THESIS

Ground States and Elementary Excitations of Quantum Antiferromagnets

Tsutomu Momoi

Department of Physics, University of Tokyo

December, 1994

Acknowledgments

I would like to express my sincerest gratitude to Professor Masuo Suzuki, for his guidance, useful discussions, critical reading of the manuscript, and above all his encouragements.

I am grateful to Professor Kenn Kubo, Professor Hidetoshi Nishimori, Professor Hal Tasaki and Dr. Tohru Koma for stimulating discussions and many fruitful suggestions for this thesis. I am also grateful to Dr. Naomichi Hatano for useful comments and critically reading this manuscript. I also thank Dr. Akira Terai, Dr. Yoshihiko Nonomura and Mr. Keisuke Totsuka for useful comments and wish to thank all members of the research group under Professor M. Suzuki.

Numerical calculations were performed on the VAX 6440 of the Meson Science Laboratory, Faculty of Science, University of Tokyo, and the HITAC S-3800 in the Computer Center, University of Tokyo. In the numerical calculations reported in Section 3.3, we partly used subroutines of TIT-PACK Ver. 2 coded by Professor H. Nishimori.

Finally, I thank my parents for mental and financial support.

List of Papers Submitted for the Requirement of the Degree

1. T. Momoi and M. Suzuki: Ground-state properties and phase diagram of the quantum XXZ antiferromagnet on a triangular lattice, J. Phys. Soc. Jpn. **61**, 3732 (1992).

2. T. Momoi: Low-lying excited states of quantum antiferromagnets on a triangular lattice, J. Stat. Phys. **75**, 707 (1994).

3. T. Momoi: Symmetry breaking in quantum antiferromagnets on a triangular lattice, J. Magn. Magn. Mat. **140–144**, 1487 (1995).

4. T. Momoi: An upper bound for the spin-wave spectrum of the Heisenberg antiferromagnet, J. Phys. Soc. Jpn. **63**, 2507 (1994).

5. T. Momoi: Spectral properties and sum rules of the one-dimensional Hubbard model, Phys. Lett. A **195**, 351 (1994).

6. T. Momoi: Spectral properties of the Hubbard model, Physica B **206** & **207**, 160 (1995).

7. T. Momoi: Energy spectra of the Nambu-Goldstone modes in the Hubbard model, Phys. Lett. A **201**, 261 (1995).

Paper Added in Reference

1. T. Momoi and M. Suzuki: Vector chiral order in the quantum XXZ antiferromagnet on a triangular lattice analyzed with the super-effective-field theory, J. Phys. Soc. Jpn. **61**, 3277 (1992).

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Part I

Ground states

Chapter 1

General Introduction

1.1 Introduction

Motivation of the thesis

Quantum spin models on lattices have been attracting theoretical and experimental interests extensively, since they can describe various magnetic materials well. The interests in quantum spin systems extend from the aspects of material applications to purely statistical mechanical ones.

For *quantum antiferromagnets*, e.g. the Heisenberg model, it has been expected that quantum effects strongly appear at low temperatures and hence low-temperature properties may be quite different from those of the classical limit. Though the question has been long studied, understanding of *quantum antiferromagnets* from the statistical mechanical point of view is still subtle and progressing now. One of the reasons is that the models contain nontrivial quantum many-body problems, though the model Hamiltonians have simple forms. It is also because phase transitions can occur only in the infinite limit of system-size. For these reasons, we expect rigorous treatment to resolve the problem and we also need advanced approximate studies that give a reliable answer to delicate questions.

To understand properties of a system at low temperatures theoretically, we first need knowledge of ground-state properties of the Hamiltonian. We next need knowledge of elementary excitations in the system at $T = 0$. These are what we would like to discuss in the present thesis. In Part I, we study ground-state properties of quantum antiferromagnets on various lattices. We are especially interested in whether spontaneous breakdown of symmetries of the model Hamiltonian occurs in the thermodynamic limit. In Part II, we discuss natures of elementary excitations at $T = 0$. Throughout this thesis, we are consistently interested in the problem how quantum effects appear in physical properties of the relevant system.

Scope of the thesis

This thesis presents both exact and approximate results which have some bearing on low-temperature properties of quantum antiferromagnets. We consider only standard models with nearest-neighbor interactions. Our discussions are mainly based on rigorous results. These results occasionally provide a new physical insight and a fresh way of looking at a particular problem. Moreover, rigorous results sometimes serve as an aid to intuitive ideas, providing certain checks and standards of comparison for approximate arguments. However, there are sometimes limitations in rigorous studies for technical reasons. This is the case of quantum antiferromagnets on a triangular lattice. Then we give several approximate analyses, which will be reported in Chapter 3.

We will give a brief proof for rigorous results, if they are new or closely related to our own results. On the other hand, concerning well-established rigorous results, we may avoid being too nervous on mathematics. Furthermore, we omit studies on the infinite-volume states using C^*-algebras. However, since understanding of equilibrium states is very important in discussions about symmetry breaking, we sometimes refer to them without proof. (If the reader is seriously interested in rigorous quantum statistical mechanics, see the texts by Ruelle [126], and Bratteli and Robinson [19], for example.)

1.2 Models of quantum antiferromagnets

Here we present the model Hamiltonians treated in the present thesis. Various antiferromagnetic compounds are well described by the Heisenberg model. The Hamiltonian of the spin-S Heisenberg antiferromagnet on a finite lattice $\Lambda \subset \mathbf{Z}^d$ is given by

$$H_\Lambda = J \sum_{\langle i,j \rangle \in \Lambda} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z), \tag{1.1}$$

where the summation runs over all nearest-neighbor sites and S_i^α $(\alpha = x, y, z)$ denote spin operators at the site i that satisfy

$$[S_i^\alpha, S_j^\beta] = i\delta_{ij}\epsilon_{\alpha\beta\gamma} S_i^\gamma \tag{1.2}$$

with $\boldsymbol{S}^2 = S(S+1)$. This Hamiltonian (1.1) has the spin-$SU(2)$ symmetry. We also discuss the anisotropic Heisenberg model, *i.e.*, the XXZ model. The Hamiltonian of the spin-S XXZ antiferromagnet is given by

$$H_\Lambda = J \sum_{\langle i,j \rangle \in \Lambda} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z), \tag{1.3}$$

where $0 \le \lambda < 1$. This Hamiltonian has the spin-$O(1)$ symmetry.

1.3 Equilibrium states of quantum lattice systems

In this section we briefly summarize universal natures of the equilibrium states [126]. From the Hamiltonian H_Λ, the equilibrium state on the lattice Λ is obtained as

$$\omega_\Lambda(\cdots) = \frac{\mathrm{Tr}\cdots\exp(-\beta H_\Lambda)}{\mathrm{Tr}\exp(-\beta H_\Lambda)}. \tag{1.4}$$

This state is invariant under the time evolution; for any operators A, we have

$$\omega_\Lambda(A(t)) = \omega_\Lambda(A), \tag{1.5}$$

where

$$A(t) = \exp(itH_\Lambda)A\exp(-itH_\Lambda). \tag{1.6}$$

The state ω_Λ also satisfies *the Kubo-Martin-Schwinger condition*

$$\omega_\Lambda(AB(i\beta)) = \omega_\Lambda(BA) \tag{1.7}$$

for arbitrary operators A and B. Since we are interested in bulk properties of the system, we take the thermodynamic limit to make boundary effects of finite lattices disappear. Mathematically speaking, phase transitions can only occur in the thermodynamic limit. Hence we take the infinite-volume limit of ω_Λ and thereby obtain the equilibrium state

$$\omega(\cdots) = \lim_{\Lambda \nearrow \mathbf{Z}^d} \omega_\Lambda(\cdots). \tag{1.8}$$

Again the state $\omega(\cdots)$ satisfies conditions (1.5) and (1.7), where $A(t)$ denotes the time evolution of the local operator A in the thermodynamic limit.

When the system has a unique pure phase in the thermodynamic limit, the state ω is an ergodic state and has the cluster property

$$\lim_{|x| \nearrow \infty} \Big\{ \omega\Big(\alpha_x(A)B\Big) - \omega\Big(\alpha_x(A)\Big)\omega(B) \Big\} = 0 \tag{1.9}$$

for arbitrary local observables A and B, where α_x means the translation by x. On the other hand, if the state does not have the cluster property, there may be multiple phases.

Spontaneous symmetry breaking

In the case that a symmetry is broken, we obtain completely different states by changing a parameter of the Hamiltonian slightly and then taking the thermodynamic limit. Occurrence of the symmetry breaking depends on the dimensionality, the temperature and the symmetry of the Hamiltonian. Sometimes it is expected that the spin size, frustration effects and the connectivity of the lattice also affect the occurrence. We will discuss this subject in Chapters 2 and 3.

The interactions of the Hamiltonian are invariant under a large group G (for example $SU(2)$), and consequently the equilibrium state ω is invariant under G. If the symmetry breaking occurs, we obtain a state with broken symmetries and it has a symmetry H_α smaller than G. The symmetry breaking can be understood by writing ω as the superposition

$$\omega(\cdots) = \int d\alpha\omega_\alpha(\cdots), \tag{1.10}$$

where $\{\omega_\alpha\}$ are ergodic states with broken symmetries and the cluster property, and $d\alpha$ is the measure on G/H_α. It is expected that, if the symmetry is spontaneously broken, the symmetric mixed state ω is decomposed into ergodic states (or pure phases).

Chapter 2

Ground states of quantum antiferromagnets on bipartite lattices — rigorous results —

In this chapter, we briefly review rigorous results on ground-state properties of quantum antiferromagnets on hypercubic lattices. We also give our new results as Propositions. Section 2.1 contains correlation inequalities. The spin-correlation functions have been rigorously bounded from above and below. Since the correlation functions provide information about the strength of both long-range correlations and fluctuations, one can prove or rule out the existence of the antiferromagnetic long-range order using these inequalities. We discuss the absence of the long-range order in one-dimensional systems in Section 2.2, and symmetry breaking in two- and higher-dimensional systems in Section 2.3. In Section 2.3.2, we show that various physical quantities have classical values in the large-S limit. Section 2.4 contains exact results on the ground state and low-lying excited states of a finite-volume system. The rigorous inequalities given in this chapter will be used again in Part II of this thesis. Thus the contents of the present chapter also give an introduction to the following chapters.

2.1 Correlation inequalities

Here, we review useful rigorous inequalities. Using these inequalities, one can derive rigorous bounds for the spin-correlation functions of the Heisenberg and XXZ antiferromagnets on a hypercubic lattice. We discuss the correlation functions both in the pure ground state and in the symmetric (or mixed) one.

Let H denote the Hamiltonian. The thermal average is given by

$$\langle B \rangle = \frac{\mathrm{Tr}[B \exp(-\beta H)]}{\mathrm{Tr}\exp(-\beta H)} \tag{2.1}$$

for an arbitrary operator B. We discuss the following two correlation functions: The direct correlation function

$$\frac{1}{2}\langle AC + CA \rangle \tag{2.2}$$

and Kubo's canonical correlation function (or the Duhamel two-point function)

$$\beta(A, C) = \int_0^\beta d\lambda \langle e^{\lambda H} A e^{-\lambda H} C \rangle. \tag{2.3}$$

First we give various useful inequalities and mathematical preparations in Sections 2.1.1–2.1.3. Then, in Section 2.1.4, we show upper and lower bounds for the spin correlation functions of the Heisenberg and XXZ antiferromagnets at $T = 0$.

2.1.1 Bogoliubov inequality and it's extension to $T = 0$

We start from the Bogoliubov inequality and it's extension to $T = 0$. Bogoliubov first gave lower bounds for the correlation functions [17].

Theorem 2.1.1. (Bogoliubov): Let A and C be arbitrary operators. Then we have

$$|\langle [A, C] \rangle|^2 \leq \beta(\Delta A^\dagger, \Delta A) \cdot \langle [[C^\dagger, H], C] \rangle, \tag{2.4}$$

where $\Delta A = A - \langle A \rangle$, and the square brackets denote the commutator, $[A, C] = AC - CA$.

Theorem 2.1.2. (Bogoliubov): Let A and C be arbitrary operators. Then we have

$$|\langle [A, C] \rangle|^2 \leq \frac{\beta}{2} \langle \{\Delta A^\dagger, \Delta A\} \rangle \cdot \langle [[C^\dagger, H], C] \rangle, \tag{2.5}$$

where $\{A, C\} = AC + CA$.

Mermin and Wagner [94], and Hohenberg [47] used (2.5) to rule out spontaneous symmetry breaking at finite temperatures in one- and two-dimensional systems with continuous symmetries. This inequality is, however, powerless for systems at $T = 0$. Then we need other inequalities that give lower bounds of the correlation functions at $T = 0$. An example is the uncertainty relation [127, 122]:

Theorem 2.1.3. (Uncertainty relation): Let A and C be arbitrary operators. Then we have

$$|\langle [A, C] \rangle|^2 \leq \langle \{\Delta A^\dagger, \Delta A\} \rangle \cdot \langle \{\Delta C^\dagger, \Delta C\} \rangle. \tag{2.6}$$

This fundamental relation describes quantum fluctuations at arbitrary temperatures. Recently, Pitaevskii and Stringari [122] used this relation to obtain lower bounds of the correlation functions at $T = 0$. Moreover, extending the uncertainty relation, Shastry [129] showed the following inequality:

Theorem 2.1.4. (Shastry): Let A and C be arbitrary operators. Then we have

$$|\langle [A, C] \rangle|^2 \leq \langle \{\Delta C^\dagger, \Delta C\} \rangle \sqrt{\langle [[A^\dagger, H], A] \rangle \cdot \beta(\Delta A^\dagger, \Delta A)} \tanh \left\{ \frac{\beta}{2} \left[\frac{\langle [[A^\dagger, H], A] \rangle}{\beta(\Delta A^\dagger, \Delta A)} \right]^{1/2} \right\}. \tag{2.7}$$

This inequality also corresponds to an extension of the Bogoliubov inequality to $T = 0$. This inequality works even at $T = 0$. Using this inequality, Pitaevskii and Stringari [122], and Shastry [129] showed the absence of the long-range order in the ground state of the one-dimensional Heisenberg antiferromagnet. (See Section 2.2.)

In the rest of this subsection, we show a proof for these inequalities (2.4)–(2.7). Let us consider the following two-point spectral function

$$p_{A,C}(\omega) = \frac{1}{Z}\sum_{m,n}\{\exp(-\beta E_m) + \exp(-\beta E_n)\}\langle m|A|n\rangle\langle n|C|m\rangle\delta(\omega - E_n + E_m), \tag{2.8}$$

where $Z = \mathrm{Tr}\exp(-\beta H)$, and $\{|m\rangle\}$ denote the eigenstates of the Hamiltonian with the eigenvalues $\{E_m\}$. This function (2.8) is the spectral representation of the time-correlation function $\langle\{A(t), C\}\rangle$, where $A(t) = \exp(iHt)A\exp(-iHt)$. It satisfies the following convenient frequency-sum rules [143, 48]:

$$\begin{aligned}
\int_{-\infty}^{\infty} d\omega \tanh\frac{\beta\omega}{2} p_{A,C}(\omega) &= \frac{1}{Z}\sum_{m,n}\{\exp(-\beta E_m) - \exp(-\beta E_n)\}\langle m|A|n\rangle\langle n|C|m\rangle \\
&= \langle [A, C]\rangle, && (2.9)\\
\int_{-\infty}^{\infty} d\omega \frac{\tanh(\beta\omega/2)}{\omega} p_{A,C}(\omega) &= \frac{1}{Z}\sum_{m,n}\frac{\exp(-\beta E_m) - \exp(-\beta E_n)}{E_n - E_m}\langle m|A|n\rangle\langle n|C|m\rangle \\
&= \beta(A, C), && (2.10)\\
\int_{-\infty}^{\infty} d\omega \cdot \omega \tanh\frac{\beta\omega}{2} p_{A,C}(\omega) &= \frac{1}{Z}\sum_{m,n}\{\exp(-\beta E_m) - \exp(-\beta E_n)\}(E_n - E_m)\langle m|A|n\rangle\langle n|C|m\rangle \\
&= \langle [[A, H], C]\rangle, && (2.11)\\
\int_{-\infty}^{\infty} d\omega p_{A,C}(\omega) &= \frac{1}{Z}\sum_{m,n}\{\exp(-\beta E_m) + \exp(-\beta E_n)\}\langle m|A|n\rangle\langle n|C|m\rangle \\
&= \langle\{A, C\}\rangle. && (2.12)
\end{aligned}$$

Using (2.8), we can prove Theorems 2.1.1–2.1.4 as follows.

Proof of Theorem 2.1.1. Let us define the functional

$$(f(\omega)A, g(\omega)B) \equiv \int d\omega f^\dagger(\omega)g(\omega)p_{A^\dagger,B}(\omega) \tag{2.13}$$

for elements in the tensor-product space $\mathcal{F}\otimes\mathcal{A}$, where $\mathcal{F}$ denotes the space of the functions of ω, and $\mathcal{A}$ denotes the space of the operators. Equation (2.13) satisfies the definition of the inner product as follows.

1) $(f(\omega)A, f(\omega)A) = \int d\omega|f(\omega)|^2 p_{A^\dagger,A}(\omega) \geq 0,$

2) $(\lambda f(\omega)A, g(\omega)B) = \lambda^*(f(\omega)A, g(\omega)B),$

3) $(f(\omega)A + g(\omega)B, h(\omega)C) = (f(\omega)A, h(\omega)C) + (g(\omega)B, h(\omega)C),$

for arbitrary $f(\omega)A$, $g(\omega)B$ and $h(\omega)C$ in $\mathcal{F}\otimes\mathcal{A}$. We hence have the Schwarz inequality

$$\left|\int_{-\infty}^{\infty} d\omega f^{\dagger}(\omega)g(\omega)p_{A^{\dagger},C}(\omega)\right|^{2} \leq \int_{-\infty}^{\infty} d\omega|f(\omega)|^{2}p_{A^{\dagger},A}(\omega)\cdot\int_{-\infty}^{\infty} d\omega|g(\omega)|^{2}p_{C^{\dagger},C}(\omega). \quad (2.14)$$

Inserting $f(\omega)=\sqrt{\tanh(\beta\omega/2)/\omega}$ and $g(\omega)=\sqrt{\omega\tanh(\beta\omega/2)}$ in (2.14), we obtain

$$|\langle[A,C]\rangle|^{2} \leq \beta(A^{\dagger},A)\langle[[C^{\dagger},H],C]\rangle, \quad (2.15)$$

where we have used the sum rules (2.9)–(2.11). Transforming the operator A into ΔA and using the relation $[\Delta A, C]=[A,C]$, we obtain (2.4). ■

Proof of Theorem 2.1.2. First, note that

$$\tanh x \leq x \quad (2.16)$$

for $x \geq 0$. Inserting $x=\beta(E_n-E_m)/2$ into (2.16) and using the sum rules (2.10) and (2.12), we have

$$\beta(\Delta A^{\dagger},\Delta A) \leq \frac{\beta}{2}\langle\{\Delta A^{\dagger},\Delta A\}\rangle. \quad (2.17)$$

Then, we obtain (2.5), using (2.4) and (2.17). ■

Proof of Theorem 2.1.3. When $f(\omega)=\tanh(\beta\omega/2)$ and $g(\omega)=1$ in (2.14), we have

$$|\langle[A,C]\rangle|^{2} \leq \langle\{C^{\dagger},C\}\rangle\int_{-\infty}^{\infty} d\omega\tanh^{2}\frac{\beta\omega}{2}p_{A^{\dagger},A}(\omega), \quad (2.18)$$

where we have used the sum rules (2.9) and (2.12). Since the function $p_{A^{\dagger},A}(\omega)$ is a summation of the delta functions with positive coefficients, the integration with respect to ω conserves the inequality of the integrand as

$$\int_{-\infty}^{\infty} d\omega\tanh^{2}\frac{\beta\omega}{2}p_{A^{\dagger},A}(\omega) \leq \int_{-\infty}^{\infty} d\omega p_{A^{\dagger},A}(\omega). \quad (2.19)$$

Hence (2.18) becomes

$$|\langle[A,C]\rangle|^{2} \leq \langle\{C^{\dagger},C\}\rangle\cdot\langle\{A^{\dagger},A\}\rangle. \quad (2.20)$$

Transforming A into ΔA and C into ΔC, we have (2.6) ■

Proof of Theorem 2.1.4. Let us consider (2.18). The integration in the right-hand side of (2.18) is rewritten in the from

$$\int_{-\infty}^{\infty} d\omega\tanh^{2}\frac{\beta\omega}{2}p_{A^{\dagger},A}(\omega) = \int_{0}^{\infty} d\omega\tanh^{2}\frac{\beta\omega}{2}\Big\{p_{A^{\dagger},A}(\omega)+p_{A,A^{\dagger}}(\omega)\Big\}. \quad (2.21)$$

We define the positive measure $d\mu(\omega)$ by

$$d\mu(\omega) = \tanh\frac{\beta\omega}{2}\Big\{p_{A^{\dagger},A}(\omega)+p_{A,A^{\dagger}}(\omega)\Big\}. \quad (2.22)$$

Applying Jensen's inequality to the convex function $\tanh x$, we obtain

$$\int_0^\infty \tanh \frac{\beta\omega}{2} d\mu(\omega) \Big/ \int_0^\infty d\mu(\omega) < \tanh \left[\beta \int_0^\infty \omega d\mu(\omega) \Big/ 2 \int_0^\infty d\mu(\omega)\right]. \tag{2.23}$$

From the Schwarz inequality we have

$$\int_0^\infty d\mu(\omega) < \left[\int_0^\infty \omega d\mu(\omega) \int_0^\infty \omega^{-1} d\mu(\omega)\right]^{1/2} = \left\{\langle[[A^\dagger, H], A]\rangle \cdot \beta(A^\dagger, A)\right\}^{1/2}, \tag{2.24}$$

where we have used the sum rules (2.10) and (2.11). We arrive at (2.7), using (2.18), (2.21), (2.23) and (2.24). ■

2.1.2 Falk–Bruch inequality

Another useful inequality was derived by Falk and Bruch [31]. This inequality gives an upper bound for $\langle\{A^\dagger, A\}\rangle$.

Theorem 2.1.5. (Falk and Bruch): Let A be an arbitrary operator. Then we have

$$\beta(A^\dagger, A) \geq \beta\langle\{A^\dagger, A\}\rangle \frac{\tanh y}{2y}, \tag{2.25}$$

where y is the solution of

$$y \tanh y = \frac{\beta\langle[[A^\dagger, H], A]\rangle}{2\langle\{A^\dagger, A\}\rangle}. \tag{2.26}$$

Proof of Theorem 2.1.5. Let x be the variable defined by

$$x = y \tanh y = \frac{\beta\langle[[A^\dagger, H], A]\rangle}{2\langle\{A^\dagger, A\}\rangle}. \tag{2.27}$$

Then, y is a function of x. We consider the function

$$f(x) = \frac{1}{y} \tanh y, \tag{2.28}$$

which is well-defined, monotone-decreasing and convex with respect to x in the region $(0, \infty)$. (See Ref. [27].) Clearly, the function f satisfies

$$f(y \tanh y) = \frac{1}{y} \tanh y. \tag{2.29}$$

In order to transform the function $f(x)$, we next consider the function

$$\begin{aligned} h(x) &= \frac{1}{Z} \mathrm{Tr}[A^\dagger e^{-xH} A e^{-(\beta-x)H}] \\ &= \frac{1}{Z} \sum_{m,n} |\langle n|A|m\rangle|^2 \exp[-\beta E_m + x(E_m - E_n)]. \end{aligned} \tag{2.30}$$

The final equation means that $h(x)$ is a Laplace transform of a positive measure $d\mu(t)$,

$$h(x) = \int e^{xt} d\mu(t). \tag{2.31}$$

Using this measure, the correlation functions and the double commutator can be written as

$$\begin{aligned} \langle\{A^\dagger, A\}\rangle &= h(\beta) + h(0) = \int (e^{\beta t} + 1) d\mu(t), && (2.32)\\ \beta(A^\dagger, A) &= \int_0^\beta h(x)dx = \int \frac{1}{t}(e^{\beta t} - 1) d\mu(t), && (2.33)\\ \langle[[A^\dagger, H], A]\rangle &= h'(\beta) - h'(0) = \int t(e^{\beta t} - 1) d\mu(t). && (2.34) \end{aligned}$$

Thus we rewrite the variable x in the form

$$x = \beta \int t(e^{\beta t} - 1) d\mu(t) \Big/ 2 \int (e^{\beta t} + 1) d\mu(t). \tag{2.35}$$

Let $d\nu(t)$ be the measure such that

$$d\nu(t) = (e^{\beta t} + 1) d\mu(t) \Big/ \int (e^{\beta t} + 1) d\mu(t). \tag{2.36}$$

Then we have

$$x = \frac{\beta}{2} \int t \tanh \frac{\beta t}{2} d\nu(t). \tag{2.37}$$

Since $f(x)$ is convex and $d\nu(t)$ is a probability measure, we have

$$\begin{aligned} f(x) &= f\left(\int \frac{\beta t}{2} \tanh \frac{\beta t}{2} d\nu(t)\right) \le \int f\left(\frac{\beta t}{2} \tanh \frac{\beta t}{2}\right) d\nu(t) \\ &= \int \frac{2}{\beta t} \tanh \frac{\beta t}{2} d\nu(t) = \frac{2\beta(A^\dagger, A)}{\beta\langle\{A^\dagger, A\}\rangle}, && (2.38) \end{aligned}$$

where we have used Jensen's inequality. ■

In the zero-temperature limit, Theorem 2.1.5 is reduced to the following form.

Theorem 2.1.6. (Kennedy, Lieb and Shastry): Let A be an arbitrary operator. Then the inequality

$$\langle 0|\{\Delta A, \Delta A^\dagger\}|0\rangle^2 \le \chi_A^{T=0} \cdot \langle 0|[[A^\dagger, H], A]|0\rangle \tag{2.39}$$

holds at $T = 0$, where $|0\rangle$ denotes the ground state and $\chi_A^{T=0} = \lim_{\beta \nearrow \infty} \beta(\Delta A^\dagger, \Delta A)$.

Let us consider the spectral function

$$S_{A,C}(\omega) \equiv \sum_n \{\langle 0|A|n\rangle\langle n|C|0\rangle + \langle 0|C|n\rangle\langle n|A|0\rangle\}\delta(\omega - E_n + E_0). \tag{2.40}$$

This spectral function satisfies the following useful sum rules [48, 68]:

$$\int_{-\infty}^{\infty} d\omega S_{A,C}(\omega) = \langle 0|\{A,C\}|0\rangle, \tag{2.41}$$

$$\int_{-\infty}^{\infty} d\omega \omega^{-1} S_{A,C}(\omega) = \lim_{\beta\nearrow\infty} \beta(A,C), \tag{2.42}$$

$$\int_{-\infty}^{\infty} d\omega \omega S_{A,C}(\omega) = \langle 0|[[A,H],C]|0\rangle. \tag{2.43}$$

Here we show a brief and straightforward proof of Theorem 2.1.6 by Kennedy, Lieb and Shastry [68].

Proof of Theorem 2.1.6. The functional

$$(f(\omega), g(\omega)) = \int_{-\infty}^{\infty} d\omega f^{\dagger}(\omega) g(\omega) S_{\Delta A^{\dagger},\Delta A}(\omega) \tag{2.44}$$

satisfies the definition of the inner product, and hence it satisfies the Schwarz inequality

$$\left|\int_{-\infty}^{\infty} d\omega f^{\dagger}(\omega) g(\omega) S_{\Delta A^{\dagger},\Delta A}(\omega)\right|^2 \\ \leq \int_{-\infty}^{\infty} d\omega |f(\omega)|^2 S_{\Delta A^{\dagger},\Delta A}(\omega) \cdot \int_{-\infty}^{\infty} d\omega |g(\omega)|^2 S_{\Delta A^{\dagger},\Delta A}(\omega). \tag{2.45}$$

Inserting $f(\omega) = \sqrt{\omega}$ and $g(\omega) = 1/\sqrt{\omega}$ in (2.45) and using the sum rules (2.41)–(2.43) we have (2.39). ■

2.1.3 Dyson–Lieb–Simon inequality (Gaussian domination)

Theorems 2.1.1–2.1.6 are applicable to a wide class of quantum lattice systems, *i.e.*, to arbitrary quantum models on arbitrary lattices. From these inequalities, however, we cannot obtain any upper bound for the Duhamel two-point function $\beta(\Delta A^{\dagger}, \Delta A)$. Up to now, upper bounds of $\beta(\Delta A^{\dagger}, \Delta A)$ are obtained for limited models, which include the quantum antiferromagnets on d-dimensional $L \times \cdots \times L$ hypercubic lattices $\Lambda \subset \mathbf{Z}^d$. We consider the spin-$S$ Heisenberg antiferromagnet. The Hamiltonian is given by

$$H_\Lambda = J \sum_{\langle i,j\rangle \in \Lambda} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z), \tag{2.46}$$

where $J > 0$ and the summation runs over all nearest-neighbor sites. We also consider the spin-S XXZ antiferromagnet,

$$H_\Lambda = J \sum_{\langle i,j\rangle \in \Lambda} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z), \tag{2.47}$$

where $J > 0$ and $0 \leq \lambda < 1$. For these models, we are interested in the spin correlations $\beta(S_{-k}^{\alpha}, S_k^{\alpha})$ and $\langle\{S_{-k}^{\alpha}, S_k^{\alpha}\}\rangle/2$, where $S_k^{\alpha} = L^{-d/2}\sum_{j\in\Lambda} S_j^{\alpha} \exp(ikr_j)$ for $\alpha = x$, y and z.

