{k-1} \hat{S}_\ell^+ \hat{S}_\ell^-\right) \exp\left(i\pi \sum_{\ell=1}^{j-1} \hat{S}_\ell^+ \hat{S}_\ell^-\right) \hat{S}_j^- \\
&= \hat{S}_j^- \exp\left(i\pi \sum_{\ell=j}^{k-1} \hat{S}_\ell^+ \hat{S}_\ell^-\right) \hat{S}_k^+ \hat{S}_k^+ \exp\left(i\pi \sum_{\ell=j}^{k-1} \hat{S}_\ell^+ \hat{S}_\ell^-\right) \hat{S}_k^- \\
&= (\hat{S}_j^- \hat{S}_j^+ - \hat{S}_j^+ \hat{S}_j^-) \exp\left(i\pi \sum_{\ell=j}^{k-1} \hat{S}_\ell^+ \hat{S}_\ell^-\right) = 0, \quad k > j. \quad (4.11)
\end{aligned}$$

In the same way, we derive relation

$$\{c_j, c_k^\dagger\} = \{c_k, c_j^\dagger\}^\dagger = 0, \quad k < j \quad (4.12)$$

$$\{c_k, c_j^\dagger\} = \hat{S}_k^- \hat{S}_k^+ + \hat{S}_k^+ \hat{S}_k^- = 1. \quad (4.13)$$

Thus we have successfully proved the fermionic commutation relations and now we can transform the relevant terms in the Hamiltonian

For $1 \leq j \leq N-1$ one obtains

$$\begin{aligned}
\hat{S}_j^- \hat{S}_{j+1}^+ &= \exp\left(-i\pi \sum_{\ell=1}^{j-1} c_\ell^\dagger c_\ell\right) c_j c_{j+1}^\dagger \exp\left(i\pi \sum_{\ell=1}^j c_\ell^\dagger c_\ell\right) \\
&= c_j \exp\left(-i\pi \sum_{\ell=1}^{j-1} c_\ell^\dagger c_\ell\right) \exp\left(i\pi \sum_{\ell=1}^j c_\ell^\dagger c_\ell\right) c_{j+1}^\dagger \\
&= c_j \exp(i\pi c_j^\dagger c_j) c_{j+1}^\dagger = c_j (1 - 2c_j^\dagger c_j) c_{j+1}^\dagger \\
&= -(1 - 2c_j^\dagger c_j) c_j c_{j+1}^\dagger = -c_j c_{j+1}^\dagger = c_{j+1}^\dagger c_j \quad (4.14)
\end{aligned}$$

and similarly we have

$$\hat{S}_{j+1}^- \hat{S}_j^+ = (\hat{S}_j^- \hat{S}_{j+1}^+)^\dagger = c_j^\dagger c_{j+1}. \quad (4.15)$$

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Here one should notice that in deriving previous equations, we have used the following relations

$$\begin{aligned}
[c_j^\dagger c_j, c_k^\dagger c_k] &= 0, & (c_j^\dagger c_j)^2 &= c_j^\dagger c_j, \\
[c_j^\dagger c_j, c_k] &= -\delta_{jk} c_k, & [c_j^\dagger c_j, c_k^\dagger] &= -\delta_{jk} c_k^\dagger, \\
\{1 - 2c_j^\dagger c_j, c_j\} &= 0, & \{1 - 2c_j^\dagger c_j, c_j^\dagger\} &= 0,
\end{aligned} \tag{4.16}$$

$$\begin{aligned}
\left[\exp\left(\pm i\pi \sum_{j=n}^m c_j^\dagger c_j\right), c_k \right] &= \left[\exp\left(\pm i\pi \sum_{j=n}^m c_j^\dagger c_j\right), c_k^\dagger \right] = 0, \\
k &\notin [n, m]
\end{aligned} \tag{4.17}$$

$$\begin{aligned}
\left\{ \exp\left(\pm i\pi \sum_{j=n}^m c_j^\dagger c_j\right), c_k \right\} &= \left\{ \exp\left(\pm i\pi \sum_{j=n}^m c_j^\dagger c_j\right), c_k^\dagger \right\} = 0, \\
k &\in [n, m].
\end{aligned} \tag{4.18}$$