Dyson, Lieb and Simon [27] first obtained an upper bound of $\beta(S_{-k}^{\alpha}, S_k^{\alpha})$. We show the upper bound in the following.

Let us consider the XXZ model on the lattice Λ with a staggered magnetic field. The Hamiltonian is defined by

$$H_\Lambda(B) = J \sum_{\langle i,j\rangle\in\Lambda} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z) - B\mathcal{O}_\Lambda, \tag{2.48}$$

where $0 \le \lambda \le 1$, and $\mathcal{O}_\Lambda$ denotes the order-parameter operator

$$\mathcal{O}_\Lambda = \sum_{i\in A} S_i^x - \sum_{i\in B} S_i^x. \tag{2.49}$$

The thermal average is given by

$$\langle A\rangle_{\Lambda,B}^T = \frac{\mathrm{Tr}[A\exp\{-\beta H_\Lambda(B)\}]}{\mathrm{Tr}\exp\{-\beta H_\Lambda(B)\}}. \tag{2.50}$$

Theorem 2.1.7. (Dyson, Lieb and Simon): Let $H_\Lambda(B)$ be the Hamiltonian defined by (2.48). Then, for arbitrary values of B, we have

$$\beta(S_{-k}^\alpha, S_k^\alpha)_{\Lambda,B} \le \frac{1}{2Jd(1+\gamma_k)} \qquad (\alpha = x, y), \tag{2.51}$$

$$\beta(S_{-k}^z, S_k^z)_{\Lambda,B} \le \frac{1}{2J\lambda d(1+\gamma_k)}, \tag{2.52}$$

where

$$\beta(A,C)_{\Lambda,B} = \int_0^\beta d\lambda\,\langle A\exp\{-\lambda H_\Lambda(B)\}C\exp\{\lambda H_\Lambda(B)\}\rangle_{\Lambda,B}^T \tag{2.53}$$

and

$$\gamma_k = \frac{1}{d}\sum_{\nu=1}^{d}\cos k_\nu. \tag{2.54}$$

Since the proof of this theorem is very complicated, we only show its brief sketch. (If the reader is seriously interested in the proof, see the original paper [27].) The important step by Dyson *et al.* is an extension of the method by Fröhlich, Simon and Spencer [35]. Fröhlich *et al.* used the following inequality in the proof of the classical cases:

$$\begin{aligned}&\left\{\int \exp[-(x-y-a)^2]d\mu(x)d\nu(y)\right\}^2\\ &\quad\le \int \exp[-(x-y)^2]d\mu(x)d\mu(y)\cdot\int \exp[-(x-y)^2]d\nu(x)d\nu(y),\end{aligned} \tag{2.55}$$

where $d\mu$ and $d\nu$ denote measures. This inequality was extended to the quantum case by Dyson *al et.* in the following form.

Lemma 2.1.8. (Gaussian domination): Let $\mathcal{H}_1$ be a finite-dimensional vector space and let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_1$. Let A be the operator $A_1 \otimes 1$ and $\tilde{A}$ be $1 \otimes A_1$ for an arbitrary operator A_1 on $\mathcal{H}_1$. Then for arbitrary self-adjoint operators A, B, $C_1, \cdots, C_l$ with real matrix representations and for arbitrary real numbers $h_1, \cdots, h_l$, we have

$$\begin{aligned}&\left(\mathrm{Tr}\left\{\exp\left[A + \tilde{B} - \sum_{i=1}^{l}(C_i - \tilde{C}_i - h_i)^2\right]\right\}\right)^2 \\ &\quad \le \mathrm{Tr}\left\{\exp\left[A + \tilde{A} - \sum_{i=1}^{l}(C_i - \tilde{C}_i)^2\right]\right\} \cdot \mathrm{Tr}\left\{\exp\left[B + \tilde{B} - \sum_{i=1}^{l}(C_i - \tilde{C}_i)^2\right]\right\}. \qquad (2.56)\end{aligned}$$

We only introduce this lemma without any proof. This lemma is applicable to antiferromagnetic quantum spin systems that have the “bond-reflection symmetry”; namely, the lattice is invariant under the reflection with a flat plane that only cuts bonds and divides the lattice into two lattices. Using this lemma, Theorem 2.1.7 can be derived [27].

Remark: Theorem 2.1.7 is not exactly equal to what was obtained by Dyson, Lieb and Simon. They only discussed the system without any magnetic field. We, however, find that their theorems and lemmas are applicable to the Hamiltonian $H_\Lambda(B)$ in (2.48) as well.

Note that, if the system has a Néel order in the thermodynamic limit, the susceptibility $\lim_{\Lambda \nearrow \mathbf{Z}^d} \beta(S^\alpha_{-k}, S^\alpha_k)_{\Lambda,B}$ would discretely change depending on B at $B = 0$. However, the bounds (2.51) and (2.52) do not depend on B. This indicates that these bounds are not optimal ones.

Using Theorems 2.1.5 and 2.1.7, Dyson, Lieb and Simon proved the existence of the antiferromagnetic long-range order in the three-dimensional Heisenberg antiferromagnet at sufficiently low temperatures [27]. After that, extending this proof, Jordão-Neves and Fernando-Perez [60] proved the long-range order in the two-dimensional system at the zero temperature. Further discussions about ground-state properties are given in Section 2.3. Owing to the applicability of Theorem 2.1.7, we can obtain rigorous proofs only for systems on lattices that have *the bond-reflection symmetry*. Thus we cannot apply this theorem to models on a triangular lattice or on a kagomé lattice. Recently, using Lemma 2.1.8, Kubo and Kishi obtained bounds for the Duhamel two-point functions of the quantum antiferromagnets on the square lattice with next-nearest-neighbor antiferromagnetic interactions, *i.e.*, the so-called J_1–J_2 model [70], and in the negative-U Hubbard model on arbitrary lattices [76].

2.1.4 Bounds of correlation functions at $T = 0$

Here we show bounds of the correlation functions in the ground states of the Heisenberg and XXZ antiferromagnets. Using the rigorous bounds given in the previous three subsections, we can obtain upper and lower bounds of the spin correlation functions. As the ground states, we consider the pure (or ergodic) states and a symmetric (or mixed) state. One of the pure ground states is given by

$$\langle \cdots \rangle_x^{T=0} = \lim_{B \searrow 0} \lim_{\Lambda \nearrow \mathbf{Z}^d} \lim_{\beta \nearrow \infty} \frac{\mathrm{Tr}[\cdots \exp\{-\beta H_\Lambda(B)\}]}{\mathrm{Tr}\exp\{-\beta H_\Lambda(B)\}}$$

$$= \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\lim_{\beta\nearrow\infty}\langle\cdots\rangle_{\Lambda,B}^{T}. \tag{2.57}$$

Because the physical equilibrium state is one of the pure (or ergodic) states, we are interested in the correlation functions in the pure state (2.57). On the other hand, in numerical studies of finite-size systems the ground state becomes a symmetric state, which is defined by

$$\langle\cdots\rangle_0^{T=0} = \lim_{\Lambda\nearrow \mathbf{Z}^d}\lim_{\beta\nearrow\infty}\frac{\mathrm{Tr}[\cdots\exp(-\beta H_\Lambda)]}{\mathrm{Tr}\exp(-\beta H_\Lambda)}. \tag{2.58}$$

(See Section 2.4.) For comparison with numerical studies, it is useful to discuss quantities in the symmetric ground state.

We first discuss the correlation functions in the pure state at $T=0$, which are given by

$$S^{\|}(k) = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\lim_{\beta\nearrow\infty}\left\langle \Delta S_{-k}^x \Delta S_k^x\right\rangle_{\Lambda,B}^T, \tag{2.59}$$

$$S_\alpha^{\perp}(k) = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\lim_{\beta\nearrow\infty}\left\langle S_{-k}^\alpha S_k^\alpha\right\rangle_{\Lambda,B}^T \tag{2.60}$$

and

$$\chi^{\|}(k) = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\lim_{\beta\nearrow\infty}\int_0^\beta d\lambda\left\langle \Delta S_{-k}^x\exp\{-\lambda H_\Lambda(B)\}\Delta S_k^x\exp\{\lambda H_\Lambda(B)\}\right\rangle_{\Lambda,B}^T, \tag{2.61}$$

$$\chi_\alpha^{\perp}(k) = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\lim_{\beta\nearrow\infty}\int_0^\beta d\lambda\left\langle S_{-k}^\alpha\exp\{-\lambda H_\Lambda(B)\}S_k^\alpha\exp\{\lambda H_\Lambda(B)\}\right\rangle_{\Lambda,B}^T \tag{2.62}$$

for $\alpha = y$ and z, where $\Delta S_k^x = S_k^x - \langle S_k^x\rangle_{\Lambda,B}^T$. Using Theorems 2.1.1–2.1.8, we can obtain both upper and lower bounds of these correlation functions.

Theorem 2.1.9. In the pure ground state, the Duhamel two-point functions (2.61) and (2.62) satisfy

$$0 \le \chi^{\|}(k) \le \frac{1}{2Jd(1+\gamma_k)}, \tag{2.63}$$

$$\frac{m_{\mathrm{s}}^2}{2Jd(\rho_x+\rho_y)(1+\gamma_k)} \le \chi_y^{\perp}(k) \le \frac{1}{2Jd(1+\gamma_k)}, \tag{2.64}$$

$$\frac{m_{\mathrm{s}}^2}{2Jd\{\rho_x(1+\lambda\gamma_k)+\rho_z(\lambda+\gamma_k)\}} \le \chi_z^{\perp}(k) \le \frac{1}{2J\lambda d(1+\gamma_k)}, \tag{2.65}$$

where

$$\gamma_k = \frac{1}{d}\sum_{\nu=1}^d \cos k_\nu, \tag{2.66}$$

$$m_{\mathrm{s}} = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\frac{1}{L^d}\langle\mathcal{O}_\Lambda\rangle_{\Lambda,B}^{T=0}, \tag{2.67}$$

$$\rho_\alpha = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\frac{1}{L^d d}\sum_{\langle i,j\rangle\in\Lambda}\left\langle -S_i^\alpha S_j^\alpha\right\rangle_{\Lambda,B}^{T=0} \tag{2.68}$$

for $\alpha = x$, y and z.

Proof of Theorem 2.1.9. The left-hand-side inequalities of (2.63)–(2.65) are derived from Theorem 2.1.1: Considering (2.14) at $T = 0$, taking the Hamiltonian as $H_\Lambda(B)$ and setting $A_k = S_k^y$ and $C = S_{Q-k}^z$ with $Q = (\pi, \cdots, \pi)$, we have

$$\langle [A, C] \rangle_{\Lambda,B}^{T=0} = \frac{1}{L^d} \langle \mathcal{O}_\Lambda \rangle_{\Lambda,B}^{T=0} \tag{2.69}$$

and

$$\left\langle [[C^\dagger, H], C] \right\rangle_{\Lambda,B}^{T=0} = \frac{2J}{L^d} \sum_{\langle i,j \rangle \in \Lambda} \left\langle -S_i^x S_j^x - S_i^y S_j^y \right\rangle_{\Lambda,B}^{T=0} (1 + \gamma_k) + \frac{B}{L^d} \langle \mathcal{O}_\Lambda \rangle_{\Lambda,B}^{T=0}. \tag{2.70}$$

In the thermodynamic limit under the infinitesimally small staggered field, we obtain

$$\lim_{B \searrow 0} \lim_{\Lambda \nearrow \mathbf{Z}^d} \langle [A, C] \rangle_{\Lambda,B}^{T=0} = m_{\mathrm{s}} \tag{2.71}$$

$$\lim_{B \searrow 0} \lim_{\Lambda \nearrow \mathbf{Z}^d} \left\langle [[C^\dagger, H], C] \right\rangle_{\Lambda,B}^{T=0} = 2Jd(\rho_x + \rho_y)(1 + \gamma_k). \tag{2.72}$$

Thus we arrive at the first inequality of (2.64). In the same way, taking $A_k = S_k^x$ and $C = S_{Q-k}^y$, we obtain the first inequality of (2.63). Furthermore, setting $A_k = S_k^z$ and $C = S_{Q-k}^y$, we have

$$\lim_{B \searrow 0} \lim_{\Lambda \nearrow \mathbf{Z}^d} \left\langle [[C^\dagger, H], C] \right\rangle_{\Lambda,B}^{T=0} = 2Jd\{\rho_x(1 + \lambda\gamma_k) + \rho_z(\lambda + \gamma_k)\}, \tag{2.73}$$

and hence the first inequality of (2.65). The right-hand-side inequalities are derived straight from Theorem 2.1.7. ■

In the Heisenberg antiferromagnet, or $\lambda = 1$, $\chi_y^\perp(k)$ and $\chi_z^\perp(k)$ are equal to each other and are called the perpendicular susceptibility $\chi^\perp(k)$. The correlation function $\chi^\parallel(k)$ is the parallel susceptibility. Both the upper and lower bounds of $\chi^\perp(k)$ in (2.64) have the same momentum dependence. If $0 \leq \lambda < 1$, on the other hand, the upper and lower bounds of the perpendicular susceptibility have different momentum dependence.

Theorem 2.1.10. In the pure ground state, the spin correlations (2.59) and (2.60) satisfy

$$0 \leq S^\parallel(k) \leq \frac{1}{2}\sqrt{\frac{\rho_y(1 - \lambda\gamma_k) + \rho_z(\lambda - \gamma_k)}{(1 + \gamma_k)}}, \tag{2.74}$$

$$\frac{m_{\mathrm{s}}^2}{2}\sqrt{\frac{\lambda(1 - \gamma_k)}{(\rho_x + \rho_y)(1 + \gamma_k)}} \leq S_y^\perp(k) \leq \frac{1}{2}\sqrt{\frac{\rho_x(1 - \lambda\gamma_k) + \rho_z(\lambda - \gamma_k)}{(1 + \gamma_k)}}, \tag{2.75}$$

$$\frac{m_{\mathrm{s}}^2}{2}\sqrt{\frac{1 - \gamma_k}{\rho_x(1 + \lambda\gamma_k) + \rho_z(\lambda + \gamma_k)}} \leq S_z^\perp(k) \leq \frac{1}{2}\sqrt{\frac{(\rho_x + \rho_y)(1 - \gamma_k)}{\lambda(1 + \gamma_k)}}. \tag{2.76}$$

Proof of Theorem 2.1.10. The left-hand-side inequalities are derived from Theorem 2.1.4: At $T=0$, equation (2.7) becomes

$$\left|\langle [A,C]\rangle_{\Lambda,B}^{T=0}\right|^2 \le \left\langle \{\Delta C^\dagger, \Delta C\}\right\rangle_{\Lambda,B}^{T=0} \sqrt{\langle [[A^\dagger, H], A]\rangle_{\Lambda,B}^{T=0} \cdot \chi_A^{T=0}}, \tag{2.77}$$

where $\chi_A^{T=0} = \lim_{\beta\nearrow\infty} \beta(\Delta A^\dagger, \Delta A)$. Setting $A_k = S^z_{k+Q}$ and $C = S^y_{-k}$, and taking the thermodynamic limit $\lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\langle\cdots\rangle_{\Lambda,B}^{T=0}$, we obtain the first inequality of (2.75). In the same way, taking $A_k = S^y_{k+Q}$ and $C = S^z_{-k}$, we have the first inequality of (2.76) and, setting $A_k = S^y_{k+Q}$ and $C = S^x_{-k}$, we have the first inequality of (2.74). The second inequalities are obtained by combining Theorems 2.1.6 and 2.1.9. ■

In the Heisenberg model ($\lambda = 1$), we have $S_y^\perp(k) = S_z^\perp(k)$ because of the isotropy of the model. The correlation function $S_\alpha^\perp(k)$ is called the perpendicular structure factor $S^\perp(k)$, and $S^\parallel(k)$ is the parallel structure factor. Both the upper and lower bounds of $S^\perp(k)$ have the same momentum dependence. For $0 \le \lambda < 1$, however, the upper and lower bounds of the perpendicular structure factor have different momentum dependence.

In the rest of this subsection, we discuss the correlation functions in the symmetric ground state (2.58),

$$S_\alpha(k) = \lim_{\Lambda\nearrow\mathbf{Z}^d}\lim_{\beta\nearrow\infty}\left\langle S^\alpha_{-k} S^\alpha_k\right\rangle^T_{\Lambda,B=0} \tag{2.78}$$

and

$$\chi_\alpha(k) = \lim_{\Lambda\nearrow\mathbf{Z}^d}\lim_{\beta\nearrow\infty}\int_0^\beta d\lambda \left\langle S^\alpha_{-k}\exp(-\lambda H_\Lambda) S^\alpha_k \exp(\lambda H_\Lambda)\right\rangle^T_{\Lambda,B=0} \tag{2.79}$$

for $\alpha = x$, y and z. Note that, if the symmetry is not spontaneously broken, there exists only one pure (or ergodic) state in the thermodynamic limit and hence there is no difference between the correlation functions (2.59) [or (2.60)] and (2.78), and between (2.61), (2.62) and (2.79).

We give correlation inequalities of the symmetric ground state in the following.

Theorem 2.1.11. In the symmetric ground state, the Duhamel two-point functions (2.79) satisfy

$$\chi_\alpha(k) \le \frac{1}{2Jd(1+\gamma_k)} \qquad (\alpha = x, y), \tag{2.80}$$

$$\chi_z(k) \le \frac{1}{2J\lambda d(1+\gamma_k)}. \tag{2.81}$$

Proof of Theorem 2.1.11. Equations (2.80) and (2.81) are derived straight from Theorem 2.1.7, by taking the thermodynamic limit $\lim\limits_{\Lambda\nearrow\mathbf{Z}^d}\lim\limits_{B\searrow 0}\langle\cdots\rangle^{T=0}_{\Lambda,B}$. ■

Theorem 2.1.12. In the symmetric ground state, the spin correlations (2.78) satisfy

$$S_\alpha(k) \le \frac{1}{2}\sqrt{\frac{\rho_1(1-\lambda\gamma_k)+\rho_2(\lambda-\gamma_k)}{(1+\gamma_k)}} \qquad (\alpha = x, y), \tag{2.82}$$

$$S_z(k) \leq \frac{1}{2}\sqrt{\frac{2\rho_1(1-\gamma_k)}{\lambda(1+\gamma_k)}}, \tag{2.83}$$

where

$$\rho_1 = \lim_{\Lambda \nearrow \mathbf{Z}^d} \lim_{B \searrow 0} \frac{1}{L^d d} \sum_{\langle i,j \rangle \in \Lambda} \left\langle -S_i^x S_j^x \right\rangle_{\Lambda,B}^{T=0}, \tag{2.84}$$

$$\rho_2 = \lim_{\Lambda \nearrow \mathbf{Z}^d} \lim_{B \searrow 0} \frac{1}{L^d d} \sum_{\langle i,j \rangle \in \Lambda} \left\langle -S_i^z S_j^z \right\rangle_{\Lambda,B}^{T=0}. \tag{2.85}$$

Proof of Theorem 2.1.12. We obtain (2.82) and (2.83) following the proof of Theorem 2.1.9, with only the order of taking limits changed. First we take the limit $B \searrow 0$, and then take the thermodynamic limit. Thereby we have (2.82) and (2.83). ■

Note that, if the symmetry is spontaneously broken in the pure state $\langle \cdots \rangle_x^{T=0}$, the two correlation functions $S_\alpha(k)$ and $S_\alpha^\perp(k)$ (or $S^\parallel(k)$) have different upper bounds. For example, in Section 2.3.2, we show the difference in the large-S limit of the two- and three-dimensional Heisenberg antiferromagnets.

2.2 Absence of long-range order in $d = 1$ systems

In this and the next sections, we show how the rigorous inequalities were used in rigorous proofs of the existence or absence of the long-range order. In this section, we discuss the long-range order in the one-dimensional systems.

In the one-dimensional quantum antiferromagnets, the spin correlations are not strong enough to produce the long-range order. It was rigorously shown that the one-dimensional spin-S Heisenberg and XXZ antiferromagnets do not have the antiferromagnetical long-range order. Hence the infinite-volume ground state would be unique and symmetric. Here, we briefly show the rigorous proof as well as results of the exact solutions.

Rigorous proof

Pitaevskii and Stringari first presented a method of proving the absence of the long-range order [122]. After that, Shastry [129] rigorously proved it, using Theorem 2.1.10. The proof is as follows.

In the finite system Λ with the periodic boundary condition, the momentum summation of the spin correlations becomes

$$\frac{1}{L}\sum_k \left\langle S_{-k}^y S_k^y \right\rangle_{\Lambda,B}^T = \frac{1}{L}\sum_{i=1}^{L} \left\langle (S_i^y)^2 \right\rangle_{\Lambda,B}^T = \left\langle (S_1^y)^2 \right\rangle_{\Lambda,B}^T, \tag{2.86}$$

where we have used the sublattice-translation invariance. Since $k = \pi$ is the singular point of the correlation functions in the thermodynamic limit, we exclude it from the momentum summation and thereby we have

$$\frac{1}{L}\sum_{k\neq\pi}\left\langle S^y_{-k}S^y_k\right\rangle^T_{\Lambda,B} = \frac{1}{L}\sum_{k}\left\langle S^y_{-k}S^y_k\right\rangle^T_{\Lambda,B} - \frac{1}{L}\left\langle S^y_{-\pi}S^y_\pi\right\rangle^T_{\Lambda,B}$$
$$= \left\langle (S^y_1)^2\right\rangle^T_{\Lambda,B} - \frac{1}{L^2}\left\langle\left(\sum_{i\in A}S^y_i - \sum_{i\in B}S^y_i\right)^2\right\rangle^T_{\Lambda,B}. \tag{2.87}$$

Taking the thermodynamic limit $\lim\limits_{B\searrow 0}\lim\limits_{\Lambda\nearrow\mathbf{Z}}\langle\cdots\rangle^{T=0}_{\Lambda,B}$ and replacing the summation $L^{-1}\sum_{k\neq\pi}$ with $(2\pi)^{-1}\int_{-\pi}^{\pi}dk$, we have

$$\int_{-\pi}^{\pi}\frac{dk}{2\pi}S^\perp_y(k) = \left\langle (S^y_1)^2\right\rangle^{T=0}_x - \lim_{B\searrow 0}\lim_{\Lambda\nearrow\mathbf{Z}}\frac{1}{L^2}\left\langle\left(\sum_{i\in A}S^y_i - \sum_{i\in B}S^y_i\right)^2\right\rangle^{T=0}_{\Lambda,B}$$
$$\leq \left\langle (S^y_1)^2\right\rangle^{T=0}_x. \tag{2.88}$$

Thus we know that the right-hand-side of (2.88) is bounded from above by the norm of $(S^y_1)^2$, *i.e.* S^2. On the other hand, we integrate both sides of the first inequality in (2.75) to obtain the lower bound as

$$\frac{m_\mathrm{s}^2}{2}\sqrt{\frac{\lambda}{\rho_x+\rho_y}}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\sqrt{\frac{1-\gamma_k}{1+\gamma_k}} \leq \int_{-\pi}^{\pi}\frac{dk}{2\pi}S^\perp_y(k). \tag{2.89}$$

The momentum integral in the left-hand-side of (2.89) diverges. For the consistency between the lower and upper bounds to be kept, the staggered magnetization m_s must be vanishing for $0<\lambda\leq 1$.

In the classical limit, the ground state has a Néel order where spins lay in the xy plane. In the ground state of the one-dimensional quantum models, however, the order is vanishing owing to quantum fluctuations. Thus the disorder of the ground state is a purely quantum effect. Indeed, the vanishing of the order was proved on the basis of the uncertainty relation, because Shastry's inequality originated from the relation.

Antiferromagnetic Spin-1/2 Heisenberg and *XY* chains

Among plenty of quantum antiferromagnets, the antiferromagnetic spin-1/2 chains are the special models, because the exact solutions are known and asymptotic forms of the correlation functions were obtained from the solutions.

The one-dimensional spin-1/2 Heisenberg antiferromagnet was first solved by Bethe [14] using a hypothesis, which was later proved by Yang and Yang [149]. From Bethe's solution, the ground-state energy [51], the magnetization curve [41] and the spin-wave spectrum [22] were evaluated exactly. Asymptotic forms of the correlation functions were first studied by Luther and Peschel [88] in the continuum limit. Izergin and Korepin [58] calculated the correlation functions from the Bethe-ansatz solution and showed the power decay of the spin correlations.

The one-dimensional spin-1/2 *XY* model was solved by Lieb, Schulz and Mattis [86]. They transformed the model to a free-fermion system and then obtained all the eigenstates.

Katsura [64] evaluated various thermodynamic quantities. After that McCoy [90] calculated the spin correlation functions and showed the asymptotic form

$$\langle S_i^x S_j^x \rangle_0^{T=0} \sim \frac{1}{|i-j|^{1/2}}. \tag{2.90}$$

Furthermore, Araki and Matsui [8] proved the uniqueness of the ground state of the infinite-volume system.

2.3 Symmetry breaking in $d \geq 2$ systems

In this section, we discuss the long-range order in the two- and higher-dimensional systems. It has been rigorously shown that the symmetry breaking occurs at $T = 0$ in the spin-S Heisenberg antiferromagnet on the cubic lattice and in the $S \geq 1$ Heisenberg antiferromagnet on the square lattice. We briefly show the rigorous proof using correlation inequalities. Furthermore, we discuss the large-S limit of the Heisenberg model and show that physical quantities have the classical values in this limit.

2.3.1 Existence of long-range order

A rigorous proof for the existence of the long-range order was first given by Dyson, Lieb and Simon [27]. They proved the long-range order of the three-dimensional Heisenberg antiferromagnet at sufficiently low temperatures. Extending their proof, Jordão-Neves and Fernando-Perez [60] proved long-range order in the ground state of the two-dimensional $S \geq 1$ Heisenberg model, and Kennedy, Lieb and Shastry [68] proved it for the three-dimensional Heisenberg model with arbitrary spins. After that the rigorous proof was extended to the XY model with $d \geq 2$ and arbitrary spins by Kennedy, Lieb and Shastry [69], and to the XXZ model by Kubo and Kishi [75] and by Nishimori and Ozeki [119].

Let us discuss the antiferromagnetic Heisenberg model with $B = 0$. Considering the d-dimensional case of (2.87), we have

$$\frac{1}{L^d} \sum_{k \neq Q} \left\langle S_{-k}^x S_k^x \right\rangle_{\Lambda, B=0}^{T=0} = \left\langle (S_1^x)^2 \right\rangle_{\Lambda, B=0}^{T=0} - \frac{1}{L^{2d}} \left\langle (\mathcal{O}_\Lambda)^2 \right\rangle_{\Lambda, B=0}^{T=0}, \tag{2.91}$$

where $Q = (\pi, \cdots, \pi)$ and

$$\mathcal{O}_\Lambda = \sum_{i \in A} S_i^x - \sum_{i \in B} S_i^x. \tag{2.92}$$

Taking the thermodynamic limit and changing the summation $L^{-d} \sum_{k \neq Q}$ into $(2\pi)^{-d} \int dk^d$, we obtain

$$\int' \frac{dk^d}{(2\pi)^d} S_x(k) = \left\langle (S_1^x)^2 \right\rangle_0^{T=0} - \sigma^2, \tag{2.93}$$

where $k = Q$ is excluded from the integral region and σ^2 denotes the long-range order parameter,

$$\sigma^2 = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{L^{2d}} \left\langle (\mathcal{O}_\Lambda)^2 \right\rangle_{\Lambda, B=0}^{T=0}. \tag{2.94}$$

Because of (2.93) and the isotropy of the model, we have

$$\int' \frac{dk^d}{(2\pi)^d} \sum_{\alpha=x,y,z} S_\alpha(k) = \left\langle (S_1^x)^2 + (S_1^y)^2 + (S_1^z)^2 \right\rangle_0^{T=0} - 3\sigma^2$$
$$= S(S+1) - 3\sigma^2. \tag{2.95}$$

On the other hand, integrating both sides of the inequalities of Theorem 2.1.12 with k except $k = Q$, we obtain the upper bound of (2.95) as

$$\int' \frac{dk^d}{(2\pi)^d} \sum_{\alpha=x,y,z} S_\alpha(k) \leq \frac{3\sqrt{\rho_1}}{\sqrt{2}} I_d, \tag{2.96}$$

where

$$I_d = \int \frac{dk^d}{(2\pi)^d} \sqrt{\frac{1-\gamma_k}{1+\gamma_k}}. \tag{2.97}$$

The integral I_d is finite for $d \geq 2$. Combing (2.95) and (2.96), we obtain

$$\sigma^2 \geq \frac{S(S+1)}{3} - \frac{\sqrt{\rho_1}}{\sqrt{2}} I_d. \tag{2.98}$$

Here the value of $(-3\rho_1)$ is the ground-state energy per bond; see (2.84). Since the Hamiltonian is a summation of local operators, the expectation values of energy are bounded by the norm of the local operators. Anderson [4] thus obtained the inequality $-3\rho_1 \geq -S(S+1/2d)$. Then, (2.98) becomes

$$\sigma^2 \geq \frac{S(S+1)}{3} - \frac{\sqrt{S(2dS+1)}}{2\sqrt{3d}} I_d. \tag{2.99}$$

This inequality shows $\sigma^2 > 0$ for $S \geq 1$ both in two and three dimensions. Estimating (2.98) more carefully, one can show the existence of the long-range order in the three-dimensional $S \geq 1/2$ Heisenberg antiferromagnet as well [68].

Recently, the occurrence of the symmetry breaking was rigorously proved. (Note that the above arguments do not show the spontaneous breakdown of the symmetry, but only show the existence of the long-range order.) Kaplan, Horsch and von der Linden [62] showed that, if $\sigma^2 > 0$ in the symmetric ground state, then the pure ground state has a non-vanishing staggered magnetization, $m_{\mathrm{s}} > 0$. Later, Koma and Tasaki [73] showed the relation $m_{\mathrm{s}} \geq \sqrt{3}\sigma$ at any temperatures.

Two-dimensional $S = 1/2$ Heisenberg model

Finally, we would like to mention the long-range order of the two-dimensional $S = 1/2$ Heisenberg antiferromagnet. Since the discovery of the high-T_{c} superconductivity in $\mathrm{La}_{2-x}\mathrm{Sr}_x\mathrm{CuO}_4$, this model has been studied extensively, because the model is expected to describe the compound without doping. Though there is no rigorous proof for this model (up to now), many theoretical and numerical studies suggested the existence of the antiferromagnetic long-range order, from quantum Monte-Carlo simulations [124, 83], spin-wave expansions [5, 77, 21] and series expansions [132]. (As a review, see [89] for example.)

2.3.2 The large-S limit of the Heisenberg model

Here we discuss the large-S limit of the Heisenberg antiferromagnet on the square and cubic lattices. First, we show the S dependence of m_{s}, ρ_x, ρ_y and ρ_z in the $S \nearrow \infty$ limit. We can obtain bounds for physical quantities using the rigorous inequalities [104]. The results indicate that the large-S limit of the quantum Heisenberg model corresponds to the classical model.

Proposition 2.3.1. In the large-S limit of the Heisenberg antiferromagnets on the square and cubic lattices, we have

$$\lim_{S\nearrow\infty} m_{\mathrm{s}}/S = 1, \tag{2.100}$$

$$\lim_{S\nearrow\infty} \rho_x/S^2 = 1, \tag{2.101}$$

$$\lim_{S\nearrow\infty} \rho_y/S^2 = \lim_{S\nearrow\infty} \rho_z/S^2 = 0. \tag{2.102}$$

Proof of Proposition 2.3.1. The quantities m_{s}, ρ_x, ρ_y and ρ_z are bounded from above by the norms of local operators. Hence, we have

$$m_{\mathrm{s}} \leq S \tag{2.103}$$

and

$$\rho_\alpha \leq S^2 \qquad (\alpha = x, y, z). \tag{2.104}$$

The ground-state energy per bond, $(-\rho_x - \rho_y - \rho_z)$, is also bounded in the form [4]

$$(\rho_x + \rho_y + \rho_z) \leq S(S + 1/2d). \tag{2.105}$$

To obtain lower bounds of m_s, we use Koma and Tasaki's inequality [73], $m_{\mathrm{s}} \geq \sqrt{3}\sigma$, and (2.99). Thus, we obtain

$$\left[S(S+1) - \sqrt{3S(2dS+1)}I_d/2\sqrt{d}\right]^{1/2} \leq m_{\mathrm{s}} \leq S \tag{2.106}$$

for $S \geq 1$. Taking the large-S limit, one obtains (2.100).

To bound ρ_x, ρ_y and ρ_z from below, we use (2.76), from which we find

$$\frac{{m_{\mathrm{s}}}^2}{(\rho_x + \rho_z)^{1/2}} \leq (\rho_x + \rho_y)^{1/2}. \tag{2.107}$$

Using $\rho_y = \rho_z$, we obtain

$${m_{\mathrm{s}}}^2 \leq \rho_x + \rho_y. \tag{2.108}$$

Combining (2.108) and (2.105), we have

$${m_{\mathrm{s}}}^2 + \rho_y \leq S(S + 1/2d), \tag{2.109}$$

where we have used $\rho_y = \rho_z$. Using (2.104), (2.108) and (2.109), we obtain bounds for ρ_α ($\alpha = x, y, z$) in the form

$$2{m_\mathrm{s}}^2 - S(S + 1/2d) \le {m_\mathrm{s}}^2 - \rho_y \le \rho_x \le S^2. \tag{2.110}$$

Taking the large-S limit and using (2.100), we obtain (2.101) and (2.102). ■

Using Proposition 2.3.1, we can obtain the correlation functions: In the large-S limit of the Heisenberg antiferromagnets on the square and cubic lattices, the upper bounds of $\chi^\perp(k)$ and $S^\perp(k)$ become equal to the lower bounds, respectively, and hence we have

$$\chi^\perp(k) = \frac{1}{2Jd(1+\gamma_k)}, \tag{2.111}$$

$$S^\perp(k) = \frac{S}{2}\sqrt{\frac{1-\gamma_k}{1+\gamma_k}}. \tag{2.112}$$

On the other hand, $\chi^\parallel(k)$ and $S^\parallel(k)$ are bounded in the form

$$0 \le \chi^\parallel(k) \le \frac{1}{2Jd(1+\gamma_k)}, \tag{2.113}$$

$$0 \le S^\parallel(k) \le O(S^{1/2})\sqrt{\frac{1-\gamma_k}{1+\gamma_k}}. \tag{2.114}$$

As we have mentioned at the end of Section 2.1, the structure factors in the pure ground state and in the symmetric ground state have different upper bounds. In the symmetric ground state, we have $\rho_1 = \rho_2 = S^2/3$, and hence

$$S_\alpha(k) \le \frac{S}{\sqrt{6}}\sqrt{\frac{1-\gamma_k}{1+\gamma_k}}. \tag{2.115}$$

Thus $S_\alpha(k)$ is smaller than $S^\perp(k)$.

2.4 Ground states and low-lying excited states of finite-size systems

Ground states of finite-volume systems are studied and discussed in numerical calculations. In this section we hence show exact results for these states, which provide useful information for the numerical approaches to these systems. We discuss the spin-S Heisenberg and XXZ antiferromagnets on a d-dimensional $L \times \cdots \times L$ hypercubic lattice $\Lambda \subset \mathbf{Z}^d$. Let H_Λ be the Hamiltonian defined by (2.46) or (2.47).

In Section 2.4.1, we discuss properties of ground states and low-lying excited states on the finite-volume lattice Λ. It is known that the ground state of H_Λ is unique and symmetric. Quantum numbers of various low-lying states can be determined as well. We show that these states have the same spatial symmetry as the Néel-ordered states.

In Section 2.4.2, we discuss finite-size effects on the low-lying states. It was shown for a class of quantum antiferromagnets that, if the ground state has a long-range order, low-lying excited states of a growing number converge to the ground state in the infinite-volume limit. In the Heisenberg antiferromagnet on Λ, we show that the number of the low-lying states that are counterpart of the infinite-volume ground state is, at least, of $o(N^2)$ (a number lower order than N^2), where $N = L^d$.

2.4.1 Marshall–Lieb–Mattis theorem

First we discuss the Heisenberg model ($\lambda = 1$). Exact information about the ground state and some low-lying states was obtained by Marshall [92], and by Lieb and Mattis [85] in the following form.

Theorem 2.4.1. (Marshall–Lieb–Mattis): Let H_Λ be the Hamiltonian of the Heisenberg antiferromagnet on the lattice Λ.
(1) The ground state is unique and it has the eigenvalue $S_{\text{total}} = 0$. Let $|\Phi_{\text{GS}}\rangle$ be the ground state. Then, all coefficients of $U|\Phi_{\text{GS}}\rangle$ in the bases that are eigenstates of $\{S_i^z\}$ are non-negative, where $U = \exp\left(i\pi \sum_{i\in B} S_i^z\right)$.
(2) The lowest state in the subspace of $S^z_{\text{total}} = m$ has the total spin $S_{\text{total}} = m$, and it is not degenerate. Let $|m, m\rangle$ be the lowest state. Then, all coefficients of $U|m, m\rangle$ are non-negative.

Thus the ground state $|\Phi_{\text{GS}}\rangle$ is symmetric, *i.e.*, it is invariant under any global rotation of spins. Using this theorem, we can specify other quantum numbers of these states. Let us discuss a system with periodic boundary conditions and let the length L be an even integer. The Hamiltonian is invariant under any sublattice translation and under any translation of the point group G of the lattice. Eigenvalues of these translations are determined for low-lying states as follows [103]:

Proposition 2.4.2. Let H_Λ be the Hamiltonian of the Heisenberg antiferromagnet on the lattice Λ and let $|s, m\rangle$ be the lowest state in the subspace $S_{\text{total}} = s$ and $S^z_{\text{total}} = m$, where m is limited to $-s \le m \le s$. Then, the states $|s, m\rangle$ are invariant under elements of the sublattice translation and the group G.

The point group G is C_{4V} for the square lattice and O_h for the cubic lattice [78]. The elements of G preserve the sublattice structure, namely, translate the sublattice A to A and B to B. Hence the Néel-ordered states are invariant under elements of the sublattice translation and the group G. This proposition thus shows that all states $|s, m\rangle$ have the same spatial symmetry as Néel ordered states.

Proof of Proposition 2.4.2. Any element T_s of the sublattice translation satisfies $(T_s)^L = 1$, where the identity mapping is denoted by 1. The sublattice translation T_s, hence, takes the eigenvalues $t_s = \exp(i2\pi l/L)$, where $l = 0, 1, \ldots, L-1$. The eigenstates with $t_s = \exp(i2\pi l/L)$ and with $t_s = \exp(-i2\pi l/L)$ are degenerate. According to Theorem 2.4.1, the state $U|s, s\rangle$ is not degenerate in the $S^z_{\text{total}} = s$ subspace and it takes non-negative coefficients in the bases of the eigenstates of $\{S_i^z\}$. Hence $U|s, s\rangle$ should have the eigenvalue $t_s = 1$. Since U and T_s commute, the state $|s, s\rangle$ is invariant under any T_s. In the same way, for any element $R \in G$, we obtain $RU|s, s\rangle = U|s, s\rangle$. Since R and U commute, the state $|s,s\rangle$ is invariant under any R.

The states $|s,m\rangle$ $(-s \leq m < s)$ are also invariant under any sublattice translation T_s and under any element $R \in G$, since the operator $\sum_i S_i^-$ commutes with T_s and R. ■

Next we discuss the XXZ model with $-1 < \lambda < 1$. In this case, the total spin-angular-momentum S_{total} is not a good quantum number and only S^z_{total} is. Affleck and Lieb [3] determined the eigenvalue S^z_{total} of the ground state as follows:

Theorem 2.4.3. (Affleck–Lieb): Let H_Λ be the Hamiltonian of the XXZ antiferromagnets with $-1 < \lambda < 1$ on the lattice Λ.
(1) The ground state of H_Λ uniquely exists in the subspace of $S^z_{\text{total}} = 0$. Let $|\Phi_{\text{GS}}\rangle$ be the ground state. Then, all coefficients of $U|\Phi_{\text{GS}}\rangle$ are non-negative.
(2) The lowest state in the subspace of $S^z_{\text{total}} = m$ is non-degenerate. Let $|m\rangle$ be the lowest state. Then, all coefficients of $U|m\rangle$ are non-negative.

Using this theorem, we specify quantum numbers of $|m\rangle$ in the following form [103].

Proposition 2.4.4. Let H_Λ be the Hamiltonian of the XXZ antiferromagnets with $-1 < \lambda < 1$ on the lattice Λ, and let $|m\rangle$ be the lowest state in the subspace of $S^z_{\text{total}} = m$. Then, the states $|m\rangle$ with arbitrary m have the same spatial symmetry as Néel ordered states.

Proof of Proposition 2.4.4. This is derived in the same way as the proof of Proposition 2.4.2. ■

It should be remarked that Theorems 2.4.1 and 2.4.3 work only for finite systems; the uniqueness of the ground state cannot be applied to the infinite-volume system.

Though topics of this thesis are limited to quantum antiferromagnets, we give a comment on ferromagnets. We can show the uniqueness of the ground state and various exact results for low-lying states of the ferromagnetic XXZ model as well. Results and proofs are given in Section 3.3.A, and they are used in Section 3.3.

2.4.2 Finite-size effect on low-lying states

As shown in Section 2.3, symmetry breaking occurs at $T = 0$ in the three-dimensional spin-S Heisenberg antiferromagnets and in the two-dimensional $S \geq 1$ models in the thermodynamic limit. Furthermore, many theoretical and numerical studies indicate that the spin-1/2 Heisenberg antiferromagnet has the long-range order. Hence, there exist multiple ground states in the thermodynamic limit.

On the other hand, the ground state on a finite-volume lattice Λ is unique, as shown in Theorems 2.4.1 and 2.4.3. It is expected that, to make the symmetry breaking occur in the infinite-volume limit, plenty of low-lying states converge to the unique ground state as the system size increases. Horsch and von der Linden [50] first showed the existence of a low-lying excited state whose energy converges to that of the ground state. Recently, Koma and Tasaki [74] proved that, if the system has the long-range order, ever increasing numbers of low-lying states converge to the ground state.

Let us discuss Koma and Tasaki's theorems. Though their original theorems are applicable to a wide class of quantum models with continuous symmetry, we consider only the spin-S XXZ model with $-1 < \lambda \leq 1$ on the lattice Λ. Let $|\Phi_{\mathrm{GS}}\rangle$ be the unique normalized ground state of H_Λ. The long-range order parameter μ is given in

$$\frac{1}{N^2}\langle\Phi_{\mathrm{GS}}|(O_\Lambda)^2|\Phi_{\mathrm{GS}}\rangle = (\mu S)^2, \tag{2.116}$$

where $0 \leq \mu \leq 1$ and $N = L^d$. Consider the following trial state

$$|\Psi_s\rangle = \frac{(O^+)^s|\Phi_{\mathrm{GS}}\rangle}{\|(O^+)^s|\Phi_{\mathrm{GS}}\rangle\|} \tag{2.117}$$

for a positive integer s, where $O^+ = \sum_{i\in A} S_i^+ - \sum_{i\in B} S_i^+$ and the norm of a state $|\Psi\rangle$ is defined by $\|\,|\Psi\rangle\| = \langle\Psi|\Psi\rangle^{1/2}$.

Theorem 2.4.5. (Koma and Tasaki): When $\mu > 0$, the state $|\Psi_s\rangle$ is well-defined and the expectation value of the energy of each $|\Psi_s\rangle$ is bounded as

$$\frac{1}{N}(\langle\Psi_s|H|\Psi_s\rangle - \langle\Phi_{\mathrm{GS}}|H|\Phi_{\mathrm{GS}}\rangle) \leq \frac{cJS^2}{\mu^2}\left(\frac{s}{N}\right)^2 \tag{2.118}$$

for $s < (\mu\sqrt{N}/8\sqrt{6})$, where c is a finite constant.

This theorem gives the following necessary condition for the symmetry breaking: If the symmetry breaking occurs in the infinite-volume limit, the expectation values of the excitation energy of a number of low-lying states decay faster than $1/N$. Convergence of more low-lying states was also shown in the following form.

Theorem 2.4.6. (Koma and Tasaki): When $\mu > 0$ and N is large enough such that $N \geq (8/\mu)^2$, the expectation value of the energy of each $|\Psi_s\rangle$ is bounded as

$$\frac{1}{N}(\langle\Psi_s|H|\Psi_s\rangle - \langle\Phi_{\mathrm{GS}}|H|\Phi_{\mathrm{GS}}\rangle) \leq \frac{c'JS^2}{\mu^2}\left(\frac{s}{N}\right) \tag{2.119}$$

for $s \leq (\mu^2 N/16)$, where c' is a finite constant.

This theorem covers a wider range of low-lying states than Theorem 2.4.5: Theorem 2.4.6 states that, when the ground state has the long-range order, the number of low-lying states whose energy per site converges to the ground-state energy is at least $o(N)$, *i.e.*, a number that is lower order than N. (For the definition of ground states, see Refs. [19] and [72].) The size dependence is, however, estimated more precisely in Theorem 2.4.5.

Furthermore Koma and Tasaki [74] proved that the symmetry breaking occurs by forming linear combinations of these low-lying states. Taking linear combinations, they constructed multiple ground states in which continuous symmetry is broken.

From now, we restrict the model to the spin-S Heisenberg model ($\lambda = 1$) and discuss the excitation energy of $|s, m\rangle$, where $|s, m\rangle$ denotes the lowest eigenstate in the subspace with $S_{\text{total}} = s$ and $S^z_{\text{total}} = m$. These states have been repeatedly discussed in numerical studies, since they are easily distinguishable from other states and they are easily obtained. Using Theorems 2.4.1 and 2.4.5, we can obtain upper bounds for the eigenvalues of the energy of $|s, m\rangle$ as follows:

Proposition 2.4.7. When $\mu > 0$, the excitation energy of the states $|s, m\rangle$ are bounded as

$$\frac{1}{N}(\langle s, m|H_\Lambda|s, m\rangle - \langle \Phi_{\text{GS}}|H_\Lambda|\Phi_{\text{GS}}\rangle) \le \frac{cJS^2}{\mu^2}\left(\frac{s}{N}\right)^2 \tag{2.120}$$

for $s < (\mu\sqrt{N}/8\sqrt{6})$ and m in the range $-s \le m \le s$, where c is a finite constant.

Proof of Proposition 2.4.7. The state $|\Psi_s\rangle$ defined by (2.117) has the eigenvalue $S^z_{\text{total}} = s$, but does not have a definite value of S_{total}. From Theorem 2.4.1, however, we know that the state $|s, s\rangle$ is the lowest eigenstate in the $S^z_{\text{total}} = s$ subspace. We thus find that the energy of $|s, s\rangle$ is bounded in the form

$$\langle s, s|H_\Lambda|s, s\rangle \le \langle \Psi_s|H_\Lambda|\Psi_s\rangle. \tag{2.121}$$

Using (2.118), we obtain (2.120) with $m = s$. Since the states $|s, m\rangle$ with the fixed s and m in the range $-s \le m \le s$ have the same energy because of the $SU(2)$ symmetry, we obtain the desired relation (2.120). ∎

In the same way, using Theorem 2.4.6, we obtain the following theorem.

Proposition 2.4.8. When $\mu > 0$ and N is large such that $N \ge (8/\mu)^2$, the excitation energy of the states $|s, m\rangle$ are bounded as

$$\frac{1}{N}(\langle s, m|H_\Lambda|s, m\rangle - \langle \Phi_{\text{GS}}|H_\Lambda|\Phi_{\text{GS}}\rangle) \le \frac{c'JS^2}{\mu^2}\left(\frac{s}{N}\right) \tag{2.122}$$

for $s \le (\mu^2 N/16)$ and m in the range $-s \le m \le s$, where c' is a finite constant.

Proof of Proposition 2.4.8. This is derived in the same way as the proof of Proposition 2.4.8 using Theorem 2.4.6 instead of Theorem 2.4.5. ∎

This proposition states that, when the ground state $|0, 0\rangle$ has the long-range order, the states $|s, m\rangle$ with $s \sim o(N)$ have the same energy per site as the ground state in the thermodynamic limit. Note that the allowed values of m are $-s, \ldots, s$ and that the total number of such low-lying states is $\sum_{s=0}^{o(N)}(2s + 1) \sim (o(N))^2 \sim o(N^2)$. Thus taking into account the $SU(2)$ symmetry, we find that the number of the low-lying states which converge to the ground state grows faster than any number that is of a lower order than N^2.

All the states $|s, m\rangle$ with $s \sim o(N)$ become the ground states in the thermodynamic limit. Remember that these states $|s, m\rangle$ have the same spatial symmetry as the Néel-ordered states, as shown in the Proposition 2.4.2. Infinite-volume ground states with the Néel order may be constructed by forming linear combinations of these low-lying states.

Chapter 3

Ground states of quantum antiferromagnets on the triangular lattice

In this chapter, we discuss ground-state properties of quantum antiferromagnets on a triangular lattice. The Heisenberg and XXZ antiferromagnets are considered.

In Section 3.2, we study ground states of the spin-S XXZ antiferromagnets. We show exact ground states of an anisotropic XXZ antiferromagnet ($\lambda = -0.5$). These states have perfect orders and most of them have the so-called 120° structure. Ground-state properties in the region $-0.5 < \lambda \leq 1$ are discussed using the spin-wave expansion. Thereby it is found that quantum fluctuations in the ground states are enhanced as λ increases from -0.5 to 1. The phase diagram of the relevant system at low temperatures is also discussed using the spin-wave theory.

In Section 3.3, we study low-lying states of the XY and Heisenberg antiferromagnets on finite-volume lattices to clarify whether spontaneous symmetry breaking occurs in the thermodynamic limit. We propose approximate forms of low-lying states, modifying the exact ground states at $\lambda = -0.5$. These approximate states have a long-range order. It is shown that the present approximation accurately describes true low-lying states. With the help of this approximation, we discuss the contribution of low-lying states to symmetry breaking of two types, namely creation of the spontaneous sublattice magnetization and the spontaneous chirality. Furthermore, we numerically study the low-lying states of finite systems. It is found that the necessary conditions for the symmetry breaking to occur are satisfied in the XY and Heisenberg antiferromagnets.

3.1 Introduction

It has been expected that ground-state properties of the Heisenberg antiferromagnet on a triangular lattice are quite different from the properties on bipartite lattices. Anderson [7] first pointed out that quantum fluctuations may appear strongly in quantum antiferromagnets on a triangular lattice. Since these systems have frustration caused by the antiferromagnetic interactions, the quantum fluctuations may be much stronger than in the quantum antiferromagnets on the square lattice [32, 91].

After Anderson's seminal discussions, many authors have been interested in ground-state properties of the spin-S Heisenberg and XXZ antiferromagnets on the triangular lattice and especially in the spin-1/2 models. The Hamiltonian of the XXZ antiferromagnet is given by

$$H = J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z), \tag{3.1}$$

where the summation runs over all the nearest-neighbor pairs.

Very few exact results are, however, known for the quantum antiferromagnets on the triangular lattice. Rigorous proofs given in Section 2.3 cannot be extended to the present model for technical reasons. Furthermore, we cannot apply the Marshall–Lieb–Mattis condition given in Section 2.4.1 to the antiferromagnets on the triangular lattice. Studies from other methods are hence needed.

In the classical limit, ground states have the so-called 120° structure, as shown in Figure 3.1. These ground states have two kinds of orders: One is the sublattice order, whose order parameter is

$$\mathcal{M}_{\mathrm{s}} = \sum_{i \in A} S_i^x + \sum_{i \in B} \Big(-\frac{1}{2} S_i^x + \frac{\sqrt{3}}{2} S_i^y \Big) + \sum_{i \in C} \Big(-\frac{1}{2} S_i^x - \frac{\sqrt{3}}{2} S_i^y \Big), \tag{3.2}$$

and the other is the chiral order,

$$\chi = \sum_{\langle i \to j \rangle} (\boldsymbol{S}_i \times \boldsymbol{S}_j)^z. \tag{3.3}$$

Here A, B and C denote the sublattices of the triangular lattice and the symbol $i \to j$ goes from the sublattice A to B, B to C and C to A. In the classical Heisenberg model ($\lambda = 1$), every state that is obtained from the global $SU(2)$ transformation of spins in Figure 3.1 belongs to the ground states. In the classical XY model, the ground states are obtained by the global $U(1)$ transformation, *i.e.*, global spin rotation along the z-axis, of Figure 3.1, and by the global Z_2 transformation, *i.e.*, global 180° rotation of spins along the x-axis of Figure 3.1. Furthermore, the ground-state manifold of the classical XXZ antiferromagnet in the region $-0.5 < \lambda < 1$ is exactly the same as that of the classical XY model [98].

For the quantum models, many authors have been interested in the problem how quantum effects change ground-state properties. There are two viewpoints in the studies of the ground states of the quantum antiferromagnets. The first one is that the quantum fluctuations are so strong and hence the ground state has no long-range order: Anderson first pointed out possibilities of the resonating-valence-bond state as the ground state [7, 32]. Kalmeyer and Laughlin also discussed a spin-liquid state [61] from this aspect. The second viewpoint is that the ground state has a long-range order with the so-called 120° structure, though the quantum fluctuations reduce the sublattice magnetization. Trial wave functions which have the 120° structure are discussed by Miyashita [97] and by Huse and Elser [53]. Furthermore, the spin-wave expansions [120, 96, 110, 82, 80] and the series expansion [132] suggested the existence of a long-range order. Since the estimates of the ground-state energy from these studies are almost equal to each other in the Heisenberg model, it is difficult to judge which picture is correct.

Apart from the above arguments, several authors [37, 118, 55, 12, 82] studied the ground states of the Heisenberg model in finite-volume lattices using the exact-diagonalization

Figure 3.1: 120° structure. A ground-state configuration of the classical antiferromagnets on a triangular lattice.

method. Two papers [12, 82] reported the calculations up to $N = 36$, but the conclusions do not coincide with each other; Bernu *et al.* [12] reported that the sublattice order is almost equal to the value obtained by the spin-wave expansion, but in contrast Leung and Runge's result [82] is contradictory to the existence of the sublattice order. Thus this issue concerning the existence of the long-range order is not yet settled down.

Furthermore, for the spin-1/2 XY model, several authors have studied ground-state properties. Results from studies of finite-volume lattices with different size using the exact diagonalization method are not consistent with each other [37, 118, 82]. (This is partially because the size of calculated clusters is not large enough to predict properties of infinite-volume systems, and partially because they have not used proper finite-size fitting-forms. See Section 3.3.3.) The chiral-order phase-transition at finite temperatures has been also studied in the XY model. Studies from the Monte-Carlo method [93] and from a cluster mean-field approximation [136] reported that the chiral order exists at finite temperatures. On the other hand, the study using high-temperature series-expansions found no critical point [38].

To clarify this confusing understanding, we give a new reliable viewpoint in Section 3.2. In Section 3.2.1, we present exact ground states of anisotropic XXZ models with $\lambda \leq -0.5$. These ground states at $\lambda = -0.5$ have long-range orders with the 120° structure and have the perfect sublattice magnetization. In Section 3.2.2, we study ground-state properties of the model with $-0.5 < \lambda \leq 1$ using the spin-wave expansion [5, 77], and thereby we find that the quantum fluctuations are enhanced as λ increases from -0.5 to 1. In this study we discuss the ground states, changing λ from -0.5 to 1. Our approach to the study of frustrated quantum spin systems is contrary to the approach of Fazekas and Anderson [32]. They studied the ground states changing λ from infinity to 1. In Section 3.2.3, we also study thermal properties of these models using the spin-wave expansion and thereby obtain a phase diagram at low temperatures.

We present another study to confirm the existence of the long-range order in the XY and Heisenberg models at $T = 0$. As we have commented before, the study of the ground states of finite-volume lattices is not enough to obtain a reliable conclusion for lack of system size. Then we study low-lying excited states of finite systems. As discussed in Section 2.4.2, low-lying excited states play important roles in symmetry breaking in the thermodynamic limit; symmetry is broken by making a linear combination of the finite-volume ground state and low-lying excited states.

It has been discussed that, when symmetry breaking occurs, growing numbers of low-lying states converge to the ground states faster than the softest magnon excitation [5, 12, 10]. Several numerical calculations showed the existence of the low-lying excited states whose values of the excitation energy decay in a form faster than $1/N$ in the spin-1/2 Heisenberg antiferromagnet on a triangular lattice [12, 82]. Bernu *et al.* [12] discussed the spatial quantum numbers of the low-lying states that construct the ordered infinite-volume ground states. They found the existence of a whole set of low-lying states in finite systems. Azaria *et al.* [10] studied the finite-size dependence of these low-lying states. They found that low-lying states satisfy the scaling property which indicates the existence of a long-range order.

In quantum antiferromagnets on the triangular lattice, the mechanism of symmetry breaking is complicated, since there are two types of symmetry breaking. In the Heisenberg antiferromagnet both the sublattice magnetization and the chirality relate to the breakdown of the $O(3)$ symmetry. In the XY antiferromagnet the $U(1) \times Z_2$ symmetry can be broken. These symmetry breakings are related to each other.

In Section 3.3, we discuss low-lying states, to understand mechanism of each symmetry breaking independently and to clarify whether spontaneous symmetry breaking occurs at $T = 0$ in the thermodynamic limit. We give approximate forms of the low-lying states, in which the degrees of freedom of the sublattice magnetization and the chirality are separated. These approximate states accurately describe the true low-lying states. Using our approximation, we can understand how rearrangements of the low-lying states bring on each symmetry breaking. Furthermore, numerically studying the low-lying states of finite systems, we discuss the occurrence of symmetry breaking.

In Section 3.4, we argue the relation between the long-range order parameter σ and the spontaneous sublattice magnetization m. It has been discussed [73] that, for bipartite systems, the relation is given by $m = \sqrt{3}\sigma$ in the Heisenberg antiferromagnet and by $m = \sqrt{2}\sigma$ in the XY antiferromagnet. In the antiferromagnets on the triangular lattice, however, the factor of the relation becomes $\sqrt{2}$ times as large as the above. We obtain $m = \sqrt{6}\sigma$ for the Heisenberg model and $m = 2\sigma$ for the XY model.