After expressing the special cyclic boundary term ($\hat{S}_N^- \hat{S}_1^+ + \hat{S}_1^- \hat{S}_N^+$) in terms of c 's and substituting Eqs.(4.14) and (4.15) into Eq.(4.2), we can rewrite the Hamiltonian of the system as

$$\hat{\mathcal{H}} = \frac{1}{2} \sum_j (c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}) + \hat{\mathcal{H}}_b \tag{4.19}$$

where

$$\hat{\mathcal{H}}_b = -\frac{1}{2} (c_1^\dagger c_N + c_N^\dagger c_1) \left[1 + \exp\left(\pm i\pi \sum_{j=1}^N c_j^\dagger c_j\right) \right] \tag{4.20}$$

represents the boundary term, which gives an $\mathcal{O}(N^{-1})$ contributions to the macroscopic physical quantities and for this reason will be neglected in further calculations.

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Applying this simplification, we are left with the problem of diagonalization of the following bilinear form

$$\hat{\mathcal{H}} = \frac{1}{2} \sum_j (c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}), \quad (4.21)$$

which describes free spinless fermions on a cyclic chain with nearest neighbor hopping.

In order to diagonalize the Hamiltonian (4.21) we rewrite it in the form

$$\hat{\mathcal{H}} = \sum_{jk} c_j^\dagger A_{jk} c_k, \quad (4.22)$$

where the elements of the matrix \mathbf{A} are given by

$$A_{jk} = \frac{1}{2} (\delta_{j,k+1} + \delta_{k,j+1}). \quad (4.23)$$

Taking into account the translational invariance of the lattice, we find the eigenvectors and eigenvalues of \mathbf{A} to be

$$\phi_{qj} = \frac{1}{\sqrt{N}} e^{iqj}, \quad \Lambda_q = \cos(q), \quad (4.24)$$

with $q = \frac{2\pi n}{N}$ and $N/2 \leq n \leq N/2 - 1$. The eigenfunctions ϕ_{qk} form an orthonormal and complete set, thus we can introduce new operators obeying the canonical anticommutation rule

$$\eta_q = \sum_j \phi_{qj}^* c_j, \quad \eta_q^\dagger = \sum_j \phi_{qj} c_j^\dagger. \quad (4.25)$$

Using the following inverse transformations

$$c_j = \sum_q \phi_{qj} \eta_q, \quad c_j^\dagger = \sum_q \phi_{qj} \eta_q^\dagger \quad (4.26)$$

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the Hamiltonian (4.22) can be rewritten in the diagonal form

$$\hat{\mathcal{H}} = \sum_q \Lambda_q \eta_q^\dagger \eta_q. \quad (4.27)$$

Since some of the eigenvalues of \mathbf{A} will be negative, we perform an additional transformation

$$\xi_q = \eta_q, \quad \Lambda_q \geq 0 \quad (4.28)$$

$$\xi_q = \eta_q^\dagger, \quad \Lambda_q < 0 \quad (4.29)$$

and obtain

$$\begin{aligned} \hat{\mathcal{H}} &= \sum_{q, \Lambda_q \geq 0} \Lambda_q \xi_q^\dagger \xi_q + \sum_{q, \Lambda_q < 0} \Lambda_q \xi_q^\dagger \xi_q \\ &= \sum_{q, \Lambda_q} |\Lambda_q| \xi_q^\dagger \xi_q - \sum_{q, \Lambda_q < 0} |\Lambda_q| \\ &= \sum_{q, \Lambda_q} |\Lambda_q| \left(\xi_q^\dagger \xi_q - \frac{1}{2} \right). \end{aligned} \quad (4.30)$$

Here the ξ operators again obey the canonical anticommutation rules.

As usually, the ground state $|0\rangle$ satisfies equation

$$\xi_q |0\rangle = 0, \quad \forall q \quad (4.31)$$

and the operator ξ_q^\dagger generates an elementary fermion excitation with energy $|\Lambda_q|$ above the ground state.