3.2 Ground-state properties of the Heisenberg and XXZ antiferromagnets[1]

In Section 3.2.1, we show exact ground states of the quantum XXZ antiferromagnets with $\lambda = -0.5$ and $\lambda < -0.5$. These ground states have perfect orders. In Section 3.2.2, we

[1]The contents of this section were published in [110].

study ground-state properties of the XXZ antiferromagnet with $-0.5 < \lambda \leq 1$, using the spin-wave expansion. In Section 3.2.3, the phase diagram at finite temperatures is also studied using the spin-wave approximation.

3.2.1 Exact ground states of anisotropic *XXZ* models

Here we show the exact ground states of the spin-1/2 XXZ antiferromagnet on the triangular lattice in the region $\lambda \leq -0.5$. We briefly derive them and discuss properties of them.

Case of $\lambda = -0.5$

First we consider the ground states in the spin-1/2 XXZ antiferromagnet with $\lambda = -0.5$. We choose the quantize axes of the Hamiltonian as follows

$$H = J\sum_{\langle i,j\rangle}\Big(S_i^z S_j^z + S_i^x S_j^x - \frac{1}{2}S_i^y S_j^y\Big), \tag{3.4}$$

where the summation runs over all nearest-neighbor pairs of sites and S^α ($\alpha = x, y, z$) are the spin operators. Let us consider the following two states

$$|\Phi_1\rangle = U\Big(\bigotimes_i |\uparrow\rangle_i\Big), \tag{3.5}$$

$$|\Phi_2\rangle = U^\dagger\Big(\bigotimes_i |\uparrow\rangle_i\Big), \tag{3.6}$$

where $2S_i^z|\uparrow\rangle_i = |\uparrow\rangle_i$ and $2S_i^z|\downarrow\rangle_i = -|\downarrow\rangle_i$, and U denotes the unitary operator

$$U = \exp\Big(i\frac{2\pi}{3}\sum_{i\in B} S_i^y - i\frac{2\pi}{3}\sum_{i\in C} S_i^y\Big). \tag{3.7}$$

As shown later, these states belong to the ground states of the Hamiltonian (3.4). The operator U rotates all the spins on the sublattice B through the angle $2\pi/3$ and on the sublattice C through the angle $-2\pi/3$ about the y axis. Transformed with this operator, states (3.5) and (3.6) have the 120° structure.

These states have a form similar to the trial wavefunction proposed by Miyashita [97] and by Betts and Miyashita [15] as the ground state of the XY antiferromagnet.

From now we show that the states $|\Phi_1\rangle$ and $|\Phi_2\rangle$ belong to the ground states. Let us divide the triangular lattice into triangular cells, as shown in Figure 3.2, and the Hamiltonian into cell Hamiltonians defined on triangular cells in the form

$$H = \sum_{\triangle(i,j,k)\in\Lambda} H_{\triangle(i,j,k)}, \tag{3.8}$$

where the summation runs over all the upward triangular cells and $H_{\triangle(i,j,k)}$ denotes the local Hamiltonian on the triangular cell labeled with the sites i, j and k. Transforming

Figure 3.2: A triangular lattice is divided into shaded triangular cells. The cell-Hamiltonians are defined on each shaded cell.

$H_{\triangle(1,2,3)}$ with the operator U, we obtain

$$U^\dagger H_{\triangle(1,2,3)} U = -\frac{J}{2} \sum_{\langle i,j\rangle \in \triangle(1,2,3)} (S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y) + \frac{\sqrt{3}J}{2} \sum_{(i\to j)\in\triangle(1,2,3)} (S_i^z S_j^x - S_i^x S_j^z). \tag{3.9}$$

Exactly diagonalizing (3.9), we can easily evaluate all eigenstates and eigenvalues, and thereby we find that the state $|\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \otimes |\uparrow\rangle_3$ is one of eigenstates of $U^\dagger H_{\triangle(1,2,3)} U$ and it takes the lowest eigenvalue $-1.5J$. (It should be remarked that the second term of the right-hand-side of (3.9) has no effect on the state $|\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \otimes |\uparrow\rangle_3$.) Since U is unitary, the state $U(|\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \otimes |\uparrow\rangle_3)$ belongs to the ground states of $H_{\triangle(1,2,3)}$. In the same way, we can show that the state $U(\otimes_i |\uparrow\rangle_i)$ is one of the lowest eigenstates of every local Hamiltonians $H_{\triangle(i,j,k)}$ and it has the same eigenvalue $-1.5J$. We hence find that $U(\otimes_i |\uparrow\rangle_i)$ belongs to the ground states of the total Hamiltonian (3.4).

In the same way, we can show that the state $U(\bigotimes_i |\uparrow\rangle_i)$ is one of the eigenstates of the Hamiltonian H and it takes the minimum energy $-1.5JN$, where N denotes the number of sites. We hence find that the state $|\Phi_2\rangle$ is also one of the ground states of the Hamiltonian (3.4).

These ground states are not fluctuated by quantum effects and they have fully-ordered sublattice-magnetization and chirality; We have

$$\langle \Phi_1 | U M U^\dagger | \Phi_1 \rangle = \langle \Phi_2 | U^\dagger M U | \Phi_2 \rangle = \frac{1}{2} N, \tag{3.10}$$

where

$$M = \sum_i S_i^z, \tag{3.11}$$

and $UMU^\dagger$ and $U^\dagger MU$ are hence order-parameter operators of the sublattice magnetization. The signs of the chirality are opposite to each other as follows:

$$\langle\Phi_1|\chi|\Phi_1\rangle = -\langle\Phi_2|\chi|\Phi_2\rangle = -\frac{3}{4}N, \tag{3.12}$$

where χ denotes the order parameter of the chiral order

$$\chi = \frac{2}{\sqrt{3}}\sum_{(i\to j)}(S_i^z S_j^x - S_i^x S_j^z). \tag{3.13}$$

Next we show other ground states. Let us consider the following states

$$\begin{aligned} |\Phi_1(\theta,\phi)\rangle &= UR_3(\theta,\phi)\Big(\bigotimes_i |\uparrow\rangle_i\Big) \\ &= UR_3(\theta,\phi)U^\dagger|\Phi_1\rangle, \qquad (3.14) \\ |\Phi_2(\theta,\phi)\rangle &= U^\dagger R_3(\theta,\phi)\Big(\bigotimes_i |\uparrow\rangle_i\Big) \\ &= U^\dagger R_3(\theta,\phi)U|\Phi_2\rangle \qquad (3.15) \end{aligned}$$

with various values of θ and ϕ, where R_3 denotes the global $O(3)$-rotation operator

$$R_3(\theta,\phi) = \exp\Big(i\theta\sum_i S_i^y\Big)\exp\Big(i\phi\sum_i S_i^x\Big). \tag{3.16}$$

These states also belong to the ground states. This can be shown using the fact that the state $|\uparrow\rangle_1\otimes|\uparrow\rangle_2\otimes|\uparrow\rangle_3$ is one of the ground states of the transformed Hamiltonian

$$\begin{aligned} R_3^\dagger(\theta,\phi)U^\dagger H_{\triangle(1,2,3)}UR_3(\theta,\phi) &= -\frac{J}{2}\sum_{\substack{\langle i,j\rangle\in\\ \triangle(1,2,3)}}(S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y) \\ +\frac{\sqrt{3}J}{2}\sum_{\substack{(i\to j)\in\\ \triangle(1,2,3)}}&\{\cos\phi(S_i^z S_j^x - S_i^x S_j^z) - \sin\phi(S_i^x S_j^y - S_i^y S_j^x)\} \qquad (3.17) \end{aligned}$$

and it is also one of the ground states of $R_3^\dagger UH_{\triangle(1,2,3)}U^\dagger R_3$.

The transformation $UR_3U^\dagger$ corresponds to closing the umbrella of spins which has the 120° structure. It should be remarked that the Hamiltonian (3.4) is not invariant under the transformation $UR_3U^\dagger$,

$$(UR_3U^\dagger)^\dagger H(UR_3U^\dagger) \neq H. \tag{3.18}$$

Only the ground-state energy is invariant under the irregular $O(3)$ transformation $UR_3U^\dagger$, *i.e.*,

$$\langle\Phi_i|(UR_3U^\dagger)^\dagger H(UR_3U^\dagger)|\Phi_i\rangle = \langle\Phi_i|H|\Phi_i\rangle \tag{3.19}$$

for $i = 1$ and 2.

The states $|\Phi_1(\theta,\phi)\rangle$ with various values of θ and ϕ have negative values of the chirality in the form

$$\langle\Phi_1(\theta,\phi)|\chi|\Phi_1(\theta,\phi)\rangle = -\frac{3}{4}N\cos^2\phi \tag{3.20}$$

and in contrast $|\Phi_2(\theta,\phi)\rangle$ has the positive chirality. The transformation $UR_3U^\dagger$ changes the absolute value of the chirality between 3/4 and 0, but never changes the sign. Thus the ground states have degeneracy of the chirality and the irregular $O(3)$ symmetry. This degeneracy of the ground states is the same as that of the corresponding classical model [98].

Most of $|\Phi_1(\theta,\phi)\rangle$ and $|\Phi_2(\theta,\phi)\rangle$ have a scalar chiral order,

$$\langle\Phi_1(\theta,\phi)|E_{123}|\Phi_1(\theta,\phi)\rangle = -\frac{3\sqrt{3}}{16}\sin\phi\cos^2\phi, \tag{3.21}$$

where E_{123} denotes the order-parameter operator of the scalar chiral order [145]

$$E_{123} = \boldsymbol{S}_1\cdot(\boldsymbol{S}_2\times\boldsymbol{S}_3). \tag{3.22}$$

Ferromagnetic Ising-like model ($\lambda < -0.5$)

Next we consider the XXZ model in the region $\lambda < -0.5$, in which the z-component spin-interactions, *i.e.*, ferromagnetic Ising interactions, are dominant. Here we choose the quantized axes of the Hamiltonian as follows

$$H = J\sum_{\langle i,j\rangle}(S_i^xS_j^x + S_i^yS_j^y + \lambda S_i^zS_j^z). \tag{3.23}$$

The ground states are given by

$$|\Phi_3\rangle = \bigotimes_i|\uparrow\rangle_i, \tag{3.24}$$

$$|\Phi_4\rangle = \bigotimes_i|\downarrow\rangle_i, \tag{3.25}$$

where the states $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of the operator S^z. These states have a perfect ferromagnetic order and they are exactly the same as the ground states of the classical model [98].

From now we prove that these two states belong to the ground states. Clearly, $|\Phi_3\rangle$ and $|\Phi_4\rangle$ are the eigenstates of the Hamiltonian (3.23) and the eigenvalues of both states are $3\lambda JN$. To show that the states (3.24) and (3.25) have the lowest energy, we again divide the Hamiltonian (3.23) into the cell-Hamiltonians

$$H_{\triangle(i,j,k)} = J\sum_{\langle l,m\rangle\in\triangle(i,j,k)}(S_l^xS_m^x + S_l^yS_m^y + \lambda S_l^zS_m^z). \tag{3.26}$$

Clearly the states (3.24) and (3.25) are also the eigenstates of these cell-Hamiltonians. Exactly diagonalizing the cell-Hamiltonian $H_{\triangle(i,j,k)}$, we easily find that the states $|\uparrow\rangle_i\otimes|\uparrow\rangle_j\otimes|\uparrow\rangle_k$ and $|\downarrow\rangle_i\otimes|\downarrow\rangle_j\otimes|\downarrow\rangle_k$ are the ground states of $H_{\triangle(i,j,k)}$ in $\lambda\le -0.5$ and the eigenvalue is $3\lambda J$. Thereby we find that the operator $H_{\triangle(i,j,k)} - 3\lambda J$ is positive semidefinite in the spin-space on the total lattice. This result shows that any eigenvalue of the Hamiltonian H is larger than $3\lambda JN$ or just equals to it. Thus the eigenvalues of $|\Phi_3\rangle$ and $|\Phi_4\rangle$ are the minimum energy of H. We hence find that the states $|\Phi_3\rangle$ and $|\Phi_4\rangle$ belong to the ground states of the total Hamiltonian (3.23).

As shown in the above proof, the states $|\Phi_3\rangle$ and $|\Phi_4\rangle$ also belong to the ground states of the XXZ model with $\lambda = -0.5$. In this case, $|\Phi_3\rangle$ and $|\Phi_4\rangle$ correspond to $|\Phi_1(\theta,\phi=\pi/2)\rangle$ and $|\Phi_1(\theta,\phi=-\pi/2)\rangle$, respectively.

3.2.2 Spin-wave expansion

Here we study ground-state properties of the spin-S XXZ antiferromagnets in the region $-0.5 < \lambda \leq 1$ using the spin-wave approximation [5, 77, 120]. As shown in the previous section, the ground states of the spin-1/2 XXZ antiferromagnet with $\lambda = -0.5$ have perfect long-range orders. Increasing λ from -0.5, we discuss how quantum effects are introduced into the ground states and how their physical values become different from those of the corresponding classical model. We calculate various physical values using the spin-wave expansion up to the first order of $1/S$.

In the ground states of the classical XXZ model with $-0.5 < \lambda < 1$, spins have the 120° structure in the xy plane. We define the quantized axes so that they have the 120° structure and we expand the quantum Hamiltonian from one of the ground states of the classical model. Oguchi [120] first applied this method to the Heisenberg model on the triangular lattice.

We choose the quantized axes in the xy plane and thereby we have

$$H = J \sum_{\langle i,j \rangle} (S_i^z S_j^z + S_i^x S_j^x + \lambda S_i^y S_j^y), \tag{3.27}$$

where S_i^α $(\alpha = x, y, z)$ denote spin operators. In this case, the order-parameter operator of the sublattice magnetization is given by

$$M_{\rm s} = \sum_{i \in A} S_i^z + \sum_{i \in B} \Big(-\frac{1}{2} S_i^z + \frac{\sqrt{3}}{2} S_i^x \Big) + \sum_{i \in C} \Big(-\frac{1}{2} S_i^z - \frac{\sqrt{3}}{2} S_i^x \Big) \tag{3.28}$$

and that of the chirality is

$$\chi = \frac{1}{2\sqrt{3} S^2} \sum_{(i \to j)} (\boldsymbol{S}_i \times \boldsymbol{S}_j)^y. \tag{3.29}$$

To change the quantized axes so that they have the 120° structure, we transform the Hamiltonian with the operator

$$U = \exp\Big(i \frac{2\pi}{3} \sum_{i \in B} S_i^y - i \frac{2\pi}{3} \sum_{i \in C} S_i^y \Big). \tag{3.30}$$

Thereby we obtain

$$U^\dagger H U = -\frac{J}{2} \sum_{\langle i,j \rangle} (S_i^z S_j^z + S_i^x S_j^x - 2\lambda S_i^y S_j^y) + \frac{\sqrt{3} J}{2} \sum_{(i \to j)} (S_i^z S_j^x - S_i^x S_j^z). \tag{3.31}$$

In this case, the thermal average of an observable A is given by

$$\langle A \rangle^T = \frac{\mathrm{Tr}[U^\dagger A U \exp(-\beta U^\dagger H U)]}{\mathrm{Tr} \exp(-\beta U^\dagger H U)}. \tag{3.32}$$

We transform the order-parameter operators with the operator U as follows

$$U^\dagger M_{\rm s} U = \sum_i S_i^z \tag{3.33}$$

and

$$U^\dagger \chi U = \frac{1}{4S^2} \sum_{\langle i,j \rangle} (S_i^z S_j^z + S_i^x S_j^x) - \frac{1}{4\sqrt{3}S^2} \sum_{(i\to j)} (S_i^z S_j^x - S_i^x S_j^z). \tag{3.34}$$

To expand spin operators, we use the Holstein-Primakoff transformation [49]

$$\begin{aligned} S_i^+ &= \sqrt{2S - a_i^\dagger a_i}\, a_i, \\ S_i^- &= a_i^\dagger \sqrt{2S - a_i^\dagger a_i}, \\ S_i^z &= S - a_i^\dagger a_i. \end{aligned} \tag{3.35}$$

where $a_i^\dagger$ denotes the creation operator of a boson at the site i. Fluctuations around the state $|\Phi_1\rangle$ are included as bosons. Thus we can obtain an expansion from one of the ground states of the model at $\lambda = -0.5$.

Using the Holstein-Primakoff transformation (3.36) and expanding the Hamiltonian (3.31) with respect to $1/S$ up to the first order, we obtain

$$\begin{aligned} U^\dagger H U = &- \frac{3NJS(S+1)}{2} + \frac{3JS}{4} \sum_k \{2 - (1-2\lambda)\gamma_k\}(a_k^\dagger a_k + a_k a_k^\dagger) \\ &- \frac{3J(1+2\lambda)S}{4} \sum_k \gamma_k (a_{-k} a_k + a_k^\dagger a_{-k}^\dagger), \end{aligned} \tag{3.36}$$

where $\{k\}$ denote wave vectors in the first Brillouin zone of the triangular lattice and

$$\gamma_k = \frac{1}{3}\Big\{\cos k_1 + \cos\Big(-\frac{1}{2}k_1 + \frac{\sqrt{3}}{2}k_2\Big) + \cos\Big(-\frac{1}{2}k_1 - \frac{\sqrt{3}}{2}k_2\Big)\Big\}. \tag{3.37}$$

Using the Bogoliubov transformation

$$\begin{aligned} a_k &= b_k \cosh\theta_{-k} - b_{-k}^\dagger \sinh\theta_k, \\ a_k^\dagger &= -b_{-k}\sinh\theta_k + b_k^\dagger \cosh\theta_{-k} \end{aligned} \tag{3.38}$$

and setting

$$\exp(2\theta_k) = \sqrt{\frac{1-\gamma_k}{1+2\lambda\gamma_k}}, \tag{3.39}$$

we can diagonalize the Hamiltonian (3.36) in the form

$$\begin{aligned} U^\dagger H U = &- \frac{3NJS(S+1)}{2} \\ &+ \frac{3JS}{2} \sum_k \sqrt{(1+2\lambda\gamma_k)(1-\gamma_k)}(2b_k^\dagger b_k + 1). \end{aligned} \tag{3.40}$$

In the ground state of the Hamiltonian (3.40), the number of bosons with any nonvanishing momentum is zero in the region $-0.5 \le \lambda \le 1$, since the energy spectrum of the boson is always positive. Hence the ground-state energy per bond is given by

$$E_{\mathrm{g}} = \langle H\rangle^{T=0}/3N = -\frac{S(S+1)J}{2} + \frac{SJ}{2N}\sum_k \sqrt{(1-\gamma_k)(1+2\lambda\gamma_k)}, \tag{3.41}$$

Table 3.1: Estimates of the ground-state energy per bond E_g/S^2J of the spin-1/2 XY antiferromagnet on the triangular lattice.

Method	Ground-state energy E_g/S^2J
Classical limit	-0.5
Variational method [97]	-0.523
Finite-lattice method [37, 118]	-0.545
Spin-wave theory $O(1/S^2)$ [95]	-0.536
Spin-wave theory $O(1/S)$	-0.532

in the region $-0.5 \leq \lambda \leq 1$. Evaluated values are shown in Figure 3.3 (a), and in Tables 3.1 and 3.2. The order-parameter operator of the sublattice magnetization (3.33) is transformed as

$$U^\dagger M_s U = N\Big(S+\frac{1}{2}\Big) - \frac{1}{2}\sum_k \cosh 2\theta_k (2b_k^\dagger b_k + 1) + \frac{1}{2}\sum_k \sinh 2\theta_k (b_k^\dagger b_{-k}^\dagger + b_{-k}b_k) \quad (3.42)$$

and the expectation value of the sublattice magnetization per site in the ground state is given by

$$m_s = \langle M_s\rangle^{T=0}/N = \Big(S+\frac{1}{2}\Big) - \frac{1}{4N}\sum_k \Big\{\sqrt{\frac{1-\gamma_k}{1+2\lambda\gamma_k}} + \sqrt{\frac{1+2\lambda\gamma_k}{1-\gamma_k}}\Big\}. \quad (3.43)$$

Calculated values are shown in Figure 3.3 (b). The chiral-order parameter (3.34) is written as

$$\begin{aligned} U^\dagger \chi U &= \frac{3N}{4} + \frac{3N}{4S} - \frac{3}{8S}\sum_k \{2\cosh 2\theta_k - \gamma_k \exp(-2\theta_k)\}(2b_k^\dagger b_k + 1) \\ &\quad + \frac{3}{8S}\sum_k \{2\sinh 2\theta_k + \gamma_k \exp(-2\theta_k)\}(b_{-k}^\dagger b_k^\dagger + b_k b_{-k}). \end{aligned} \quad (3.44)$$

Then the expectation value of the chiral-order parameter per site in the ground state is given by

$$q = \langle \chi\rangle^{T=0}/N = \frac{3}{4} + \frac{3}{4S} - \frac{3}{4SN}\sum_k \frac{(1+\lambda\gamma_k)\sqrt{1-\gamma_k}}{\sqrt{1+2\lambda\gamma_k}} \quad (3.45)$$

and estimates are shown in Figure 3.3 (c).

At $\lambda = -0.5$, the evaluated values of the ground-state energy, chirality and sublattice magnetization are exactly equal to the exact values given by state (3.6), though we have expanded them only up to the first order of $1/S$. The remaining higher-order terms in $1/S$ do not contribute to these physical quantities at $\lambda = -0.5$.

As λ is increased from -0.5 and the antiferromagnetic Ising interactions are introduced into the Hamiltonian, the values of the ground-state energy become lower than the classical

Figure 3.3: Evaluated values of (a) the energy per bond E_{g}/JS^2, (b) the sublattice magnetization per site m_{s}/S, and (c) the chirality per site q in the ground state of the spin-1/2 AFT XXZ model using the spin-wave expansion up to $1/S$ order. The parameter λ means the anisotropy of the z-component interactions. The symbols $*$ denote the exact results of the state $|\Phi_2\rangle$ and dashed lines denote values in the classical limit ($S \to \infty$).

Table 3.2: Estimates of the ground-state energy per bond E_g/S^2J of the spin-1/2 Heisenberg antiferromagnet on the triangular lattice.

Method	Ground-state energy E_g/S^2J
Classical limit	-0.5
Variational method (RVB state) [32]	-0.613
Variational method (120° structure) [53]	-0.715
Finite-lattice method [37, 118]	-0.729
Spin-wave theory $O(1/S^2)$ [95]	-0.729
Spin-wave theory $O(1/S)$ [120]	-0.718

values and the values of the sublattice magnetization decrease. Thus quantum fluctuations appear and become strong as λ increases. Near $\lambda = 1$, the sublattice magnetization is reduced fast depending on the parameter λ. On the other hand, the calculated values of the chirality change in a little different way. As λ is increased from -0.5, the values of the chirality become larger than the classical one. In the spin-1/2 XY model ($\lambda = 0$), the value is given by $q = 0.798$, where the corresponding classical value is 0.75. Since the eigenvalues of the chiral order parameter on a triangle-cell are ± 1 and 0 in the $S = 1/2$ case, it is possible that the value of chirality is enhanced by quantum effects. As the system approaches the Heisenberg model, the value of chirality quickly decreases in the same way as the sublattice magnetization does.

The values of the ground-state energy obtained by various methods are shown in Tables 3.1 and 3.2. In spite of our simple approximation, our results agree well with other results. In the spin-1/2 XY model, the evaluated value of the sublattice magnetization is given by $m_s = 0.448$ and the chirality is given by $q = 0.798$. In the Heisenberg model, we have $m_s = 0.238$ and $q = 0.405$. Estimates of the sublattice magnetization and the chirality by various methods are listed in Tables 3.4 and 3.5 (on page 59).

What we learnt from this study is as follows: As λ is enlarged from -0.5 to 1, quantum fluctuations are gradually introduced into the ground states and hence ground states smoothly change from the perfectly ordered state $|\Phi_2\rangle$. In the XY model, quantum fluctuations are not yet strong and values of the order parameters are fairly large. In the Heisenberg model, quantum fluctuations become strong, however the order parameters have non-vanishing values in the present approximation. We give further discussions about symmetry breaking in Section 3.3.

3.2.3 Phase diagram at low temperatures

In this section we discuss a phase diagram at finite temperatures in the spin-1/2 XXZ antiferromagnet. We study the chiral-ordered phase and the ferromagnetic phase, using the spin-wave approximation.

Villain [142] first pointed out that, in the frustrated classical XY model on two-dimensional lattices, the ground-state degeneracy of chirality causes an Ising-type phase transition at finite temperatures. After that, various authors studied the phase transition in the classical XY model [100, 81, 67]. Miyashita [98] studied the classical antiferromagnetic XXZ model on the triangular lattice using the Monte Carlo simulation and found that the chirality is ordered at sufficiently low temperatures in the region $-0.5 < \lambda < 1$ and a ferromagnetic order exists in the region $\lambda < -0.5$. At $\lambda = -0.5$, the ground states have a non-trivial degeneracy. Miyashita discussed that ferromagnetically ordered states are stable at finite temperatures in the classical model. In the classical XY model, the KT transition also occurs near the critical point of the chiral-order phase-transition [100].

In this section we only discuss orders defined by nonvanishing values of order parameters, namely the chiral order and ferromagnetic order. We study the phase diagram of the quantum XXZ antiferromagnets using the linear spin-wave approximation.

As shown in Section 3.2.2, the Hamiltonian is approximated in the form

$$U^\dagger H U = 3NE_{\mathrm{g}} + \sum_k \epsilon_k b_k^\dagger b_k \tag{3.46}$$

in the region $-0.5 \le \lambda \le 1$, where E_{g} denotes the ground-state energy defined in (3.41) and

$$\epsilon_k = 3JS\sqrt{(1+2\lambda\gamma_k)(1-\gamma_k)}. \tag{3.47}$$

The thermal average is defined by (3.32). The expectation value of the chirality at finite temperatures is given by

$$\begin{aligned}\langle\chi\rangle^T/N &= q - \frac{3}{2SN}\sum_k \frac{(1+\lambda\gamma_k)\sqrt{1-\gamma_k}}{\sqrt{1+2\lambda\gamma_k}}\langle b_k^\dagger b_k\rangle \\ &= q - \frac{3}{2SN}\sum_k \frac{(1+\lambda\gamma_k)\sqrt{1-\gamma_k}}{\sqrt{1+2\lambda\gamma_k}}\frac{1}{\exp(\beta\epsilon_k)-1},\end{aligned} \tag{3.48}$$

where q denotes the expectation value of the chirality per site at $T = 0$ given by (3.45).

In the region $-0.5 < \lambda < 1$, the dispersion relation behaves as $\epsilon_k \sim |k|$ for small k. The numerator of the integrand of (3.48) also has a zero-point at $\boldsymbol{k} = 0$. The existence of this zero-point comes from the stability of the chirality against (long-range) spin-wave excitations. The momentum summation in the second term of the right-hand-side of (3.48) is finite and hence the deviation of the chirality from ground-state values is small at low temperatures. This indicates that the chiral order remains even at finite temperatures.

At $\lambda = -0.5$, we have

$$\langle\chi\rangle^T/N = \frac{3}{4} - \frac{3}{4SN}\sum_k \frac{2-\gamma_k}{\exp(\beta\epsilon_k)-1} \tag{3.49}$$

and

$$\epsilon_k = 3JS(1-\gamma_k). \tag{3.50}$$

Since the dispersion relation is $\epsilon_k \sim k^2$ for small k, the second term (*i.e.*, the deviation of the chirality Δq) diverges as

$$\Delta q = \frac{3}{4SN}\sum_k \frac{2-\gamma_k}{\exp(\beta\epsilon_k)-1} \sim \frac{1}{\beta N}\sum_k \frac{1}{k^2} \to \infty. \tag{3.51}$$

This divergence means that the chirality is unstable at $\lambda = -0.5$ against spin-wave excitations and that the chirality is destroyed at finite temperatures. The phase boundary of the chiral order thus comes to an end at $\lambda = -0.5$, as shown in Figure 3.5.

At $\lambda = 1$, energy spectra have other zero-points at the corners of the Brillouin zone. Owing to these modes, the deviation of the chirality Δq becomes divergent as

$$\Delta q \sim \frac{1}{\beta N} \sum_k \frac{1}{(\boldsymbol{k} - \boldsymbol{k}')^2} \to \infty, \tag{3.52}$$

where $\boldsymbol{k}'$ denotes a momentum at one of the corners of the Brillouin zone, *e.g.* $(4\pi/3, 0)$. This result is consistent with the exact proof of the absence of the vector chiral order at finite temperatures [66].

Next we discuss the ferromagnetic phase. As shown in Section 3.2.1, ground states are ferromagnetically ordered in $\lambda < -0.5$. We use the Hamiltonian (3.23) and transform it into

$$U_z^\dagger H U_z = -\frac{J}{2} \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y - 2\lambda S_i^z S_j^z) - \frac{\sqrt{3}J}{2} \sum_{(i \to j)} (S_i^x S_j^y - S_i^y S_j^x), \tag{3.53}$$

where

$$U_z = \exp\Big(i\frac{2\pi}{3} \sum_{i \in B} S_i^z - i\frac{2\pi}{3} \sum_{i \in C} S_i^z \Big). \tag{3.54}$$

By the transformation U_z, spin fluctuations become space-translational invariant and spin waves with $\boldsymbol{k} \sim 0$ become dominant. Expanding the Hamiltonian with the Holstein-Primakoff transformation, we obtain

$$U_z^\dagger H U_z = 3NS^2 J\lambda + \sum_k \epsilon'_k a_k^\dagger a_k, \tag{3.55}$$

where

$$\epsilon'_k = 3SJ(-2\lambda - \gamma_k) - \sqrt{3}SJ\Big\{ \sin k_1 + \sin\Big(-\frac{1}{2}k_1 + \frac{\sqrt{3}}{2}k_2\Big) + \sin\Big(-\frac{1}{2}k_1 - \frac{\sqrt{3}}{2}k_2\Big) \Big\}. \tag{3.56}$$

The expectation value of the magnetization is given by

$$m = \Big\langle \sum_i S_i^z \Big\rangle^T = S - \frac{1}{N} \sum_k \langle a_k^\dagger a_k \rangle = S - \frac{1}{N} \sum_k \frac{1}{\exp(\beta \epsilon'_k) - 1}. \tag{3.57}$$

In the region $\lambda < -0.5$, the spectrum of the boson behaves as

$$\epsilon'_k \sim \frac{3SJ}{4}(-8\lambda - 4 + k^2). \tag{3.58}$$

A finite gap exists above the ground states, which comes from the fact that the ferromagnetic Ising interaction is dominant in $\lambda < -0.5$. In this region, the ferromagnetic order is hence stable against the spin-wave fluctuations and it can exist at sufficiently low temperatures. As λ is increased, the energy gap decreases. At $\Delta = -0.5$ it vanishes and we have

$$\epsilon'_k \sim \frac{3SJ}{4} k^2. \tag{3.59}$$

Then the deviation of the magnetization diverges as

$$\Delta m \sim \frac{1}{\beta N}\sum_k \frac{1}{k^2} \to \infty. \tag{3.60}$$

This divergence indicates that the magnetization is unstable and there is no magnetic order at finite temperatures. This result is different from that of the classical model by Miyashita [98].

Finally, we discuss possibilities of intermediate phases near $\lambda = -0.5$. As we have shown in Section 3.2.1, the ground states are non-trivially degenerate at $\lambda = -0.5$. We calculate the free energy at finite temperatures expanding from various ground states (3.15), to determine which state is most stable. It may be possible that a scalar-chiral-order phase appears at finite temperatures by quantum effects in an intermediate phase between the ferromagnetic and vector-chiral-order phases, since a scalar chiral order appears in a part of the degenerate ground-states.

We use the Hamiltonian (3.4) with $\lambda = -0.5$ and rotate the quantized axes with $R_3(\theta,\phi)$ as

$$\begin{aligned} R_3^\dagger U^\dagger H U R_3 = &-\frac{J}{2}\sum_{\langle i,j\rangle}(S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y) \\ &-\frac{\sqrt{3}J}{2}\sum_{(i\to j)}\{\cos\phi(S_i^z S_j^x - S_i^x S_j^z) - \sin\phi(S_i^y S_j^x - S_i^x S_j^y)\}. \end{aligned} \tag{3.61}$$

When $\phi = 0$, the quantized axes are in the xy plane and they have the 120° structure. As ϕ is increased, these axes close as bones of umbrella do. We expand the Hamiltonian (3.61) up to the first order of $1/S$ and thereby obtain

$$R^\dagger U^\dagger H U R = -\frac{3NJS^2}{2} + \sum_k \{3JS(1-\gamma_k) + \sqrt{3}JSg_k\sin\phi\}a_k^\dagger a_k, \tag{3.62}$$

where

$$g_k = \sin k_1 + \sin\Big(-\frac{1}{2}k_1 + \frac{\sqrt{3}}{2}k_2\Big) + \sin\Big(-\frac{1}{2}k_1 - \frac{\sqrt{3}}{2}k_2\Big). \tag{3.63}$$

This Hamiltonian is already diagonalized. The partition function of this system is given by

$$\begin{aligned} Z(\phi) &= \operatorname{Tr}\exp(-\beta R^\dagger U^\dagger H U R) \\ &= \exp\Big(\frac{3\beta NJS^2}{2}\Big)\prod_k \sum_{n_k=0}^{\infty}\exp\{-\beta\epsilon_k(\phi)n_k\}, \end{aligned} \tag{3.64}$$

where

$$\epsilon_k(\phi) = 3JS(1-\gamma_k) + \sqrt{3}JSg_k\sin\phi. \tag{3.65}$$

Hence the free energy per site is given by

$$\begin{aligned} F(\phi) &= -\frac{1}{\beta N}\log Z(\phi) \\ &= -\frac{3JS^2}{2} + \frac{1}{\beta N}\sum_k \log[1-\exp\{-\beta\epsilon_k(\phi)\}]. \end{aligned} \tag{3.66}$$

Figure 3.4: Values of the free energy $F(\phi)$ as a function of ϕ at various temperatures. These values are calculated by expanding them from various ground states (3.15) which have different values of ϕ. The ground state with $\phi = 0$ has the 120° structure and the state with $\phi = \pi/2$ corresponds to the ferromagnetically ordered state. Temperatures are written in the unit of JS^2/k_{B}.

Figure 3.5: Schematic phase diagram of the quantum XXZ antiferromagnets at finite temperatures. The parameter λ denotes the z-component anisotropy of the Hamiltonian. Phase boundaries are predicted without quantitative accuracy using the spin-wave expansions and the exact ground states.

We have evaluated $F(\phi)$ for various values of ϕ at finite temperatures. The results are shown in Figure 3.4.

The free energy $F(\phi)$ has the minimum value at $\phi = \pi/2$. This indicates that the state fluctuating around the ferromagnetic-ordered ground state (3.15) is most favored at each temperature and that the scalar chiral order can not appear at finite temperatures. However, as we have discussed before, even the ferromagnetic order can not exist at finite temperatures.

Taking into account all the above results, we obtain the phase diagram shown in Figure 3.5. We have drawn phase boundaries without quantitative accuracy on temperatures, since we have only discussed whether orders are stable against spin-wave excitations or not.

3.3 Low-lying states of finite-volume systems[2]

In this section we study low-lying states in finite-volume triangular lattices to clarify whether spontaneous symmetry breaking occurs at $T = 0$ in the thermodynamic limit. In Section 3.3.1, we give approximate forms of low-lying states and discuss properties of these states. In Section 3.3.2, with help of our approximation we discuss how rearrangements of the low-lying states bring on symmetry breakings of two types. Furthermore, in Section 3.3.3, we discuss the occurrence of symmetry breaking, studying the low-lying states of finite systems with the numerical diagonalization method. Some rigorous results for the low-lying states of *ferromagnets*, which are used in Section 3.3.1, are shown in Appendix.

3.3.1 An approximation for low-lying states

Here we give approximate forms of low-lying states of the quantum antiferromagnets on a finite-volume triangular lattice and then discuss properties of them. The ground states of antiferromagnets on finite systems are symmetric. Low-lying excited states play an important role in symmetry breaking in an infinite-volume limit. Mechanism of the symmetry breaking is discussed in the next section.

We consider the quantum *XXZ* antiferromagnets on the finite-volume lattice Λ with a periodic boundary condition. The size of the system is N, where $N = 3m$ with an integer m. The Hamiltonian is given by

$$H = J \sum_{\langle i,j\rangle \in \Lambda} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z), \tag{3.67}$$

where the summation runs over all the nearest-neighbor sites and the symbol λ denotes the anisotropy of the z-component interactions. The models in the region $-0.5 < \lambda \leq 1$ are considered.

We concentrate on low-lying states that have sublattice-translational invariance and C_{3V} invariance. (The symbol C_{3V} denotes the point group of the 120° rotation and reflection of the lattice.) Bernu *et al.* [12, 13] reported that there are many low-lying states of this type. Here we classify the states according to eigenvalues of the 60° rotation (C_6). We call the class of C_6-symmetric states *type α* and the class of C_6-antisymmetric states *type β*.

[2]The contents of this section were published in [101, 102].

As an approximation for the lowest states of type α and of type β in the $S^z_{\text{total}} = n$ (or $n + 1/2$) subspace, we consider the following states:

$$|n\alpha\rangle = \frac{(U + U^\dagger)|\mathrm{F}n\rangle}{\|(U + U^\dagger)|\mathrm{F}n\rangle\|}, \qquad |n\beta\rangle = \frac{(U - U^\dagger)|\mathrm{F}n\rangle}{\|(U - U^\dagger)|\mathrm{F}n\rangle\|} \tag{3.68}$$

for $n = 0, \pm 1, \pm 2, \ldots$, where the symbol U denotes the unitary operator

$$U = \exp\Big(i\frac{2\pi}{3}\sum_{i\in B} S^z_i - i\frac{2\pi}{3}\sum_{i\in C} S^z_i\Big) \tag{3.69}$$

and $\|(U \pm U^\dagger)|\mathrm{F}n\rangle\| = \langle \mathrm{F}n|(U \pm U^\dagger)^2|\mathrm{F}n\rangle^{1/2}$. The state $|\mathrm{F}n\rangle$ denotes the lowest state in the $S^z_{\text{total}} = n$ (or $n + 1/2$) subspace of the "ferromagnetic" XXZ model on Λ which is defined by the Hamiltonian

$$H_{\mathrm{F}} = -J \sum_{\langle i,j\rangle\in\Lambda} (S^x_i S^x_j + S^y_i S^y_j - 2\lambda S^z_i S^z_j). \tag{3.70}$$

Here the parameter λ is set equal to that in (3.67). We write the eigenvalue of H_{F} for the state $|\mathrm{F}n\rangle$ as $E_{\mathrm{f}n}$.

In the case of $\lambda = -0.5$, all states $\{|n\alpha\rangle\}$ and $\{|n\beta\rangle\}$ belong to the exact ground states which we [110] presented in Section 3.2.1. Generalizing these exact ground states to the region $-0.5 < \lambda \le 1$, we have proposed approximate forms (3.68). The approximate ground state $|0\alpha\rangle$ is also a generalization of the trial state of Betts and Miyashita [15] for the XY antiferromagnet. We first discuss properties of the approximate states (3.68). After that we verify that this approximation is good.

Here we discuss the meaning of the model (3.70). The states $|n\alpha\rangle$ and $|n\beta\rangle$ are linear combinations of $U|\mathrm{F}n\rangle$ and $U^\dagger|\mathrm{F}n\rangle$. The unitary operator U transforms the Hamiltonian (3.67) into the form

$$UHU^\dagger = -\frac{1}{2}J\sum_{\langle i,j\rangle}(S^x_i S^x_j + S^y_i S^y_j - 2\lambda S^z_i S^z_j) - \frac{\sqrt{3}}{2}J\sum_{\langle i\to j\rangle}(S^x_i S^y_j - S^y_i S^x_j), \tag{3.71}$$

where the symbol $i \to j$ goes from the sublattice A to B, B to C, and C to A. The first term in (3.71) gives the Hamiltonian (3.70). Thus the present approximation corresponds to neglecting the second term in (3.71).

In the thermodynamic limit of the ferromagnet (3.70), only $O(2)$ symmetry breaking can take place, since it has no frustration. The classical limit of the ferromagnet (3.70) in the region $-0.5 < \lambda \le 1$ has ferromagnetically ordered ground states, in which all spins are lying in the XY plane [98]. The spin-1/2 ferromagnetic XY model ($\lambda = 0$) on the triangular lattice has been studied by using the exact-diagonalization method [36, 118] and the spin-wave theory [117, 144]. The results indicate the existence of the ferromagnetic long-range order. As λ increases in the ferromagnet (3.70), quantum fluctuations are enhanced and the magnetization is reduced.

Furthermore, as shown in Section 3.3.A, we can obtain several exact results for the ferromagnet (3.70) on the finite-volume lattice Λ. The ground state is unique and it exists in the $S^z_{\text{total}} = 0$ subspace. Then it has $O(2)$-rotational invariance. (When N is an odd number, there exists trivial degeneracy; the states $|\mathrm{F}0\rangle$ and $|\mathrm{F}-1\rangle$ are degenerate.) The lowest state in the $S^z_{\text{total}} = n$ subspace, which we write as $|\mathrm{F}n\rangle$, is unique. The coefficients of $|\mathrm{F}n\rangle$ in the bases which are eigenstates of $\{\ S_i^z\ \}$ are nonnegative. All states $\{\ |\mathrm{F}n\rangle\ \}$ are translationally invariant and C_{6V}-invariant. (See Section 3.3.A.)

Using these rigorous results for the low-lying states of the ferromagnet, we can determine the spatial quantum numbers of the approximate states. We have verified in the small clusters that the spatial quantum numbers of the approximate states (3.68) are equal to those of the true states. Bernu *et al.* [12] also investigated the spatial quantum numbers of the low-lying states for the Heisenberg antiferromagnet and classified the low-lying states into three classes: Γ_1 (states with $k=0$ and even under inversion), Γ_2 (states with $k=0$ and odd under inversion), and Γ_3 [states with $k=\pm(4\pi/3,0)$]. When $S^z_{\mathrm{total}}(=n)=3l$ or $S^z_{\mathrm{total}}(=n+1/2)=3l+3/2$ with an integer l, $|n\alpha\rangle$ and $|n\beta\rangle$ belong to Γ_1 and Γ_2, respectively. Otherwise, both $|n\alpha\rangle$ and $|n\beta\rangle$ belong to Γ_3. As we show in the next section, our classification is useful in discussing the symmetry breaking about the sublattice magnetization and the chirality separately.

An advantage of our approximation is that the degrees of freedom of the Z_2(chiral) symmetry and the $O(2)$ symmetry are separated in it. Then we can discuss breakdown of each symmetry independently. The parts of the unitary operator, namely $(U \pm U^\dagger)$, can describe the chiral symmetry breaking and the parts of the low-lying states of the ferromagnet, namely $|\mathrm{F}n\rangle$ $(n=0,\pm1,\pm2,\ldots)$, can display the breakdown of the $O(2)$ symmetry.

We give a remark for the case of the Heisenberg antiferromagnet. Since the model is isotropic, a slight modification is necessary for the approximate ground state, $|0\alpha_{(\lambda=1)}\rangle$. We only give the form of an approximate ground state as follows:

$$|0\alpha'\rangle = \frac{1}{4\pi}\int d\Omega R(\mathbf{\Omega})|0\alpha_{(\lambda=1)}\rangle \Big/ \Big\| \frac{1}{4\pi}\int d\Omega R(\mathbf{\Omega})|0\alpha_{(\lambda=1)}\rangle \Big\|, \tag{3.72}$$

where $\mathbf{\Omega}$ is the unit vector with the spherical coordinates (θ,φ) and

$$R(\mathbf{\Omega}) = \exp\Big(i\varphi\sum_i S_i^z\Big)\exp\Big(i\theta\sum_j S_j^y\Big). \tag{3.73}$$

We now discuss the accuracy of our approximation. We compare the approximate low-lying states with the true ones, numerically diagonalizing finite systems. To compare with the ground state of the Heisenberg model, we use the state $|0\alpha_{(\lambda=1)}\rangle$ instead of (3.72), since it is not easy to treat (3.72) in numerical calculations. First we note that, as we have already mentioned, the spatial quantum numbers of our approximate low-lying states are equal to those of the true states: They are invariant under any sublattice translation and any translation of C_{3V}, and they have the same momentum as the true states. In the true system there indeed exist low-lying states of two types corresponding to the types α and β. Second, the approximate low-lying states have accurate expectation values of physical quantities. (See Table 3.3.) The expectation values of the energy are at most 2% higher than the exact values in the XY model and at most 7% higher in the Heisenberg model. We have calculated correlation functions of the sublattice magnetization and the chirality, excluding the autocorrelations. They are almost equal to the exact values in the $S=1/2$ XY model. In the $S=1/2$ Heisenberg model, we multiply the evaluated values by factor 1/3, since partial symmetry is broken in our approximate states (3.68), as mentioned above. (The coefficient 1/3 is derived using the arguments given in Section 3.4.) Finally

Figure 3.6: Two-fold structures in the spectrum of low-lying states.

we calculated overlaps between the exact low-lying states and the approximate ones. The results are shown in Table 3.3. In the XY model the approximate states have more than 90% overlaps with the exact states and in the Heisenberg model more than 70%. These situations are the same for the low-lying states in the $S^z_{\rm total} = 1$ and $S^z_{\rm total} = 2$ subspaces as well. Thus we find that the exact low-lying spectrum has the two-fold structures, as shown in Figure 3.6, and that the true low-lying states can be accurately described with the present approximation.

Using this approximation, we can estimate the expectation values of the energy. The ground-state energy is calculated as

$$\langle 0\alpha|H|0\alpha\rangle = \frac{E_{\rm f0} + 4E_{\rm f0}\langle {\rm F0}|U|{\rm F0}\rangle - 6\lambda J\langle {\rm F0}|U(\sum_{\langle i,j\rangle} S^z_i S^z_j)|{\rm F0}\rangle}{2 + 2\langle {\rm F0}|U|{\rm F0}\rangle}, \tag{3.74}$$

where we have used the relations $UHU^\dagger + U^\dagger HU = H_{\rm F}$ and $UHU = H_{\rm F}U^\dagger + U^\dagger H_{\rm F} - 3\lambda JU^\dagger \sum_{\langle i,j\rangle} S^z_i S^z_j$. The terms $\langle {\rm F0}|U|{\rm F0}\rangle$ and $\langle {\rm F0}|U(\sum_{\langle i,j\rangle} S^z_i S^z_j)|{\rm F0}\rangle$ correspond to the transition probabilities from the ferromagnetic ground state, $|{\rm F0}\rangle$, to the antiferromagnetic state, $U|{\rm F0}\rangle$. In the thermodynamic limit, these values are vanishing. Thus the ground-state energy is estimated as

$$\langle 0\alpha|H|0\alpha\rangle \simeq \frac{E_{\rm f0}}{2}. \tag{3.75}$$

Next we discuss the energy gaps. The energy gap between the ground state (type α) and the lowest state of type β is almost vanishing as

$$\begin{aligned}\langle 0\beta|H|0\beta\rangle - \langle 0\alpha|H|0\alpha\rangle &= \frac{-3E_{\rm f0}\langle {\rm F0}|U|{\rm F0}\rangle + 6\lambda J\langle {\rm F0}|U(\sum_{\langle i,j\rangle} S^z_i S^z_j)|{\rm F0}\rangle}{1 - \langle {\rm F0}|U|{\rm F0}\rangle^2} \\ &\simeq 0.\end{aligned} \tag{3.76}$$

The energy gap between the ground state of $S^z_{\rm total} = 0$ and the lowest state of $S^z_{\rm total} = 1$ is estimated as

$$\langle 1\alpha|H|1\alpha\rangle - \langle 0\alpha|H|0\alpha\rangle \simeq \frac{1}{2}(E_{\rm f1} - E_{\rm f0}). \tag{3.77}$$

Table 3.3: Various physical values of approximate states $|0\alpha\rangle$ and $|0\beta\rangle$ are compared with those of the exact ground state $|0\rangle$ and the lowest excited state $|1\rangle$ in the spin-1/2 (a) XY and (b) Heisenberg models. Expectation values of the energy, spin long-range order and chiral long-range order are calculated and divided with those of exact states. (See text.) Ratio of the expectation values to the true values are listed. Overlaps $|\langle 0|0\alpha\rangle|^2$ and $|\langle 1|0\beta\rangle|^2$ are also listed.

(a) XY model

size	type	ratio of energy	ratio of spin long-range order	ratio of chiral long-range order	overlaps
$N = 3$	α	1.0	1.0	1.0	1.0
	β	1.0	1.0	1.0	1.0
$N = 9$	α	0.992	1.037	0.999	0.979
	β	0.992	1.037	1.049	0.979
$N = 12$	α	0.973	1.202	1.221	0.847
	β	0.998	0.993	1.022	0.998
$N = 21$	α	0.986	1.079	1.037	0.918
	β	0.986	1.079	1.037	0.918

(b) Heisenberg model

size	type	ratio of energy	ratio of spin long-range order	ratio of chiral long-range order	overlaps
$N = 3$	α	1.0	0.333	0.333	1.0
	β	1.0	0.333	0.333	1.0
$N = 9$	α	0.932	0.665	0.437	0.788
	β	0.932	0.665	0.517	0.788
$N = 12$	α	0.929	0.435	0.567	0.799
	β	0.997	0.314	1.856	0.987
$N = 21$	α	0.936	0.582	0.777	0.464
	β	0.936	0.582	0.777	0.464

Relations between these energy gaps and the symmetry breaking of two types, namely creation of the spontaneous chirality and of the spontaneous sublattice magnetization, are discussed in the next section.

3.3.2 Contribution of low-lying states to symmetry breaking

As we have discussed in Section 2.4.2, many low-lying states converge to the ground states, as the system size is enlarged, and then linear combinations of these states make the symmetry breaking occur. Several authors [50, 74, 139, 12, 13] have discussed the mechanism of symmetry breaking in quantum Heisenberg antiferromagnets. In this section we study roles played by low-lying states of two types in symmetry breaking. Here we assume that the ground states of an infinite-volume system have a long-range order and that the symmetry breaks down. In Section 3.3.3 we study possibilities of the occurrence of symmetry breaking.

In antiferromagnets on a triangular lattice, there are two types of symmetry breaking. In the XY model, or in the XXZ model for $-0.5 < \lambda < 1$, the $O(2)$ symmetry and the Z_2(chiral) symmetry can break independently. In the Heisenberg model, both the spontaneous sublattice magnetization and the spontaneous chirality correspond to the breakdown of the $O(3)$ symmetry.

As shown in Section 3.3.1, the low-lying states on a finite-volume triangular lattice have twofold structures. The purpose of this section is to clarify the relations between the symmetry breaking of two types and the low-lying states of types α and β. Our approximation (3.68) helps us to understand the symmetry breaking of two types independently, since the degrees of freedom of the sublattice magnetization and of the chirality are separated in it.

In an infinite-volume system we can define four types of ground states, which are classified by existence of the spontaneous sublattice magnetization or the spontaneous chiral order. Here we show the definitions of four types.

1. *Symmetric states (mixed states)*,

$$\langle\cdots\rangle_1 = \lim_{N\uparrow\infty}\lim_{\beta\uparrow\infty}\frac{\mathrm{Tr}[\cdots\exp(-\beta H)]}{\mathrm{Tr}[\exp(-\beta H)]} = \omega(\cdots). \tag{3.78}$$

2. *States in which only the spontaneous chirality exists*,

$$\langle\cdots\rangle_2 = \lim_{B\downarrow 0}\lim_{N\uparrow\infty}\lim_{\beta\uparrow\infty}\frac{\mathrm{Tr}[\cdots\exp\{-\beta(H-BQ^z)\}]}{\mathrm{Tr}[\exp\{-\beta(H-BQ^z)\}]} \tag{3.79}$$

where Q^z denotes the z component of the chirality order-parameter operator

$$\boldsymbol{Q} = \frac{2}{\sqrt{3}}\sum_{\langle i\to j\rangle}(\boldsymbol{S}_i\times\boldsymbol{S}_j). \tag{3.80}$$

The summation is defined in the same way as in (3.71).

3. *States in which only the spontaneous magnetization exists*,

$$\langle\cdots\rangle_3 = \lim_{B\downarrow 0}\lim_{N\uparrow\infty}\lim_{\beta\uparrow\infty}\frac{\mathrm{Tr}[\cdots\exp\{-\beta(H-B(U\sum_i S_i^x U^\dagger + U^\dagger\sum_i S_i^x U))\}]}{\mathrm{Tr}[\exp\{-\beta(H-B(U\sum_i S_i^x U^\dagger + U^\dagger\sum_i S_i^x U))\}]}. \tag{3.81}$$

4. *Pure states*,

$$\langle\cdots\rangle_4 = \lim_{B\downarrow 0}\lim_{N\uparrow\infty}\lim_{\beta\uparrow\infty}\frac{\mathrm{Tr}[\cdots\exp\{-\beta(H-BU^\dagger\sum_i S_i^x U)\}]}{\mathrm{Tr}[\exp\{-\beta(H-BU^\dagger\sum_i S_i^x U)\}]} = \tilde{\omega}(\cdots). \tag{3.82}$$

Here the equilibrium states are defined as functionals of expectation values on an operator space. (This is familiar in studies of infinite-volume systems.) In the following, we show, using the approximate states (3.68), how each ground state is constructed of low-lying states.

1. Symmetric states (mixed states). By taking the thermodynamic limit of the finite-volume ground state, we get the symmetric ground state (3.78). No symmetry is broken in it.

2. States in which only the spontaneous chirality exists. We obtain the state $\langle\cdots\rangle_2$ by taking the thermodynamic limit under an infinitesimal effective field which is conjugate to the chiral order parameter.

An approximation of this state is given by $|2\rangle = U|\mathrm{F0}\rangle$. There remains the $O(2)$ invariance in it. Both Miyashita's trial function [97] and the variational function by Huse and Elser [53] belong to this type of ground state.

In the XY-like model, the state $U|\mathrm{F0}\rangle$ is constructed by making a linear combination of $|0\alpha\rangle$ and $|0\beta\rangle$,

$$\{|0\alpha\rangle,\ \ |0\beta\rangle\}\longrightarrow\{U|\mathrm{F0}\rangle,\ \ U^\dagger|\mathrm{F0}\rangle\}. \tag{3.83}$$

Thus with help of our approximation we find that, if the ground state (type α) and the lowest state of type β become degenerate in the infinite-volume limit and if they are rearranged between themselves, the Z_2 symmetry of the chirality is broken.

In the Heisenberg model, the degree of freedom of the chirality is continuous and the ground state is isotropic, as mentioned in (3.72). Then two states are not enough to break entirely the symmetry of the chirality. Koma and Tasaki [74] proposed an approximate state which describes breakdown of continuous symmetry and they argued that the thermodynamic limit of this approximate state is a pure state, in which continuous symmetry is broken. By applying their argument to the present case, an approximate state which has fully-ordered spontaneous chirality can be constructed in the form

$$\frac{1}{(2k+1)^{1/2}}\left\{|\Phi_{\mathrm{GS}}\rangle + \sum_{n=1}^{k}\left(\frac{(Q^+)^n|\Phi_{\mathrm{GS}}\rangle}{\|(Q^+)^n|\Phi_{\mathrm{GS}}\rangle\|}+\frac{(Q^-)^n|\Phi_{\mathrm{GS}}\rangle}{\|(Q^-)^n|\Phi_{\mathrm{GS}}\rangle\|}\right)\right\}. \tag{3.84}$$

where $Q^\pm = Q^x \pm iQ^y$ and $|\Phi_{\mathrm{GS}}\rangle$ denotes the ground state. The number k is of $o(N)$. This state has a nonvanishing expectation value of the operator Q^x. By rotating all the spins through the angle $\pi/2$ about the y axis, we obtain an approximation for the state $\langle\cdots\rangle_2$. According to the arguments by Koma and Tasaki [74], the infinite-volume limit of this approximate state become $\langle\cdots\rangle_2$. The states $(Q^\pm)^{2m}|\Phi_{\mathrm{GS}}\rangle$ belong to type α and $(Q^\pm)^{2m+1}|\Phi_{\mathrm{GS}}\rangle$ to β. Thus the state $\langle\cdots\rangle_2$ is constructed by a linear combination of low-lying states of type α and of type β.

In our approximation the expectation value of the spontaneous chirality is calculated as

$$\begin{aligned}\langle 2|Q^z|2\rangle &= \frac{E_{\mathrm{f0}}}{J}+\frac{E_{\mathrm{f0}}}{3J}\langle\mathrm{F0}|U|\mathrm{F0}\rangle - 2\lambda\langle\mathrm{F0}|\sum_{\langle i,j\rangle}S_i^zS_j^z|\mathrm{F0}\rangle\\ &\simeq \frac{E_{\mathrm{f0}}}{J} - 2\lambda\langle\mathrm{F0}|\sum_{\langle i,j\rangle}S_i^zS_j^z|\mathrm{F0}\rangle\end{aligned} \tag{3.85}$$

where the relations $UHU^{\dagger} = \dfrac{1}{2}H_{\mathrm{F}} - \dfrac{3}{4}JQ$ and $H = -H_{\mathrm{F}} + 3J\lambda \sum_{\langle i,j\rangle} S_i^z S_j^z$ are used and E_{f0} denotes the ground-state energy of the ferromagnet. As λ is increased from -0.5, the first term in (3.85) becomes large by quantum effects. The second term in (3.85), $\langle \mathrm{F0}| \sum_{\langle i,j\rangle} S_i^z S_j^z |\mathrm{F0}\rangle$, behaves as follows: At $\lambda = -0.5$ this term is vanishing, since there is no correlation between up and down spins in the ground state $|\mathrm{F0}\rangle$. As the parameter λ increases, nearest-neighbor pairs of up and down spins are favored. Then the term becomes large. Thus at $\lambda = 0$ the chirality is enhanced by the quantum effect of the first term and near $\lambda = 1$ the value is reduced by the contribution of the second term.

3. States in which only the spontaneous magnetization exists. In the state $\langle \cdots \rangle_3$ there exists the spontaneous magnetization, though there exists no spontaneous chirality.