The dispersion relation for the model under investigation is shown in Fig 4.1. As one can see there always exist gapless excitations near $q = \pm\pi/2$. The ground state energy reduced per one spin is given by

$$\begin{aligned} U_0 = \frac{\langle \hat{\mathcal{H}} \rangle}{N} &= -\frac{1}{N} \sum_q \frac{1}{2} |\Lambda_q| \\ &= \int_{-\pi}^{\pi} \frac{dq}{4\pi} |\cos(q)| = -\frac{1}{\pi} \int_0^{\pi/2} \cos(q) dq = -\frac{1}{\pi} \end{aligned} \quad (4.32)$$

4.1 Jordan-Wigner Transformation for the XY Model

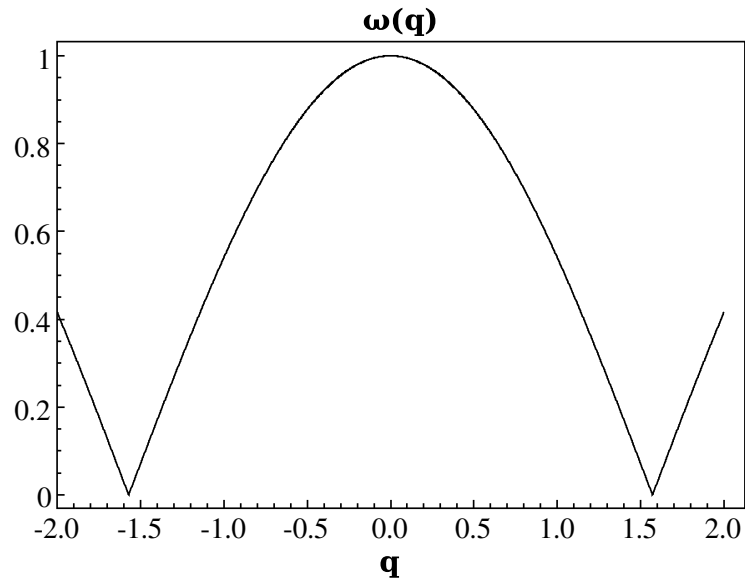


Figure 4.1: *Dispersion relation of the XY model.*

Of course, the method of fermionization can be extended to many other systems including the systems with higher spin and higher spatial dimensions. However, the analysis of these systems requires complex and tedious calculations and sometimes also the application of additional theoretical tools/methods (for example the Green function technique) that are beyond the scope of this introductory text.

Conclusion

In this work we have discussed some theoretical tools that are frequently used to investigate the localized quantum spin models.

The first approach is the standard mean-field theory, which represents the simplest possible technique usually applied to understand basic quantitative features of various theoretical models of quantum magnetism. Although this method is included in many textbooks, the formulation is usually very simplified and frequently the authors do not derive the Gibbs free energy within this method. To avoid this problem, we have used an elegant formulation based on the Bogolyubov inequality which enables to extend our approach to formulate more accurate theories (for example the Oguchi approximation or Constant Coupling Method). One should also emphasize that in deriving the partition function we have applied the Cauchy integral formula, which enables to calculate exponential function with a matrix argument. This is an unknown trick which can be used in calculations in any branch of theoretical physics.

In the Chapter 3 we have discussed the standard spin-wave theory separately for ferromagnetic and antiferromagnetic materials. We have shown in detail how to introduce the boson operators that enable to calculate several physical quantities such as magnetization, internal energy and magnetic contribution to the specific heat.

The last part is dedicated to the method of fermionization. Here we have discussed the application of Jordan-Wigner transformation to the quantum XY model with spin $1/2$. This approach represents another standard theoretical approach which is used to investigate quantum magnetism.

It is clear from the content of this supporting text that we have covered just one special part of quantum theory of magnetism, which is, however, discussed elementary enough. In order to understand further interesting features of the quantum magnetism it is necessary to study further textbooks, for example [8], [9], [10], [11]).

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