In the XY-like model, the $O(2)$-symmetry breaking occurs in the following way. First we consider the case of the ferromagnetic XXZ model (3.70). As shown in Appendix A, the finite-volume ground state of the ferromagnet is unique and it has $O(2)$-rotational invariance. It was shown in Ref. [74] that the low-lying states $|\mathrm{F}n\rangle$ $[n = \pm 1, \pm 2, \ldots, \pm o(N)]$ converge to the ground state and pure infinite-volume ground states are constructed by taking linear combinations of the low-lying states. The state $|\text{F-order}\rangle$ denotes one of the ferromagnetically ordered ground states, where $\langle \text{F-order}|S_i^x|\text{F-order}\rangle \neq 0$ and $\langle \text{F-order}|S_i^y|\text{F-order}\rangle = 0$. In the case of the antiferromagnet, with help of the approximate low-lying states, we can understand the mechanism of the $O(2)$-symmetry breaking on the analogy of the ferromagnet. Under the effective field B in (3.81), the low-lying states of type α have an energy lower than those of β have. An approximate state for $\langle \cdots \rangle_3$ is given by $(U + U^{\dagger})|\text{F-order}\rangle$, which is constructed by making a linear combination of $(U + U^{\dagger})|\mathrm{F}n\rangle$ $(n = 0, \pm 1, \pm 2, \ldots)$. In the same way, by using low-lying states of type β, another state in which only the spontaneous magnetization exists is constructed as $(U - U^{\dagger})|\text{F-order}\rangle$. Thus we find that, if the low-lying states of the same type become degenerate in the infinite-volume limit and if rearrangements occur between them, the breakdown of the $O(2)$ symmetry occurs.

For the Heisenberg model, by applying the approximation of Koma and Tasaki [74] to this model, an approximate state of $\langle \cdots \rangle_3$ is written as

$$\frac{1}{\sqrt{2k+1}} \left\{ |\Phi_{\mathrm{GS}}\rangle + \sum_{n=1}^{k} \left(\frac{(O^+)^n |\Phi_{\mathrm{GS}}\rangle}{\|(O^+)^n |\Phi_{\mathrm{GS}}\rangle\|} + \frac{(O^-)^n |\Phi_{\mathrm{GS}}\rangle}{\|(O^-)^n |\Phi_{\mathrm{GS}}\rangle\|} \right) \right\} \tag{3.86}$$

where $O^+ = U \sum_i S_i^+ U^{\dagger} + U^{\dagger} \sum_i S_i^+ U$. All the low-lying states, $(O^+)^n|\Phi_{\mathrm{GS}}\rangle$ and $(O^-)^n|\Phi_{\mathrm{GS}}\rangle$, belong to the type α. Thus we can obtain the state $\langle \cdots \rangle_3$ by taking a linear combination of the low-lying states of the same type.

4. Pure states. The pure infinite-volume ground states have the same structure as the ground states of the classical model. The $O(2)$ symmetry and Z_2 symmetry are broken in the XY model, and the $O(3)$ symmetry of the sublattice magnetization and that of the chirality are broken in the Heisenberg model.

To construct the pure infinite-volume ground states, the symmetry breaking of two types discussed in the above should occur. A number of low-lying states of both types, α and β, become degenerate to the ground state and rearrangements occur between them. This is consistent with the previous arguments by Bernu *et al.* [12] and Koma and Tasaki [74].

By discussing the symmetry breaking of two types separately, we find that the spontaneous sublattice magnetization is created by rearrangements of the low-lying states of the same type and that the spontaneous chirality is by rearrangements of pairs of low-lying states of types α and β.

It is possible that, if long-range order of one type exists in the true system, only one type of symmetry breaking occurs in the thermodynamic limit. Though the result from the renormalization group [9] indicates existence of one critical point (critical spin $S_{\rm c}$), our arguments suggest that symmetry breaking can occur separately and that an intermediate phase can appear in which symmetry breaking of only one type occurs.

An approximation for this state is given by

$$|4\rangle = U|\text{F-order}\rangle \tag{3.87}$$

and the expectation values are related to the quantities of the ferromagnet in the forms

$$\langle 4|U\sum_i S_i^x U^\dagger|4\rangle = \langle \text{F-order}|\sum_i S_i^x|\text{F-order}\rangle \tag{3.88}$$

and

$$\langle 4|Q^z|4\rangle = \langle 2|Q^z|2\rangle. \tag{3.89}$$

3.3.3 Numerical results of finite-size systems

In this section we numerically study low-lying states of finite systems to verify the occurrence of symmetry breaking discussed in Section 3.3.2. We discuss the XY and Heisenberg antiferromagnets.

First we discuss the necessary conditions for symmetry breaking to occur. Bernu *et al.* [12] have also discussed these matters. We discuss the conditions of the creation of the spontaneous sublattice magnetization and of the spontaneous chirality separately.

As discussed in Refs. [12] and [74], when the symmetry breaking occurs in the thermodynamic limit, there should exist growing numbers of low-lying states which satisfy the following two conditions.

1. The excitation energy decays in the $1/N$ form.
2. The spatial symmetry is the same as that of the ground state of the classical model, i.e., the state has sublattice-translational invariance and C_{3V} invariance.

In the thermodynamic limit, these low-lying states become ground states. In general, all the pure ground states give the same physical quantities. The sublattice magnetization and the chirality per site should be the same throughout the ground states. From this consideration and the discussions in Section 3.3.2, we obtain the necessary condition of the creation of the spontaneous sublattice magnetization as follows:

3. A number of low-lying states of type α satisfy condition 1 and they have the same macroscopic value of long-range order of the sublattice magnetization.

The necessary condition of the creation of the spontaneous chirality is as follows:

4. Pairs of low-lying states of types α and β satisfy the condition 1 and they have the same macroscopic value of long-range order of the chirality.

Figure 3.7: Size dependence of the energy gap between the lowest state (type α) and the lowest excited state (type β) in the same S^z_{total} subspace for the Heisenberg model.

Bernu *et al.* [12] studied the low-lying states of the Heisenberg model on the triangular lattice. They found many low-lying states which satisfy the conditions 1 and 2, and found that these states have similar macroscopic values for the sublattice magnetization. They estimated the sublattice magnetization of the ground state in the infinite-volume limit for the Heisenberg model. Leung and Runge [82] estimated the sublattice magnetization and chirality of the ground state for the XY and Heisenberg models.

To examine these conditions explicitly, we study the energy gaps, the sublattice magnetization and the chirality of the low-lying states in the $S = 1/2$ XY and Heisenberg models, and estimate the physical values of the low-lying states in the infinite-volume limit. The systems of the size $N = 9$, 12, 21, and 27 with periodic boundary conditions are studied, using the exact-diagonalization method. We study the low-lying states which belong to the subspaces of $S^z_{\mathrm{total}} = 0$ (or 0.5) and of $S^z_{\mathrm{total}} = 1$ (or 1.5), and which satisfy the condition 2. (The ground state and some low-lying excited states really belong to these subspaces.) As we have indicated in Section 3.3.1, there exist the C_6-symmetric (type α) and C_6-antisymmetric (type β) states. In many cases, we studied the lowest state of each subspace. There are exceptions: In the space of $S^z_{\mathrm{total}} = 0$ for $N = 12$ and $S^z_{\mathrm{total}} = 1.5$ for $N = 21$ of the Heisenberg model, we chose the first excited state of type β, since the first-excited state of type α and the lowest state of type β are degenerate and form a paired doublet, and the ground state (type α) and the first excited state of type β are in pairs.

The lowest state in the $S^z_{\mathrm{total}} = 0$ and C_6-symmetric (type α) subspace, which is the ground state, has been already calculated up to $N = 36$ in Refs. [12] and [82]. We used the data for $N = 36$ in Ref. [82].

First we discuss the energy gap. Here the energy gap is defined as the difference between the total energies of two states. The energy gap between the lowest state of type α and that of β is shown in Figure 3.7. In many cases the states of types α and β are degenerate. The energy gap between the ground state (type α) and the lowest state (type α) of the $S^z_{\mathrm{total}} = 1$

Figure 3.8: Size dependence of the energy gap between the ground state (type α) and the lowest state (type α) in S^z_{total}=1.

subspace is plotted in Figure 3.8. It decreases proportionally to N^{-1}. As we discussed in Section 3.3.2, the former energy gap is relevant to the symmetry breaking of the chirality and the latter to the breakdown of the rotational symmetry which creates the spontaneous sublattice magnetization. The latter energy gap corresponds to the singlet-triplet gap in the Heisenberg model, which was reported in Ref. [82].

It was proved that, if there is a long-range order, the energy gap decreases in the N^{-1} form or faster [50, 74]. Thus the above results are consistent with the existence of long-range order in the XY and Heisenberg antiferromagnets.

Next we consider the sublattice magnetization which is observed with the operator

$$M = \sum_{i\in A} S_i^x + \sum_{i\in B}\Big(-\frac{1}{2}S_i^x + \frac{\sqrt{3}}{2}S_i^y\Big) + \sum_{i\in C}\Big(-\frac{1}{2}S_i^x - \frac{\sqrt{3}}{2}S_i^y\Big). \tag{3.90}$$

We calculated the long-range order of the sublattice magnetization $\langle M^2\rangle/N^2$. The values of the spontaneous sublattice magnetization m are estimated, using the relation $m = \lim_{N\uparrow\infty}\sqrt{6\langle M^2\rangle}/N$ for the Heisenberg model and $m = \lim_{N\uparrow\infty} 2\sqrt{\langle M^2\rangle}/N$ for the XY model. We show a derivation of these relations in Section 3.4. We fit the data of the sublattice magnetization m to the $N^{-1/2}$ form. This finite-size correction was derived from the spin-wave theory [52] and using the effective Hamiltonian for a large spin [10]. [We also fit the long-range correlation $\langle M^2\rangle/N^2$ to the $N^{-1/2}$ form, using the data for $N = 3$, 9, 12, 21, and 27, and found that the correction term of $O(N^{-1})$ in the fitting of $\langle M^2\rangle/N^2$ is larger than that in the fitting of m. Therefore we adopted the fitting of m.] The results for the XY model are shown in Figure 3.9. We extrapolated in the $N^{-1/2}$ form, using the data for $N = 9$, 12, 21, and 27. For the ground state we also used the data for $N = 36$ which was reported in Ref. [82]. The values in the infinite-volume limit are shown in Table 3.4. They coincide with each other. Thus the condition 3 is satisfied in the XY model. The data for the Heisenberg model are shown in Figure 3.10. The values in the infinite-size limit are

Figure 3.9: Size dependence of the sublattice magnetization of the lowest state in each subspace of the XY model, which is estimated through $2\sqrt{\langle M^2 \rangle / N}$. The result for N=36 is also listed [82]. SW denotes the result from the spin-wave expansion [110].

Figure 3.10: Size dependence of the sublattice magnetization of the lowest state in each subspace of the Heisenberg model, which is estimated through $\sqrt{6\langle M^2 \rangle / N}$. The result for $N = 36$ is also listed [82]. SW denotes the result from the spin-wave expansion [96].

Figure 3.11: Size dependence of the chirality of the lowest state in each subspace of the XY model which is estimated through $\sqrt{\langle (Q^z)^2\rangle}/N$. The result for $N = 36$ is also listed [82]. SW denotes the result from the spin-wave expansion [110].

shown in Table 3.5. They are almost equal. Thus the condition 3 is also satisfied in the Heisenberg model. All the values are nonvanishing and close to the result by the spin-wave theory. On the other hand, as reported in Ref. [82], if we fit the data $\langle M^2\rangle/N^2$ to $N^{-1/2}$, we obtain the estimate $m \simeq 0$. The values seriously depend on the fitting form. Hence it may be still hard to conclude the existence of the long-range order in the Heisenberg model.

Finally we consider the chiral order, which is observed with the operator

$$\boldsymbol{Q} = \frac{2}{\sqrt{3}} \sum_{<i\to j>} \boldsymbol{S}_i \times \boldsymbol{S}_j, \tag{3.91}$$

where the symbol $i \to j$ goes from the sublattice A to B, B to C, and C to A. We calculated the long-range order of the chirality $\langle (Q^z)^2\rangle/N^2$. The values of the spontaneous chirality q are estimated using the relations $q = \lim_{N\uparrow\infty} \sqrt{3\langle (Q^z)^2\rangle}/N$ for the Heisenberg model and $q = \lim_{N\uparrow\infty} \sqrt{\langle (Q^z)^2\rangle}/N$ for the XY model. (See Section 3.4.) We show the results for the XY model in Figure 3.11 and for the Heisenberg model in Figure 3.12. For the XY model we extrapolated the expectation values of the chirality in the $N^{-3/2}$ form, which we derive from the finite-size correction of the spin-wave theory [110]. On the other hand, in the Heisenberg model the finite-size correction behaves in the $N^{-1/2}$ form, as discussed by Azaria *et al.* [10] This difference of the correction terms comes from the fact that in the Heisenberg model the chirality is sensitive to spin-wave fluctuations of long wavelength, while in the XY model the chiral order is stable against them. The extrapolated values are shown in Tables 3.4 and 3.5. In the the XY model the values are consistent with each other and nonvanishing, which suggests the existence of the chiral order. Thus the condition 4 is satisfied. In the Heisenberg model the values do not agree with each other. It is necessary to calculate larger systems to conclude that these low-lying states have the same chirality. We cannot fit the data to a form including higher-order terms, since the system sizes are

Figure 3.12: Size dependence of the chirality of the lowest state in each subspace of the Heisenberg model which is estimated through $\sqrt{3\langle (Q^z)^2\rangle /N}$. The result for $N = 36$ is also listed [82]. SW denotes the result from the spin-wave expansion [110].

too small. Thus we cannot conclude the existence of the long-range order of the chirality in the Heisenberg model.

Table 3.4: Estimates of the sublattice magnetization m and the chirality q for the $S = 1/2$ XY antiferromagnet on the triangular lattice.

	m	q
$S^z_{\rm total}$=0, type α	0.41	0.76
$S^z_{\rm total}$=0, type β	0.39	0.76
$S^z_{\rm total}$=1, type α	0.42	0.77
$S^z_{\rm total}$=1, type β	0.41	0.78
Spin-wave expansion $O(1/S)$ [110]	0.448	0.798
Spin-wave expansion $O(1/S^2)$ [82]	0.437	

To test the mechanism of symmetry breaking of the chirality which we have discussed in Section 3.3.2, we construct the state

$$|\phi\rangle = \frac{1}{\sqrt{2}}(|\alpha\rangle + i|\beta\rangle), \tag{3.92}$$

where $|\alpha\rangle$ ($|\beta\rangle$) denotes the lowest state of type α (β) in each $S^z_{\rm total}$ subspace. We observe the spontaneous chirality of this state. The expectation value of the chirality is calculated

Figure 3.13: Spontaneous symmetry breaking of the chirality of the XY model which is created by a linear combination $(|\alpha\rangle + i|\beta\rangle)/\sqrt{2}$ of the low-lying states of types α and β.

Figure 3.14: Spontaneous symmetry breaking of the chirality of the Heisenberg model which is created by a linear combination $(|\alpha\rangle + i|\beta\rangle)/\sqrt{2}$ of the low-lying states of types α and β. The values are multiplied by the factor $\sqrt{3}$.

Table 3.5: Estimates of the sublattice magnetization m and the chirality q for the $S = 1/2$ Heisenberg antiferromagnet on the triangular lattice.

	m	q
$S^z_{\mathrm{total}} = 0$, type α	0.24	0.21
$S^z_{\mathrm{total}} = 0$, type β	0.22	0.16
$S^z_{\mathrm{total}} = 1$, type α	0.24	0.54
$S^z_{\mathrm{total}} = 1$, type β	0.38	0.73
Spin-wave expansion $O(1/S)$ [120, 110]	0.238	0.405
Spin-wave expansion $O(1/S^2)$ [96]	0.250	

through the relation

$$\langle \phi | Q^z | \phi \rangle = i \langle \alpha | Q^z | \beta \rangle. \tag{3.93}$$

The estimates in the XY model are shown in Figure 3.13. They are almost equal to the values shown in Figure 3.11. This coincidence suggests the correctness of the mechanism of the chiral symmetry breaking discussed in Section 3.3.2. In the Heisenberg model we multiply the calculated values by the factor $\sqrt{3}$, since the symmetry is not fully broken in the state (3.92); the state (3.84) should be properly used instead of (3.92). The estimates are shown in Figure 3.14. Thus we can break the chiral symmetry by making a linear combination of low-lying states of type α and of type β.

From the above results we summarize that the necessary conditions 3 and 4 are satisfied in the XY model. In the Heisenberg model the necessary conditions are almost satisfied, though there remains ambiguity about whether the low-lying states have the same properties. In any case, in the above results there is no evidence which contradicts the occurrence of symmetry breaking.

3.3.A Low-lying states of the ferromagnetic *XXZ* model

In this Appendix, we show the uniqueness of the ground state and give spatial quantum numbers of the low-lying states of the spin-S XXZ ferromagnet on finite systems. We discuss the model on the finite-volume triangular lattice Λ with a periodic boundary condition. For simplicity, we restrict the number of sites to an even integer. The Hamiltonian is given by

$$H_{\mathrm{F}} = -J \sum_{\langle i,j \rangle \in \Lambda} (S^x_i S^x_j + S^y_i S^y_j + \eta S^z_i S^z_j), \tag{3.94}$$

where $J > 0$ and $\eta < 1$. The summation runs over all the nearest-neighbor sites.

The Hamiltonian (3.94) has nonpositive off-diagonal elements. The bases which have the same S^z_{total} are connected by the elements of the Hamiltonian. From the Perron-Frobenius theorem, the lowest eigenstate in each S^z_{total} subspace is unique and it has nonnegative coefficients.

Here we show that the ground state exists uniquely in the $S^z_{\rm total} = 0$ subspace. We consider the following Hamiltonian

$$H'_{\rm F} = -\sum_{i,j\in\Lambda} J_{ij}(S_i^x S_j^x + S_i^y S_j^y + \eta S_i^z S_j^z), \tag{3.95}$$

where $J_{ij} \geq 0$ for all i and j. Affleck and Lieb [3] showed that, in the antiferromagnetic XXZ chain, the ground state exists uniquely in the $S^z_{\rm total} = 0$ subspace. As they did, we transform the Hamiltonian (3.95) using the unitary operator

$$W = \exp\Big(i\frac{\pi}{2}\sum_i S_i^x\Big) \tag{3.96}$$

into the form

$$W^\dagger H'_{\rm F} W = -\sum_{i,j\in\Lambda} J_{ij}\Big\{\frac{1}{4}(1+\eta)(S_i^+S_j^- + S_i^-S_j^+) + \frac{1}{4}(1-\eta)(S_i^+S_j^+ + S_i^-S_j^-) + S_i^zS_j^z\Big\}. \tag{3.97}$$

In the region $-1 < \eta < 1$, this transformed Hamiltonian has nonpositive off-diagonal elements. It has two connected blocks, i.e., all bases in the subspaces with even $S^z_{\rm total}$ are connected by the elements of the Hamiltonian and those with odd $S^z_{\rm total}$ are connected. From the Perron-Frobenius theorem, the lowest eigenstate in each connected subspace is unique. Thus we find that the number of the ground states is at most two in the original model (3.95). The lowest states in the $S^z_{\rm total} = n$ and $S^z_{\rm total} = -n$ subspaces are degenerate. When level crossing of the ground state occurs, more than two ground states must exist, which contradicts the above result. Thus in the whole region of various parameters $\{\ J_{ij}\ \}$, the ground state should exist in the same $S^z_{\rm total}$ subspace.

For the region $\eta < -1$, as Affleck and Lieb did, we can show the above results using the unitary operator

$$W = \exp\Big(i\frac{\pi}{2}\sum_i S_i^y\Big). \tag{3.98}$$

To obtain the eigenvalue $S^z_{\rm total}$ of the ground state, we consider the case $J_{ij} = J$ for all i and j. The Hamiltonian can be written in the form

$$H'_{\rm F} = -J\{(\boldsymbol{S})^2 - (1-\eta)(S^z)^2\}, \tag{3.99}$$

where $\boldsymbol{S} = (S^x, S^y, S^z)$ and $S^\alpha = \sum_{i\in\Lambda} S_i^\alpha$ $(\alpha = x, y, z)$. The ground state of this model is unique and it has the eigenvalues $S_{\rm total} = SN$ and $S^z_{\rm total} = 0$. [137] From the above results, we find that the ground state of the original model (3.94) in the regions $\eta < -1$ and $-1 < \eta < 1$ exists uniquely in the $S^z_{\rm total} = 0$ subspace.

This argument can be extended to the ferromagnetic XXZ model on any lattice. The ferromagnet on a bipartite lattice is equivalent to the XXZ antiferromagnet with the z-component anisotropy $-\eta$. In this case the above results are consistent with what were proved by Lieb and Mattis [85], and Affleck and Lieb [3].

Lastly, we give the spatial quantum numbers of the lowest state in each $S^z_{\rm total}$ subspace. The Hamiltonian (3.94) is invariant under any translation, rotation, and reflection. As we have shown in the above, the lowest state is nondegenerate and it has nonnegative coefficients. From this fact, we find that the lowest state has the eigenvalue 1 for any translation, rotation, and reflection, i.e., it is translationally invariant and C_{6V}-invariant.

3.4 Relations between long-range order and symmetry breaking[3]

Here we discuss the relation between spontaneous symmetry breaking m and the long-range order parameter σ. It has been discussed[99, 73] that the relation is given by $m = \sqrt{3}\sigma$ for the Heisenberg antiferromagnet and by $m = \sqrt{2}\sigma$ for the XY antiferromagnet on bipartite lattices. But these relations are not valid in the antiferromagnets on the triangular lattice. Here we show that, in the antiferromagnets on the triangular lattice, the factor becomes $\sqrt{2}$ times as large as the above.

Our arguments are based on the assumption that the symmetric infinite-volume ground state (3.78) is decomposed into the pure ground states. Koma and Tasaki[73] used this decomposition to explain the factor $\sqrt{3}$ for the Heisenberg antiferromagnets on bipartite systems.

The spontaneous sublattice magnetization m is defined as

$$m \equiv \lim_{B\downarrow 0}\lim_{N\uparrow\infty}\lim_{\beta\uparrow\infty}\frac{1}{N}\frac{\mathrm{Tr}[M\exp\{-\beta(H-BM)\}]}{\mathrm{Tr}[\exp\{-\beta(H-BM)\}]}. \tag{3.100}$$

Using the sublattice-translational invariance and equivalence of the sublattice magnetization, we have

$$m = \tilde{\omega}(S_0^x), \tag{3.101}$$

where the state $\tilde{\omega}(\cdots)$ is defined by (3.82). The long-range order parameter of the sublattice magnetization σ_m is defined by

$${\sigma_m}^2 \equiv \lim_{N\uparrow\infty}\lim_{\beta\uparrow\infty}\frac{1}{N^2}\frac{\mathrm{Tr}[M^2\exp(-\beta H)]}{\mathrm{Tr}[\exp(-\beta H)]}. \tag{3.102}$$

Using the rotational and translational invariance, we obtain

$$\begin{aligned}{\sigma_m}^2 = \lim_{|r|\uparrow\infty}\frac{1}{3}\ \{\ &\omega(S_0^xS_r^x) + \omega(-\frac{1}{2}S_0^xS_{r+\boldsymbol{e_1}}^x + \frac{\sqrt{3}}{2}S_0^xS_{r+\boldsymbol{e_1}}^y)\\ &+\omega(-\frac{1}{2}S_0^xS_{r+\boldsymbol{e_2}}^x - \frac{\sqrt{3}}{2}S_0^xS_{r+\boldsymbol{e_2}}^y)\},\end{aligned} \tag{3.103}$$

where the state ω is defined by (3.78). The sites 0 and r belong to the sublattice A and $\boldsymbol{e_1}$ ($\boldsymbol{e_2}$) denotes the unit lattice vector which belongs to the sublattice B (C).

We also define the spontaneous chirality q as

$$q \equiv \lim_{B\downarrow 0}\lim_{N\uparrow\infty}\lim_{\beta\uparrow\infty}\frac{1}{N}\frac{\mathrm{Tr}[Q^z\exp\{-\beta(H-BM)\}]}{\mathrm{Tr}[\exp\{-\beta(H-BM)\}]} = \tilde{\omega}(Q^z(0)) \tag{3.104}$$

and the long-range order parameter of the chirality σ_q as

$${\sigma_q}^2 \equiv \lim_{N\uparrow\infty}\lim_{\beta\uparrow\infty}\frac{1}{N^2}\frac{\mathrm{Tr}[(Q^z)^2\exp(-\beta H)]}{\mathrm{Tr}[\exp(-\beta H)]} = \lim_{|r|\uparrow\infty}\omega(Q^z(0)Q^z(r)), \tag{3.105}$$

[3]The contents of this section were published in [101].

where the operator $Q^z(r)$ is the z component of the chiral order-parameter operator on the unit triangular cell,

$$\boldsymbol{Q}(r) = \frac{2}{\sqrt{3}}(\boldsymbol{S}_r \times \boldsymbol{S}_{r+\boldsymbol{e}_1} + \boldsymbol{S}_{r+\boldsymbol{e}_1} \times \boldsymbol{S}_{r+\boldsymbol{e}_2} + \boldsymbol{S}_{r+\boldsymbol{e}_2} \times \boldsymbol{S}_r). \tag{3.106}$$

Now we derive the relations between m and σ_m, and between q and σ_q. Our results are as follows: For the XY model

$$m = 2\sigma_m \qquad \text{and} \qquad q = \sigma_q, \tag{3.107}$$

and for the Heisenberg model

$$m = \sqrt{6}\sigma_m \qquad \text{and} \qquad q = \sqrt{3}\sigma_q. \tag{3.108}$$

The relation $m = \sqrt{6}\sigma_m$ for the Heisenberg model has been already used by Bernu *et al.*[12].

To derive these relations, we use the following standard arguments. It is widely believed that the mixed state ω can be naturally decomposed into pure equilibrium states,[19]

$$\omega(\cdots) = \int d\alpha \omega_\alpha(\cdots), \tag{3.109}$$

where $\{\omega_\alpha\}$ denote the pure states and the parameter α describes their properties. The state $\tilde{\omega}$, which is defined in eq. (3.82), is one of ω_α. The pure states have the cluster property,[19]

$$\omega_\alpha(A_0 B_r) \xrightarrow[|r|\uparrow\infty]{} \omega_\alpha(A_0)\omega_\alpha(B_r) \tag{3.110}$$

for any local operators A and B.

XY-Like Model

In the XXZ model with $-0.5 < \Delta < 1$, it is expected that the decomposition (3.109) is of the form

$$\omega(\cdots) = \frac{1}{4\pi}\int_0^{2\pi} d\theta \{\omega_{\theta,+}(\cdots) + \omega_{\theta,-}(\cdots)\}, \tag{3.111}$$

where $\omega_{\theta,+}$ ($\omega_{\theta,-}$) denote the states which have positive (negative) chirality and in which vectors of spins on the sublattice A form the angle θ with the x axis. The state $\tilde{\omega}$ corresponds to $\omega_{\theta=0,+}$. The pure states have following expectation values of the sublattice magnetization:

$$\begin{aligned}
\omega_{\theta,+}\Big(S_0^x\Big) &= m\cos\theta, \quad \omega_{\theta,-}\Big(S_0^x\Big) = m\cos\theta, \\
\omega_{\theta,+}\Big(-\frac{1}{2}S_{\boldsymbol{e_1}}^x + \frac{\sqrt{3}}{2}S_{\boldsymbol{e_1}}^y\Big) &= m\cos\theta, \quad \omega_{\theta,-}\Big(-\frac{1}{2}S_{\boldsymbol{e_1}}^x + \frac{\sqrt{3}}{2}S_{\boldsymbol{e_1}}^y\Big) = m\cos(\theta - \frac{2\pi}{3}), \\
\omega_{\theta,+}\Big(-\frac{1}{2}S_{\boldsymbol{e_2}}^x - \frac{\sqrt{3}}{2}S_{\boldsymbol{e_2}}^y\Big) &= m\cos\theta, \quad \omega_{\theta,-}\Big(-\frac{1}{2}S_{\boldsymbol{e_2}}^x - \frac{\sqrt{3}}{2}S_{\boldsymbol{e_2}}^y\Big) = m\cos(\theta + \frac{2\pi}{3}),
\end{aligned} \tag{3.112}$$

and the chirality

$$\omega_{\theta,\pm}(Q^z(0)) = \pm q. \tag{3.113}$$

Using the decomposition (3.111) and the property (3.110), we find that the long-range order parameter of the sublattice magnetization (3.103) is transformed as

$$
\begin{aligned}
{\sigma_m}^2 &= \lim_{|r|\uparrow\infty} \frac{1}{12\pi}\int_0^{2\pi} d\theta \Big\{ \omega_{\theta,+}(S_0^x S_r^x) + \omega_{\theta,+}(-\frac{1}{2}S_0^x S_{r+\boldsymbol{e}_1}^x + \frac{\sqrt{3}}{2}S_0^x S_{r+\boldsymbol{e}_1}^y) \\
&\quad + \omega_{\theta,+}(-\frac{1}{2}S_0^x S_{r+\boldsymbol{e}_2}^x - \frac{\sqrt{3}}{2}S_0^x S_{r+\boldsymbol{e}_2}^y) + \omega_{\theta,-}(S_0^x S_r^x) \\
&\quad + \omega_{\theta,-}(-\frac{1}{2}S_0^x S_{r+\boldsymbol{e}_1}^x + \frac{\sqrt{3}}{2}S_0^x S_{r+\boldsymbol{e}_1}^y) + \omega_{\theta,-}(-\frac{1}{2}S_0^x S_{r+\boldsymbol{e}_2}^x - \frac{\sqrt{3}}{2}S_0^x S_{r+\boldsymbol{e}_2}^y)\Big\} \\
&= \frac{1}{12\pi}\int_0^{2\pi} d\theta \\
&\quad \times \Big[\omega_{\theta,+}(S_0^x)\Big\{\omega_{\theta,+}(S_0^x) + \omega_{\theta,+}(-\frac{1}{2}S_{\boldsymbol{e}_1}^x + \frac{\sqrt{3}}{2}S_{\boldsymbol{e}_1}^y) + \omega_{\theta,+}(-\frac{1}{2}S_{\boldsymbol{e}_2}^x - \frac{\sqrt{3}}{2}S_{\boldsymbol{e}_2}^y)\Big\} \\
&\quad + \omega_{\theta,-}(S_0^x)\Big\{\omega_{\theta,-}(S_0^x) + \omega_{\theta,-}(-\frac{1}{2}S_{\boldsymbol{e}_1}^x + \frac{\sqrt{3}}{2}S_{\boldsymbol{e}_1}^y) + \omega_{\theta,-}(-\frac{1}{2}S_{\boldsymbol{e}_2}^x - \frac{\sqrt{3}}{2}S_{\boldsymbol{e}_2}^y)\Big\}\Big] \\
&= \frac{m^2}{4\pi}\int_0^{2\pi} d\theta \cos^2\theta = \frac{m^2}{4}. \qquad (3.114)
\end{aligned}
$$

Thus we obtain the relation $m = 2\sigma_m$.

In the same way, the long-range order parameter of the chirality, (3.105), is estimated as

$$
\begin{aligned}
{\sigma_q}^2 &= \lim_{|r|\uparrow\infty} \frac{1}{4\pi}\int_0^{2\pi} d\theta \Big\{\omega_{\theta,+}(Q^z(0)Q^z(r)) + \omega_{\theta,-}(Q^z(0)Q^z(r))\Big\} \\
&= \frac{1}{4\pi}\int_0^{2\pi} d\theta\{\omega_{\theta,+}(Q^z(0))^2 + \omega_{\theta,-}(Q^z(0))^2\} = q^2. \qquad (3.115)
\end{aligned}
$$

Thus we get the relation $q = \sigma_q$.

Heisenberg Model

For the Heisenberg model it is expected that the mixed state $\omega(\cdots)$ is decomposed as

$$\omega(\cdots) = \frac{1}{8\pi^2}\int d\Omega \int_0^{2\pi} d\phi\, \omega_{\boldsymbol{\Omega},\phi}(\cdots), \qquad (3.116)$$

where the vector $\boldsymbol{\Omega}$ is perpendicular to the plane to which all spins are parallel, and the angle ϕ denotes rotation with respect to the vector $\boldsymbol{\Omega}$. The direction of the vector $\boldsymbol{\Omega}$ and that of the chirality are the same, which are described with the spherical coordinates (θ, φ). The state $\tilde{\omega}$ corresponds to the state $\omega_{\varphi=0,\phi=0}$. The pure states have the following expectation values of the sublattice magnetization

$$
\begin{aligned}
&\omega_{\boldsymbol{\Omega},\phi}\Big(S_0^x\Big) = m(\cos\varphi\cos\theta\cos\phi - \sin\varphi\sin\phi), \qquad (3.117) \\
&\omega_{\boldsymbol{\Omega},\phi}\Big(-\frac{1}{2}S_{\boldsymbol{e}_1}^x + \frac{\sqrt{3}}{2}S_{\boldsymbol{e}_1}^y\Big) \\
&\quad = m\Big\{\cos\Big(\varphi - \frac{2\pi}{3}\Big)\cos\theta\cos\Big(\phi + \frac{2\pi}{3}\Big) - \sin\Big(\varphi - \frac{2\pi}{3}\Big)\sin\Big(\phi + \frac{2\pi}{3}\Big)\Big\}, \\
&\omega_{\boldsymbol{\Omega},\phi}\Big(-\frac{1}{2}S_{\boldsymbol{e}_2}^x - \frac{\sqrt{3}}{2}S_{\boldsymbol{e}_2}^y\Big) \\
&\quad = m\Big\{\cos\Big(\varphi + \frac{2\pi}{3}\Big)\cos\theta\cos\Big(\phi - \frac{2\pi}{3}\Big) - \sin\Big(\varphi + \frac{2\pi}{3}\Big)\sin\Big(\phi - \frac{2\pi}{3}\Big)\Big\},
\end{aligned}
$$

and the chirality

$$\omega_{\mathbf{\Omega},\phi}(\boldsymbol{Q}(0)) = q\mathbf{\Omega}. \tag{3.118}$$

Using the decomposition (3.116) and the property (3.110), we find that the long-range order parameter of the sublattice magnetization is transformed as

$$\begin{aligned}
{\sigma_m}^2 &= \frac{1}{24\pi^2}\int d\Omega \int_0^{2\pi} d\phi\, \omega_{\mathbf{\Omega},\phi}(S_0^x) \\
&\quad \times \{\omega_{\mathbf{\Omega},\phi}(S_0^x) + \omega_{\mathbf{\Omega},\phi}(-\frac{1}{2}S_{\boldsymbol{e}_1}^x + \frac{\sqrt{3}}{2}S_{\boldsymbol{e}_1}^y) + \omega_{\mathbf{\Omega},\phi}(-\frac{1}{2}S_{\boldsymbol{e}_2}^x - \frac{\sqrt{3}}{2}S_{\boldsymbol{e}_2}^y)\} \\
&= \frac{m^2}{6}.
\end{aligned} \tag{3.119}$$

Thus we obtain the relation $m = \sqrt{6}\sigma_m$.

Using the decomposition (3.116) and the property (3.110), we find that the long-range order parameter of the chirality is transformed as

$$\begin{aligned}
{\sigma_q}^2 &= \frac{1}{3}\lim_{|r|\uparrow\infty} \omega(\boldsymbol{Q}(0)\boldsymbol{Q}(r)) \\
&= \frac{q^2}{24\pi^2}\int d\Omega \int_0^{2\pi} d\phi \mathbf{\Omega}^2 = \frac{q^2}{3},
\end{aligned} \tag{3.120}$$

where the isotropy of the state is used. Thus we get the relation $q = \sqrt{3}\sigma_q$.

3.5 Summary and discussions

To summarize, we have studied ground-state properties of the quantum Heisenberg and XXZ antiferromagnets on the triangular lattice.

In Section 3.2, we showed exact ground states of the XXZ antiferromagnets in the region $\lambda \leq -0.5$, and studied the ground-state and thermal properties in the region $-0.5 < \lambda \leq 1$ using the spin-wave theory. Most of the exact ground states at $\lambda = -0.5$ have the long-range order with the 120° structure. These ground states have the perfect sublattice magnetization. These exact ground states give a new reliable standpoint to understand ground-state properties of the XXZ antiferromagnets. As λ increases from -0.5 to 1, quantum effects smoothly appear in the ground states. Near $\lambda = 0$, values of the sublattice magnetization decrease slightly, but on the other hand values of the chirality become larger than the classical limit. Thus in the antiferromagnetic XY model the ground state is not so fluctuating with quantum effects and it has the sublattice order. Furthermore, the chirality is ordered even at finite temperatures. Near the antiferromagnetic Heisenberg model, quantum effects become strong, and the values of the magnetization and the chirality rapidly decay. Estimates of both the magnetization and the chirality are non-vanishing in the Heisenberg model, though the λ dependence of these quantities suggests that the Heisenberg model is near the critical point.

To clarify whether symmetry breaking occurs or not in the XY and Heisenberg antiferromagnets, we studied low-lying states of the quantum antiferromagnets on finite-volume triangular lattices in Section 3.3. We gave approximate forms of low-lying states, which have twofold structures. It was found that these approximate states resemble the true states in various properties. We classified the low-lying states by the eigenvalues of C_6, namely C_6-symmetric and C_6-antisymmetric. States of both types exist in pairs in the true low-lying spectrum. We discussed how rearrangements of the low-lying states of two types bring on the symmetry breaking. The spontaneous chirality is created by taking a linear combination of pairs of low-lying states of types α and β. The spontaneous sublattice magnetization is obtained by making a linear combination of low-lying states of the same type.

Numerically studying low-lying states of finite systems, we discussed whether the necessary conditions of the symmetry breaking are satisfied or not. We found that the conditions are satisfied in the XY antiferromagnet. The estimate of the sublattice magnetization is $m = 0.41$ and that of the chirality is $q = 0.77$. These values are less than the spin-wave results by 7% and 4%, respectively. In the Heisenberg antiferromagnet the conditions are almost satisfied, although the estimates of the sublattice magnetization and the chirality do not converge well for lack of system size. The sublattice magnetization is estimated as $m = 0.22$–0.38 and the chirality as $q = 0.16$–0.73, where the results from the spin-wave expansion are $m = 0.25$ and $q = 0.45$. Since the extrapolated results seriously depend on fitting forms, it is still hard in the present study to conclude definitely the existence of long-range order in the Heisenberg model. However, it should be remarked that there are plenty of low-lying states that converge to the ground state faster than the softest magnon excitation and these states have twofold structures that are needed to create the 120° structure in ground states. Furthermore, Bernu *et al.* also found existence of towers of low-lying states that create the Néel order in the infinite-volume limit [13]. We believe that these results support the existence of symmetry breaking.

We also studied the phase diagram at low temperatures using the spin-wave theory and found that the chiral order is stable against spin-wave excitations in the region $-0.5 < \lambda < 1$. The results given by the spin-wave expansion indicate that the system of $\lambda = -0.5$ has no order at finite temperatures. For $\lambda < -0.5$, the ferromagnetic Ising interaction is dominant and then the ferromagnetic order exists at sufficiently low temperatures.

We give a remark that the real system of the XXZ model with $\lambda = -0.5$ may have some order at finite temperatures. Indeed, as shown in Section 3.2.1, the Hamiltonian itself is not invariant with any continuous transformation that changes the sign of the magnetization or the chirality. If any order appears at finite temperatures, it may be the ferromagnetic order, since the free energy of the ferromagnetic phase is lower than that of the chiral phase. To test this possibility, a more delicate study is needed.

We did not argue the KT transition in this chapter. Ding and Makivic [25, 26] found KT transition in spin-1/2 ferromagnetic XY model. Hence it is expected that KT-type transition may occur accompanied with or independently on the chiral-order phase transition. The relation between the KT transition and the chiral order phase-transition is also an interesting problem. To reveal this relation, further studies from other approaches are needed.

Part II

Elementary excitations

Chapter 4

Spin-wave excitations of the Heisenberg and $\boldsymbol{XXZ}$ antiferromagnets

In this chapter, we discuss properties of elementary excitations in the Heisenberg antiferromagnets on hypercubic lattices. Section 4.1 contains a brief review about properties of the spin-wave excitations in one-dimensional antiferromagnets. In Section 4.2, we show an upper bound for the lowest threshold of the spin-wave spectrum in two- and three-dimensional quantum antiferromagnets. The spin-wave spectrum is bounded as $\varepsilon(\boldsymbol{k}) \leq c|\boldsymbol{k}|$, where c gives an upper bound for the spin-wave velocity. In the large-S limit, our upper bound coincides with the spin-wave spectrum given by the spin-wave theory. In Appendix, we show various upper bounds of the excitation spectrum. Some of them will be used in the next chapter.

4.1 One-dimensional system

It is instructive to discuss elementary excitations in the $S = 1/2$ Heisenberg chain first, because there are exact solutions.

$\boldsymbol{S = 1/2}$ Heisenberg model

Spin-wave excitations of the one-dimensional Heisenberg antiferromagnet were evaluated by des Cloizeaux and Pearson [22], using the Bethe-ansatz solution. They showed that the lowest one-particle excitation has the dispersion law

$$\varepsilon(k) = \frac{\pi J}{2}|\sin k| \qquad -\pi \leq k \leq \pi. \tag{4.1}$$

After that, Faddeev and Takhtajan [30] argued that the natural one-particle excitation is a doublet of spin-1/2 spin waves, *i.e.*, kinks, and it satisfies the dispersion law shown in Figure 4.1. Roughly speaking, elementary excitations are created by spin flips in local domains and each local region has two domain walls, *i.e.*, kinks, at both ends, since we are considering the one-dimensional system. Thus in the one-dimensional system natural excitations are pairs of kinks.

Figure 4.1: Dispersion law of the one-particle excitation. The lower threshold behaves as $\omega = \pi J|\sin k|/2$ and the upper one $\omega = \pi J|\sin k/2|$.

$S \geq 1$ Heisenberg model

For general spin models, Haldane [43, 44] first argued that excitation spectra of the one-dimensional Heisenberg antiferromagnets differ according to whether the spin is an integer or a half-odd-integer; spin-integer models have a unique ground state with a finite excitation gap on it, but on the other hand spin-half-integer models have no gap. After that, excitations in $S \geq 1$ models were studied extensively in literature [71, 18, 116, 3, 2, 45]. Various approximate and numerical results indicate that Haldane's conjecture is correct. Later his conjecture to spin-half-integer models was rigorously proved by Affleck and Lieb [3].

Spectral properties of $S(k, \omega)$

In experiments, excitation spectra are observed through the dynamical structure factor

$$S(k,\omega) = \sum_n |\langle 0|S_k^z|n\rangle|^2 \delta(\omega - E_n + E_0), \tag{4.2}$$

where $|0\rangle$ ($|n\rangle$) denotes the ground state (an eigenstate) of the Hamiltonian. This spectral function has information about excited states created by the operation of S_k^z. To compare results from theoretical and experimental studies on the excitation spectrum, many authors have been interested in properties of $S(k,\omega)$. Neutron scattering experiments at low temperatures showed existence of sharp excitations with the dispersion law (4.1) for all momenta [29, 54] and also found the broad continuum around $k = \pi$ [114].

However, in theoretical studies, it is hard to calculate $S(k,\omega)$ from the Bethe-ansatz solution exactly. The $S = 1/2$ XY model is an exception: The function $S(k,\omega)$ of the spin-1/2 XY model was evaluated and the results show that $S(k,\omega)$ only contains the one-particle excitations [115, 112]. On the other hand, it is expected for the Heisenberg model that $S(k,\omega)$ contains both the one-particle and multi-particle excitations, and hence $S(k,\omega)$ has a continuum spectrum above the one-particle excitation spectrum. Hohenberg and Brinkman [48] studied $S(k,\omega)$ of the $S = 1/2$ Heisenberg antiferromagnet using sum rules and showed that most of spectral weight of $S(k,\omega)$ concentrates near lowest frequency $\varepsilon(k)$ at small k. (We will give related discussions on the Hubbard model in Section 5.1. See also Section 4.A.)

4.2 Two and three dimensional systems[1]

In this section we discuss the spin-wave spectrum in the two and three dimensional Heisenberg antiferromagnets. We show upper bounds for the spin-wave spectrum on Néel-ordered ground states.

4.2.1 Introduction

As we have discussed in Chapter 2, quantum Heisenberg and XXZ antiferromagnets on the square and cubic lattices have Néel-ordered ground states. For these systems, the Nambu-Goldstone theorem for quantum spin systems [79, 148] states that there are gapless elementary excitations. The spin-wave theory [5, 77] succeeded in giving a precise description of the Goldstone bosons, *i.e.*, magnons, in the Heisenberg antiferromagnet. The linear spin-wave theory predicts that spin-wave excitations have the gapless k-linear dispersion relation $\varepsilon(\boldsymbol{k}) \simeq 2\sqrt{d}SJ|\boldsymbol{k}|$ for small k. Recently neutron-scattering experiments [1, 46] in La_2CuO_4 reported that magnon excitations follow the dispersion given by the spin-wave theory.

4.2.2 Upper bounds of the spin-wave spectrum

The purpose of this section is to estimate the excitation spectrum of the spin-S Heisenberg and XXZ antiferromagnets on the d-dimensional $L \times \cdots \times L$ hypercubic lattice $\Lambda \subset \mathbf{Z}^d$ for $d \geq 2$. We prove an upper bound for the lowest threshold of the spectrum of elementary excitations on ground states with broken symmetries. Our upper bound has the same momentum dependence as the dispersion relation given by the spin-wave theory. For $S \gg 1$, the upper bound coincides with the result of the spin-wave approximation.

The Hamiltonian is given by

$$\mathcal{H}_\Lambda = J \sum_{\langle i,j \rangle \in \Lambda} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z), \tag{4.3}$$

where $0 \leq \lambda \leq 1$ and the summation runs over all the nearest-neighbor sites. Let us consider the system under the small staggered magnetic field,

$$\mathcal{H}_\Lambda(B) = \mathcal{H}_\Lambda - B\mathcal{M}_\Lambda, \tag{4.4}$$

[1]The contents of this section were published in [104].

where

$$\mathcal{M}_\Lambda = \sum_{i\in A} S_i^x - \sum_{i\in B} S_i^x. \tag{4.5}$$

We define the normalized ground state of $\mathcal{H}_\Lambda(B)$ as $|\Phi_{\mathrm{GS},B}\rangle$. We take a thermodynamic limit applying an infinitesimally small field B.

As an excited state, we consider the following standard trial state

$$|\Psi_B(\boldsymbol{k})\rangle = S_k^z|\Phi_{\mathrm{GS},B}\rangle / \|S_k^z|\Phi_{\mathrm{GS},B}\rangle\|, \tag{4.6}$$

where $S_k^z = L^{-d/2}\sum_j S_j^z \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_j)$, $\boldsymbol{k} = (k_1, k_2, \ldots, k_d)$ and $\|S_k^z|\Phi_{\mathrm{GS},B}\rangle\| = \langle\Phi_{\mathrm{GS},B}|S_{-k}^z S_k^z|\Phi_{\mathrm{GS},B}\rangle^{1/2}$. When spins lie in the xy plane, the operation of S_i^z flips the spin at the site i. The excitation energy of $|\Psi_B(\boldsymbol{k})\rangle$ is given by

$$\varepsilon(\boldsymbol{k}) = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\{\langle\Psi_B(\boldsymbol{k})|\mathcal{H}_\Lambda(B)|\Psi_B(\boldsymbol{k})\rangle - \langle\Phi_{\mathrm{GS},B}|\mathcal{H}_\Lambda(B)|\Phi_{\mathrm{GS},B}\rangle\} \tag{4.7}$$

and the staggered magnetization is

$$m_{\mathrm{s}} = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\frac{1}{L^d}\langle\Phi_{\mathrm{GS},B}|\mathcal{M}_\Lambda|\Phi_{\mathrm{GS},B}\rangle. \tag{4.8}$$

We take the momentum $\boldsymbol{k}$ as $\boldsymbol{k} \neq 0$, $\boldsymbol{k} \neq (\pi, \ldots, \pi)$ and $k_m = 2\pi l_m/L$ $(0 \le l_m \le L-1)$, so that $|\Phi_{\mathrm{GS},B}\rangle$ and $|\Psi_B(\boldsymbol{k})\rangle$ are orthogonal. This trial state is called the Bijl-Feynman single-mode approximation [16, 33]. A similar trial state was studied by Horsch and von der Linden in the two-dimensional system with no magnetic field [50]. Using the state (4.6), we show an upper bound of the spin-wave spectrum as follows.

Theorem 4.2.1 (Momoi): If the ground state has a Néel order, *i.e.*, if $m_{\mathrm{s}} > 0$, the energy spectrum $\varepsilon(\boldsymbol{k})$ is bounded as

$$\varepsilon(\boldsymbol{k}) \le \frac{2dJ(\rho_x+\rho_y)}{{m_{\mathrm{s}}}^2}\sqrt{\rho_x(1+\lambda\gamma_k)+\rho_z(\lambda+\gamma_k)}\sqrt{1-\gamma_k}, \tag{4.9}$$

where

$$\rho_\alpha = -\lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\frac{1}{L^d d}\sum_{\langle i,j\rangle\in\Lambda}\langle\Phi_{\mathrm{GS},B}|S_i^\alpha S_j^\alpha|\Phi_{\mathrm{GS},B}\rangle \tag{4.10}$$

for $\alpha = x$, y and z, and

$$\gamma_k = \frac{1}{d}\sum_{i=1}^{d}\cos k_i. \tag{4.11}$$

Proof of Theorem 4.2.1. As in ref. [50], the excitation energy of $|\Psi_B(\boldsymbol{k})\rangle$ is calculated as

$$\begin{aligned}
&\langle\Psi_B(\boldsymbol{k})|\mathcal{H}_\Lambda(B)|\Psi_B(\boldsymbol{k})\rangle - \langle\Phi_{\mathrm{GS},B}|\mathcal{H}_\Lambda(B)|\Phi_{\mathrm{GS},B}\rangle \\
&= \frac{\langle\Phi_{\mathrm{GS},B}|[[S_{-k}^z, \mathcal{H}_\Lambda(B)], S_k^z]|\Phi_{\mathrm{GS},B}\rangle}{2\langle\Phi_{\mathrm{GS},B}|S_{-k}^z S_k^z|\Phi_{\mathrm{GS},B}\rangle} \\
&= \frac{2J(1-\gamma_k)\langle\Phi_{\mathrm{GS},B}|\sum_{\langle i,j\rangle\in\Lambda}(-S_i^x S_j^x - S_i^y S_j^y)|\Phi_{\mathrm{GS},B}\rangle + B\langle\Phi_{\mathrm{GS},B}|\mathcal{M}_\Lambda|\Phi_{\mathrm{GS},B}\rangle}{2L^d\langle\Phi_{\mathrm{GS},B}|S_{-k}^z S_k^z|\Phi_{\mathrm{GS},B}\rangle}.
\end{aligned} \tag{4.12}$$

The excitation energy in the thermodynamic limit is given by

$$\varepsilon(\boldsymbol{k}) = \frac{2Jd(\rho_x+\rho_y)(1-\gamma_k)}{2S_\perp^z(\boldsymbol{k})}, \tag{4.13}$$

where $S_\perp^z(\boldsymbol{k})$ denotes the structure factor of the Néel-ordered ground state,

$$S_\perp^z(\boldsymbol{k}) = \lim_{B\searrow 0}\lim_{\Lambda\nearrow \mathbf{Z}^d}\langle\Phi_{\mathrm{GS},B}|S_{-k}^z S_k^z|\Phi_{\mathrm{GS},B}\rangle. \tag{4.14}$$

To bound the structure factor from below, we use (2.76) of Theorem 2.1.10,

$$2S_\perp^z(\boldsymbol{k}) \geq \frac{{m_\mathrm{s}}^2\sqrt{1-\gamma_k}}{\sqrt{\rho_x(1+\lambda\gamma_k)+\rho_z(\lambda+\gamma_k)}}. \tag{4.15}$$

Combining (4.13) and (4.15), we obtain (4.9). ■

We thus find that the lowest spin-wave spectrum is bounded from above by a gapless k-linear dispersion relation. When $\lambda=1$, our upper bound (4.9) has the same momentum dependence as the spin-wave spectrum given by the linear spin-wave theory. This theorem also shows the upper bound of the spin-wave velocity v_s in the form

$$v_\mathrm{s} \leq \sqrt{2d(1+\lambda)(\rho_x+\rho_z)}(\rho_x+\rho_y)J/{m_\mathrm{s}}^2. \tag{4.16}$$

The expectation value $\varepsilon(\boldsymbol{k})$ can be bounded from below as well. In Theorem 2.1.10, the transverse structure factor $S_\perp^z(\boldsymbol{k})$ is bounded from above in the form

$$2S_\perp^z(\boldsymbol{k}) \leq \left[\frac{(\rho_x+\rho_y)(1-\gamma_k)}{\lambda(1+\gamma_k)}\right]^{1/2}. \tag{4.17}$$

Using this inequality, we obtain

$$\varepsilon(\boldsymbol{k}) \geq 2dJ\sqrt{\lambda(\rho_x+\rho_y)(1-{\gamma_k}^2)}. \tag{4.18}$$

(We remark that this gives only a lower bound for the expectation value of the single-mode approximation and not for the spin-wave spectrum.) Both the upper and lower bounds have the k-linear dispersion relation for small k and hence $\varepsilon(\boldsymbol{k})$ has the gapless k-linear dispersion relation.

Finally, we discuss the large-S limit of the spectrum. For the Heisenberg antiferromagnet, we have Proposition 2.3.1,

$$\lim_{S\nearrow\infty} m_\mathrm{s}/S = 1, \tag{4.19}$$

$$\lim_{S\nearrow\infty} \rho_x/S^2 = 1, \tag{4.20}$$

$$\lim_{S\nearrow\infty} \rho_y/S^2 = \lim_{S\nearrow\infty} \rho_z/S^2 = 0. \tag{4.21}$$

From these rigorous results, we find that the upper bound coincides with the lower bound in the large-S Heisenberg model and hence we obtain

$$\varepsilon(\boldsymbol{k}) = 2dSJ\sqrt{1-{\gamma_k}^2}. \tag{4.22}$$

This spectrum has the same dispersion relation as that given by the spin-wave theory [5, 77]. This shows that the single-mode approximation gives a precise spin-wave spectrum in the large-S limit. For the large-S XXZ model ($0 \le \lambda < 1$), it is expected that the ground state becomes the Néel state and we have $\rho_x \simeq S^2$, $\rho_y \simeq O(S)$, $\rho_z \simeq O(S)$ and $m_{\rm s} \simeq S$, though we have not proved it. Then we expect that the upper bound for the spectrum behaves as $2dJS\sqrt{(1+\lambda\gamma_k)(1-\gamma_k)}$. This spectrum coincides with that given by the linear spin-wave theory for the XXZ model [117].

Recently, Stringari obtained a better upper bound of the spin-wave spectrum [135]. He discussed the lowest threshold $\omega(k)$ of the dynamical structure factor $S(k,\omega)$ using sum rules. (See also Appendix.) His upper bound is as follows.

Theorem 4.2.2 (Stringari): If the ground state has a Néel order, the lowest frequency $\omega(\boldsymbol{k})$ is bounded as

$$\omega(\boldsymbol{k}) \le \frac{2dJ\sqrt{\rho_x+\rho_y}}{m_{\rm s}}\sqrt{\rho_x(1+\lambda\gamma_k)+\rho_z(\lambda+\gamma_k)}\sqrt{1-\gamma_k}. \tag{4.23}$$

This upper bound has the same momentum dependence as our upper bound, but the coefficient is smaller by the multiplicative factor $m_{\rm s}/\sqrt{\rho_x+\rho_y}$. We discuss the relation between (4.9) and (4.23) in Appendix. The difference between two bounds partly comes from multi-magnon states included in the Feynman state (4.6). In the large-S limit, both upper bounds become equal to the excitation spectrum given by the spin-wave approximation. This indicates that state (4.6) in the large-S limit only contains one-magnon excitations. (See Appendix.)

4.A Various upper bounds for the excitation spectrum

In this Appendix, we show various upper bounds for the excitation spectrum at $T=0$. These upper bounds relate to Theorems 4.2.1 and 4.2.2, and to the study by Hohenberg and Brinkman [48], which we referred to on page 73. Furthermore, we use these bounds in Chapter 5.

Let us write the ground state in the thermodynamic limit as $\langle\cdots\rangle$. We consider only an ergodic (or a pure) state. Then in two- and three-dimensional systems, the state $\langle\cdots\rangle$ may have broken symmetries. Sometimes we also write the state as $|0\rangle$.

We discuss the excitation spectrum of the dynamical structure factor at $T=0$

$$S(k,\omega) = \frac{1}{\pi}\int dt \langle A_k A_{-k}^\dagger(t)\rangle \exp(i\omega t), \tag{4.24}$$

where $A_k = |\Omega|^{-1/2}\sum_{j\in\Omega} A_j \exp(ikr_j)$ and $A_{-k}^\dagger(t)$ denotes the time evolution of the operator $A_{-k}^\dagger$. (Later, we take the infinite limit $\Omega \nearrow \mathbf{Z}^d$ to avoid influence from the boundary of Ω. In this limit, boundary effects decay rapidly.) Inserting intermediate states, we can rewrite $S(k,\omega)$ in the form

$$\begin{aligned} S(k,\omega) &= 2\sum_n |\langle 0|A_{-k}^\dagger|n\rangle|^2 \delta(\omega - E_n + E_0) \\ &= \sum_n \{|\langle 0|A_k|n\rangle|^2 + |\langle 0|A_{-k}^\dagger|n\rangle|^2\}\delta(\omega - E_n + E_0), \end{aligned} \tag{4.25}$$

where $\{|n\rangle\}$ denote the eigenstates of the Hamiltonian with the eigenvalues $\{E_n\}$. The last equality holds when the Hamiltonian is real. The spectral function $S(k,\omega)$ has information about excitations created by the operator A_k.

Let $\omega(\boldsymbol{k})$ be the lowest threshold of positive regions in $S(k,\omega)$ with fixed k. We expect that $\omega(k)$ corresponds to the lowest frequency of the excitation spectrum. To obtain upper bounds of $\omega(k)$, we use frequency average of ω^2 with spectral weight $\omega^{-1}S(k,\omega)$, which was discussed first by Wagner [143]. Using this frequency average, we can obtain an upper bound of $\omega(k)$ in the following form [48, 135, 105].

Theorem 4.A.1: The lowest frequency $\omega(k)$ is bounded as

$$[\omega(k)]^2 \leq \frac{\displaystyle\int_{-\infty}^{\infty} d\omega\omega S(k,\omega)}{\displaystyle\int_{-\infty}^{\infty} d\omega\omega^{-1} S(k,\omega)} = \frac{\langle[[A_k,H],A^\dagger_{-k}]\rangle}{\chi_A(k)}, \tag{4.26}$$

where $\chi_A(k)$ denotes the Duhamel two-point function (or Kubo's canonical correlation) of A_k at $T=0$

$$\chi_A(k) = \sum_n \left\{\frac{|\langle 0|A_k|n\rangle|^2}{E_n - E_0} + \frac{|\langle 0|A^\dagger_{-k}|n\rangle|^2}{E_n - E_0}\right\}. \tag{4.27}$$

Proof of Theorem 4.A.1. The spectral function $S(k,\omega)$ has the following property

$$S(k,\omega) = S_0(k)\delta(\omega-\omega(k)) + S_{\mathrm{c}}(k,\omega), \tag{4.28}$$

where $S_{\mathrm{c}}(k,\omega)$ comes from the continuum spectrum above $\omega(k)$ and $S_{\mathrm{c}}(k,\omega)=0$ for $\omega \leq \omega(k)$. Since coefficients of the delta functions in $S(k,\omega)$ are nonnegative, we have

$$\begin{aligned}\int_{-\infty}^{\infty} d\omega\omega S(k,\omega) &= \omega(k)S_0(k) + \int_{\omega(k)}^{\infty} d\omega\omega S_{\mathrm{c}}(k,\omega)\\ &\geq [\omega(k)]^2\Big\{\omega(k)^{-1}S_0(k) + \int_{\omega(k)}^{\infty} d\omega\omega^{-1}S_{\mathrm{c}}(k,\omega)\Big\}\\ &= [\omega(k)]^2\int_{-\infty}^{\infty} d\omega\omega^{-1}S(k,\omega).\end{aligned} \tag{4.29}$$

The function $S(k,\omega)$ is equivalent to (2.40) if $A=A_k$ and $C=A^\dagger_{-k}$. Hence $S(k,\omega)$ satisfies sum rules (2.41)–(2.43). Using frequency-sum rules (2.42) and (2.43), we obtain (4.26). ■

In the one-dimensional Heisenberg model, Hohenberg and Brinkman exactly evaluated the frequency average at small k, and then showed that the average is almost equal to the lowest frequency [48]. For two- and three-dimensional systems, however, there is no exact solution and hence we cannot directly estimate the average. To bound $\chi_A(k)$ from below, we use the Bogoliubov inequality (Theorem 2.1.1) and thereby we obtain

$$\omega(k) \leq \frac{\langle[A_k,[H,A^\dagger_{-k}]]\rangle^{1/2}\langle[B_k,[H,B^\dagger_{-k}]]\rangle^{1/2}}{|\langle[A_k,B_k]\rangle|}, \tag{4.30}$$

which is satisfied by any operator B_k. Wagner first discussed this inequality and later Stringari [135] used it to obtain Theorem 4.2.2. Recently we also studied this spectral average in the Hubbard models [105, 107], which is shown in Chapter 5.

The inequality (4.26) can be extended to the following forms

$$[\omega(k)]^{m-l} \leq \frac{\displaystyle\int_{-\infty}^{\infty} d\omega \omega^m S(k,\omega)}{\displaystyle\int_{-\infty}^{\infty} d\omega \omega^l S(k,\omega)} \tag{4.31}$$

for integers l and m such that $l < m$. Here we define the right-hand side of (4.31) as $F(l,m)$. From the Schwarz inequality, we have

$$F(l,m) \leq F(m, 2m-l). \tag{4.32}$$

Repeatedly using (4.32), we obtain a sequence of upper bounds in the form

$$\omega(k) \leq F(-1,0) \leq [F(-1,1)]^{1/2} \leq F(0,1) \leq [F(0,2)]^{1/2} \leq F(1,2) \leq \cdots. \tag{4.33}$$

Finally we discuss the relation between our bound (4.9) and Stringari's bound (4.23). From the second and third inequalities of (4.33), we obtain

$$\omega(k) \leq \left[\frac{\langle[[A_k, H], A^\dagger_{-k}]\rangle}{\chi_A(k)}\right]^{1/2} \leq \frac{\langle[[A_k, H], A^\dagger_{-k}]\rangle}{\langle\{A_k, A^\dagger_{-k}\}\rangle}, \tag{4.34}$$

where we have used sum rules (2.41)–(2.43). Note that the last equation is nothing but the excitation energy of Feynman's trial state [16, 33]

$$|\Psi(k)\rangle = \frac{A_k|0\rangle}{\|A_k|0\rangle\|} \tag{4.35}$$

and we also used this trial state in Theorem 4.2.1. Thus, our bound (4.9) comes from the third equation of (4.34). On the other hand, Stringari obtained the bound (4.23) from the second equation of (4.34). Thus, the difference between the bounds (4.9) and (4.23) may originate from the second inequality in (4.34). In $F(0,1)$, upper frequencies are added with larger weight than in $[F(-1,1)]^{1/2}$. Then, if there are multi-magnon excitations in $S(k,\omega)$, the frequency average $F(0,1)$ becomes larger than $[F(-1,1)]^{1/2}$. In contrast, if $S(k,\omega)$ only contains one-particle excitations, both upper bounds in (4.34) become equal to the lowest frequency at small k.

Chapter 5

Spin and charge excitations of the Hubbard model

Though this thesis is devoted to discussions of the quantum antiferromagnets, we would like to mention excitations of the Hubbard model in this chapter. The Hubbard model describes itinerant electron systems and on the other hand the Heisenberg antiferromagnet is a model of localized electrons. Both models are equivalent in a certain limit and hence they are closely related to each other. Furthermore, our discussions in this chapter are based on the method which we have shown in Chapter 4. Thus the contents of this chapter closely relate to the topics of this thesis.

We discuss only the short-range repulsive Hubbard model. The Hamiltonian is defined by

$$H = -t \sum_{\langle i,j \rangle \in \Lambda} \sum_{\sigma=\uparrow,\downarrow} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + U \sum_{i \in \Lambda} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i \in \Lambda} (n_{i\uparrow} + n_{i\downarrow}), \tag{5.1}$$

where $c_{i\sigma}^{\dagger}$ denotes the creation operator of an electron at the site i with spin σ, and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. The first term gives the kinetic energy of electrons and the second term gives the potential energy by the on-site electron-electron interactions.

In Section 5.1 we study spectral properties of dynamical structure factors of the one-dimensional Hubbard model at $T = 0$, using sum rules and the Bethe-ansatz solution. Sum rules help us to obtain information about dynamic quantities from static quantities. We estimate the spectral weight on the lowest frequencies of spin and charge excitations at small momentum. It is found that there exists a strong or broad continuum spectrum above the lowest frequency at small momentum in the spin excitations of the dilute limit and in the charge excitations near half-filling. The spectral weight on the lowest frequency is negligible in these two regions. In other regions, most of the spectral weight concentrates near the lowest frequency.

In Section 5.2 we study energy spectra of the Nambu-Goldstone modes in the Hubbard model at $T = 0$, assuming breakdown of continuous symmetries. Using the frequency average discussed in Section 4.A, we obtain rigorous upper bounds of the energy spectra of the Nambu-Goldstone modes in magnetic order phases and in superconducting phases of the two- and three-dimensional Hubbard models. Since rigorous results are rare for interacting electron systems, the present results are useful to verify approximate theories.

5.1 One-dimensional system[1]

5.1.1 Introduction

The Hubbard model has been attracting theoretical and experimental interests, because it is the simplest model of interacting electrons. The one-dimensional repulsive Hubbard model is defined by the following Hamiltonian

$$H = -t\sum_{i=1}^{L}\sum_{\sigma=\uparrow,\downarrow}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + c_{i+1\sigma}^{\dagger}c_{i\sigma}) + U\sum_{i=1}^{L}n_{i\uparrow}n_{i\downarrow} - \mu\sum_{i=1}^{L}(n_{i\uparrow} + n_{i\downarrow}), \tag{5.2}$$

where $c_{i\sigma}^{\dagger}$ denotes the creation operator of an electron at the site i with spin σ and $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$. We consider a system with the size L under the periodic boundary condition and then take the infinite-volume limit.

Since Lieb and Wu [87] exactly solved the one-dimensional Hubbard model using the nested Bethe-ansatz method [150], various static quantities were exactly calculated for this model [121, 23, 138, 130, 141]. Ovchinnikov [121] calculated the spectrum of the lowest spin-wave excitation at half-filling and Coll [23] studied it for arbitrary filling. Spin-wave excitations have gapless k-linear modes in arbitrary filling. On the other hand the charge-fluctuation spectrum has a gap at half-filling and consequently the ground state is an insulator [87]. For doped cases, Coll [23] showed that charge-density excitations have gapless k-linear modes. Later, Woynarovich [146] found charge excitations of another type, which have optical modes. Spin and charge excitations have different velocities in doped systems. Takahashi [138] evaluated the magnetic susceptibility at half-filling and Shiba [130] evaluated for all filling. Usuki, Kawakami and Okiji [141] obtained the charge susceptibility. Recently, asymptotic forms of the space and time correlation functions were obtained using the conformal field theory [65, 128, 34].

On the other hand, it is difficult to calculate dynamical quantities directly from the Bethe-ansatz solution. The main purpose of the present section is to study spectral properties of the dynamical structure factor at $T = 0$,

$$S(k,\omega) = 2\sum_{n}|\langle 0|A_k|n\rangle|^2\delta(\omega - E_n + E_0), \tag{5.3}$$

where A_k is the Fourier transform of a local operator A_i, i.e., $A_k = L^{-1/2}\sum_{i=1}^{L}A_i\exp(ikr_i)$, and $|n\rangle$ ($|0\rangle$) denotes an eigenstate (the ground state) of the Hamiltonian. We recall the long standing question about strength of the spectral weight that is carried on by the lowest k-linear mode. (See Section 4.1.) We use frequency-sum rules of $S(k,\omega)$, which relate the dynamical structure factor to static quantities [143, 48]. Using this relation, we can obtain information about $S(k,\omega)$ from static quantities [48].

5.1.2 Spectral properties of $S(k,\omega)$

Here, we discuss the dynamical structure factor at small k in the one-dimensional repulsive Hubbard model at $T = 0$, using the Bethe-ansatz solution and using sum rules. We

[1]The contents of this section were published in [105, 106].

study excitations of spin and charge degrees of freedom, setting A_i as S_i^x and $(n_{i\uparrow}+n_{i\downarrow})-\langle 0|(n_{i\uparrow}+n_{i\downarrow})|0\rangle$, respectively. Using the frequency average (4.26), we find that $S(k,\omega)$ has singular behavior in two regions: There is a strong or broad continuum spectrum above the lowest frequency in the dynamical spin-structure factor of the dilute limit and in the dynamical charge-structure factor near half-filling. In other cases, the spectral weight of $S(k,\omega)$ concentrates near the lowest frequency of the excitation spectrum.

Methods

Here we show methods including sum rules and the Bethe-ansatz solution.

First we discuss the frequency average (4.26),

$$[\omega_{\rm av}(k)]^2 = \frac{\displaystyle\int_0^\infty \mathrm{d}\omega\omega S(k,\omega)}{\displaystyle\int_0^\infty \mathrm{d}\omega\omega^{-1} S(k,\omega)} = \frac{\langle 0|[[A_k,H],A_{-k}^\dagger]|0\rangle}{\chi(k)}, \tag{5.4}$$

where $\chi(k)$ denotes the Duhamel two-point function (or Kubo's canonical correlation) of A_k in the ground state,

$$\chi(k) = \sum_n \left\{ \frac{|\langle 0|A_k|n\rangle|^2}{E_n-E_0} + \frac{|\langle 0|A_{-k}^\dagger|n\rangle|^2}{E_n-E_0} \right\}. \tag{5.5}$$

As shown in Theorem 4.A.1, the square root of this mean value gives an upper bound of the lowest frequency of the excitation spectrum $\omega(k)$, i.e.,

$$\omega(k) \le \omega_{\rm av}(k). \tag{5.6}$$

Comparing $\omega_{\rm av}(k)$ with $\omega(k)$, we discuss distribution of spectral weight in $S(k,\omega)$. If the spectral weight in $S(k,\omega)$ is concentrated near $\omega(k)$ at small k, we have $\omega(k)\simeq\omega_{\rm av}(k)$ for small k and, if there is a strong continuum spectrum above $\omega(k)$, we have $\omega(k)\ll\omega_{\rm av}(k)$ at small k. Using this relation, Hohenberg and Brinkman [48] studied $S(k,\omega)$ of the one-dimensional XY and Heisenberg antiferromagnets.

Next we list exact results derived from the Bethe-ansatz solution, which are used in exactly calculating the mean value. Lieb and Wu first reduced the ground-state wave function to two integral equations of distribution functions of spins and charges [87]. We write the distribution of charges with momentum k as $\rho(k)$. In the zero magnetic field, one obtains $\rho(k)$ from the following integral equation

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{2\pi}\int_{-Q}^{Q} dk'\overline{K_1}(\sin k - \sin k')\rho(k'), \tag{5.7}$$

where

$$\overline{K_1}(x) = \int_{-\infty}^{\infty} d\omega \frac{\exp(-|\omega|u/4)}{2\cosh(\omega u/4)}\exp(i\omega x) \tag{5.8}$$

with $u=U/t$. The cutoff Q relates to the chemical potential μ and it satisfies

$$\int_{-Q}^{Q} dk\rho(k) = n, \tag{5.9}$$

where n denotes the density of electrons per site. It is convenient to use a dressed energy, which was given in Refs. [141] and [147]. The dressed energy of a charge, $\epsilon_{\rm c}(k)$, is given by

$$\begin{aligned}\epsilon_{\rm c}(k) &= -2t\cos k - \mu \\ &\quad + \frac{1}{2\pi}\int_{-Q}^{Q} dk' \cos k' \overline{K_1}(\sin k - \sin k')\epsilon_{\rm c}(k').\end{aligned} \tag{5.10}$$

Using $\rho(k)$ and $\epsilon_{\rm c}(k)$, one obtains the ground-state energy per site in the form

$$\epsilon_0 = \int_{-Q}^{Q} dk\,(\mu - 2\cos k)\,\rho(k) = \frac{1}{2\pi}\int_{-Q}^{Q} dk\epsilon_{\rm c}(k). \tag{5.11}$$

In the ground state, all the states that have $\epsilon_{\rm c}(k) < 0$ are filled. Then the parameter Q satisfies $\epsilon_{\rm c}(Q) = 0$.

One can express various quantities, using $\rho(k)$ and $\epsilon_{\rm c}(k)$. Fermi velocities in the zero magnetic field are obtained in the forms [147]

$$v_{\rm c} = \frac{1}{2\pi\rho(Q)}\epsilon'_{\rm c}(Q), \tag{5.12}$$

$$v_{\rm s} = \frac{1}{2\pi}\int_{-Q}^{Q} dk \exp\left(\frac{2\pi}{u}\sin k\right)\epsilon'_{\rm c}(k) \Big/ \int_{-Q}^{Q} dk \exp\left(\frac{2\pi}{u}\sin k\right)\rho(k), \tag{5.13}$$

where $v_{\rm c}$ ($v_{\rm s}$) denotes the charge (spin-wave) velocity. The uniform magnetic susceptibility $\chi_{\rm s}$ relates to $v_{\rm s}$ as [138, 23]

$$\chi_{\rm s}(k=0) = \frac{1}{2\pi v_{\rm s}} \tag{5.14}$$

and the uniform charge susceptibility $\chi_{\rm c}$ is given by [34]

$$\chi_{\rm c}(k=0) = \frac{1}{\pi v_{\rm c}}[f(Q)]^2, \tag{5.15}$$

where $f(k)$ satisfies

$$f(k) = 1 + \frac{1}{2\pi}\int_{-Q}^{Q} dk' \overline{K_1}(\sin k - \sin k') f(k') \cos k'. \tag{5.16}$$

One obtains the kinetic energy in the form [11]

$$K \equiv \frac{1}{L} t \sum_{i,\sigma} \langle 0 | (c^\dagger_{i\sigma} c_{i+1\sigma} + c^\dagger_{i+1\sigma} c_{i\sigma}) | 0 \rangle \tag{5.17}$$

$$= t\frac{\partial \epsilon_0}{\partial t}, \tag{5.18}$$

which Baeriswyl *et al.* [11] and Carmelo and Baeriswyl [20] evaluated.

We numerically estimate these quantities, converting the integral equations into a set of matrix equations and solving the matrix equations. In the matrix equations, unknown functions are represented in terms of 1000 discrete values. We verified, changing the number of discrete elements, that a set of discrete values converge well to a certain function and, furthermore, we checked that estimates of physical quantities are equal to previously reported values and to asymptotic forms in various limits.

Figure 5.1: The uniform magnetic susceptibility as a function of the electron concentration n for various values of U. Note that we have divided the values by the susceptibility of free electrons, to clarify the singularity in the low-density limit.

The uniform magnetic susceptibility has the following asymptotic forms [130]

$$\chi_{\mathrm{s}}(0) = \begin{cases} \dfrac{U}{4\pi^2 t^2}\left(\dfrac{2\pi n}{2\pi n - \sin 2\pi n}\right) & (U/t \gg 1) \\ \dfrac{1}{4\pi t \sin(\pi n/2)} & (U/tn \ll 1). \end{cases} \tag{5.19}$$

Studying (5.14) in the dilute limit ($n \to 0$), we obtain

$$\chi_{\mathrm{s}}(0) = \frac{3U}{8\pi^4 t^2 n^2} + \frac{1}{t} O(n^{-1}). \tag{5.20}$$

Shiba derived this result in the large-U limit [130]. We find that (5.20) holds for arbitrary non-zero U in the dilute limit. On the other hand, in free electrons ($U = 0$), $\chi_{\mathrm{s}}(0)$ behaves as $\chi_{\mathrm{s}}(0) = (2\pi^2 tn)^{-1}$ in the low-density limit. Hence, if $U > 0$, $\chi_{\mathrm{s}}(0)$ has a stronger divergence, as shown in Figure 5.1, and this shows that the Coulomb interaction drastically enhances spin fluctuations in the dilute limit. This singularity indicates that an effective interaction of spins becomes large in the dilute limit.

The uniform charge susceptibility behaves as [141]

$$\chi_{\mathrm{c}}(0) = \begin{cases} \dfrac{1}{2\pi t \sin \pi n} & (U/t \gg 1, n \neq 1) \\ \dfrac{\alpha}{t(1-n)} & (n \sim 1, n \neq 1), \end{cases} \tag{5.21}$$

where α changes from 0 to $1/2\pi^2$ as U increases.

The kinetic energy has the following asymptotic form for large U [20]

$$K = \frac{2t}{\pi} \sin n\pi + \frac{4nt^2 \ln 2}{\pi U} [2\pi n - \sin(2\pi n)]. \tag{5.22}$$

For small U, we have

$$K = \frac{4t}{\pi} \sin \frac{n\pi}{2}. \tag{5.23}$$

Numerically estimating the kinetic energy, we find that (5.23) holds for small U for arbitrary filling.

Spin-wave spectrum

We discuss spin-wave excitations, setting the operator A_k of (5.3) as S_k^x. Here, $S(k,\omega)$ is the dynamical spin-structure factor, which relates to the imaginary part of magnetic susceptibility as

$$\pi S(k,\omega) = -2\mathrm{Im}\chi_{\mathrm{s}}(k,\omega) \tag{5.24}$$

for $\omega \geq 0$. The operation of S_k^x excites the spin degree of freedom. For quantum Heisenberg antiferromagnets, it has been shown that the excitation spectrum given by the state $S_k^x|0\rangle$ agrees well with the lowest frequency of the spin-wave spectrum in one-dimensional [48] and higher-dimensional [135, 104] systems.

The double commutator of (5.4) is transformed as

$$\langle 0|[[S_k^x, H], S_{-k}^x]|0\rangle = \frac{1}{2} K \cdot (1 - \cos k). \tag{5.25}$$

The numerator of (5.4) becomes the static magnetic susceptibility $\chi_{\mathrm{s}}(k)$. Assuming the continuity property of $\chi_{\mathrm{s}}(k)$ near $k = 0$, we obtain the mean value for small k in the form

$$\omega_{\mathrm{av}}(k) = \frac{1}{2} \left[\frac{K}{\chi_{\mathrm{s}}(0)} \right]^{1/2} |k|. \tag{5.26}$$

To compare this average with the lowest frequency of the spin-wave spectrum $\omega_{\mathrm{s}}(k)$, we evaluate the ratio

$$R_{\mathrm{s}} = \lim_{k \to 0} \frac{\omega_{\mathrm{av}}(k)}{\omega_{\mathrm{s}}(k)} = \pi \sqrt{K \cdot \chi_{\mathrm{s}}(0)}, \tag{5.27}$$

where we have used (5.14) and the relation $\omega_{\mathrm{s}}(k) = v_{\mathrm{s}}|k|$ for small k. We calculate the ratio R_{s} for arbitrary U and for arbitrary filling, numerically solving the Bethe-ansatz solution. The result is shown in Figure 5.2.

In case of small U/tn, the mean value agrees well with the lowest frequency $\omega_{\mathrm{s}}(k)$. Both $\omega_{\mathrm{s}}(k)$ and $\omega_{\mathrm{av}}(k)$ have the following asymptotic form

$$\omega_{\mathrm{s}}(k) = \omega_{\mathrm{av}}(k) = 2t \sin \frac{n\pi}{2} \cdot |k|. \tag{5.28}$$

This result means that the spectral weight of the dynamical spin-structure factor [or $\mathrm{Im}\chi_{\mathrm{s}}(k,\omega)$] concentrates near $\omega = \omega_{\mathrm{s}}(k)$ at small k. In the free fermion model ($U = 0$), $\mathrm{Im}\chi_{\mathrm{s}}(k,\omega)$ has peaks only on $\omega = \omega_{\mathrm{s}}(k)$ for small k. We find that the Coulomb repulsive force does not change this behavior, if the parameter U/nt is small.

In the dilute limit ($n \to 0$), the ratio R_{s} diverges in the form $R_{\mathrm{s}} \propto (U/tn)^{1/2}$. The mean value has the following asymptotic form

$$\omega_{\mathrm{av}}(k) = 2\pi^2 tn \sqrt{\frac{tn}{3U}} |k| \qquad (U/tn \gg 1), \tag{5.29}$$

Figure 5.2: Ratio of the mean value of the spin-wave spectrum to the lowest frequency of spin excitations $\omega_{\rm s}(k)$ at small k.

whereas the lowest frequency behaves as

$$\omega_{\rm s}(k) = \frac{4\pi^3 n^2 t^2}{3U}|k| \qquad (U/tn \gg 1). \tag{5.30}$$

This means that the spectral weight of the lowest frequency in the dynamical spin-structure factor becomes weak and negligible in the dilute limit. There exists a broad or strong continuum spectrum above $\omega = v_{\rm s}|k|$. We thus find that, in the dilute limit, spectral properties of the interacting model ($U > 0$) are completely different from the free model ($U = 0$). This singularity may come from the spin fluctuations that we have shown in the previous section. We will report further studies and discussions about the system in the dilute limit in ref. [108].

In the large-U region, the mean value coincides well with the lowest frequency $\omega_{\rm s}(k)$ only at half-filling. The ratio $R_{\rm s}$ at half-filling in the large-U limit is $\sqrt{2\ln 2} = 1.1774$. This value is slightly greater than the value $\sqrt{(8\ln 2 - 2)/3} = 1.0871$ of the one-dimensional Heisenberg antiferromagnet by Hohenberg and Brinkman [48]. This discrepancy comes from the difference of expectation values of the double commutator $[[S^x_{-k}, H], S^x_k]$. For doped cases, however, the average is much greater than $\omega_{\rm s}(k)$. The average becomes

$$\omega_{\rm av}(k) = \left[\frac{2\pi t^3}{U}\sin(n\pi)\right]^{1/2}|k| \qquad (U|1-n|/t \gg 1) \tag{5.31}$$

at small k, though the lowest frequency behaves as

$$\omega_{\rm s}(k) = \frac{[2\pi n - \sin(2\pi n)]t^2}{nU}|k| \qquad (U/t \gg 1). \tag{5.32}$$

We hence find that, in the large-U limit of doped cases, there exists a strong or broad continuum spin-wave spectrum for small k above the lowest frequency $\omega = v_{\rm s}|k|$.

Using the ratio R_{s}, we can observe differences between the excited state $S_k^x|0\rangle$ and the lowest spin-wave excitation. Another implication of R_{s} is that the ratio shows how the model is far from the free electron system. In the free model ($U = 0$), the state $S_k^x|0\rangle$ has a gapless k-linear dispersion relation with the velocity v_{s} and hence we have $R_{\mathrm{s}} = 1$. As the system becomes away from the free model, the ratio R_{s} turns large. An example is the one-dimensional spin 1/2 XXZ antiferromagnets. The ratio R_{s} equals to 1 in the XY model, which is equivalent to the free fermion, and the value becomes 1.0871 in the Heisenberg antiferromagnet [48]. (Note that the operator A_k should be S_k^z for the XY model.)

Charge-fluctuation spectrum

We discuss spectral weight of charge excitations, setting the operator A_k as $n_k - \langle 0|n_k|0\rangle$, where $n_k = L^{-1/2}\sum_j (n_{j\uparrow} + n_{j\downarrow})\exp(ikr_j)$. Here, $S(k,\omega)$ is the dynamical charge-structure factor and it relates to the imaginary part of charge susceptibility, $\mathrm{Im}\chi_{\mathrm{c}}(k,\omega)$. Bijl [16] and Feynman [33] first proposed the state $\rho_k|0\rangle$ as a density fluctuation in the Bose liquid, where ρ_k denotes the Fourier transform of the density operator. In the one-dimensional Hubbard model, it has been discussed that the state $n_k|0\rangle$ describes excitations created by charge-density fluctuations [28].

The double commutator of (5.4) becomes

$$\langle 0|[[n_k, H], n_{-k}]|0\rangle = 2K \cdot (1 - \cos k) \tag{5.33}$$

and the denominator of (5.4) becomes the static charge susceptibility $\chi_{\mathrm{c}}(k)$. Assuming the continuity property of $\chi_{\mathrm{c}}(k)$ at small k, we obtain the mean value (5.4) of the charge-fluctuation spectrum in the form

$$\omega_{\mathrm{av}}(k) = \left[\frac{K}{\chi_{\mathrm{c}}(0)}\right]^{1/2} |k| \tag{5.34}$$

for small k.

To compare this average with the lowest frequency of the charge-fluctuation spectrum $\omega_{\mathrm{c}}(k)$, we evaluate the ratio

$$R_{\mathrm{c}} = \lim_{k\to 0}\frac{\omega_{\mathrm{av}}(k)}{\omega_{\mathrm{c}}(k)} = \frac{\pi}{[f(Q)]^2}\sqrt{K \cdot \chi_{\mathrm{c}}(0)}, \tag{5.35}$$

where we have used the relation $\omega_{\mathrm{c}}(k) = v_{\mathrm{c}}|k|$ for small k and (5.15). We calculate the value R_{c}, numerically solving the Bethe-ansatz solution. The result is shown in Figure 5.3.

The ratio R_{c} has the divergent singularity $R_{\mathrm{c}} \propto |1-n|^{-1/2}$ in vicinity of half-filling ($n \sim 1$). The average (5.34) behaves as

$$\omega_{\mathrm{av}}(k) \propto \sqrt{1-n}|k| \tag{5.36}$$

for $U|1-n|/t \ll 1$. On the other hand, the lowest frequency of charge fluctuations has

$$\omega_{\mathrm{c}}(k) \propto (1-n)|k| \tag{5.37}$$

Figure 5.3: Ratio of the mean value of the charge-fluctuation spectrum to the lowest frequency of charge excitations $\omega_{\rm c}(k)$ at small k.

near half-filling. We thus find that the spectral weight of $\mathrm{Im}\chi_{\rm c}(k,\omega)$ on $\omega = v_{\rm c}|k|$ is weak and negligible at small k for $n \sim 1$. A strong or broad continuum spectrum exists in the region $\omega > \omega_{\rm c}(k)$ near half-filling.

If the system is doped and away from half-filling, the ratio $R_{\rm c}$ is almost equal to 1. Hence we find that, in fairly doped systems, the weight of the dynamical charge-structure factor concentrates near the lowest frequency at small k.

Woynarovich [146] showed that there are optical modes in charge excitations. According to his argument on the large U limit, optical modes come from excitations in which some electron pairs occupy the same sites and gapless k-linear modes are, on the other hand, given by charge fluctuations that do not create any doubly occupied site. Our results indicate the following: In fairly doped systems, the spectral weight of $\mathrm{Im}\chi_{\rm c}(k,\omega)$ concentrates near the k-linear acoustic mode. This is consistent with the fact that, in the low-density system, charge fluctuations having double occupancy of electrons are rare. As the electron filling becomes near half-filling, the spectral weight moves from the acoustic mode to optical modes. Finally at the half-filling, the acoustic mode disappears, and hence charge excitations have a finite gap as shown in Refs. [87], [121] and [146].

In the vicinity of half-filling, the Coulomb interaction makes the state $n_k|0\rangle$ extensively different from the lowest charge excitation. As commented in the previous section, this result means that the charge degree of freedom is far from free near the half-filling, even if U is small.

5.2 Two and three dimensional systems –energy spectra of the Nambu-Goldstone modes–[2]

5.2.1 Introduction

The Hubbard model has been attracting wide theoretical and experimental interests, since it is a simplified model of many materials, e.g. $La_{2-x}Sr_xCuO_4$, *etc.* (See [24], for example.) Various phases are expected to appear in two- and three-dimensional systems at low temperatures. There are, however, very few rigorous results that support the occurrence of symmetry breaking in the ground state of the thermodynamic limit [84]. Furthermore, approximate theories sometimes arrive at completely different conclusions. Thus our understanding of the low-temperature properties is still incomplete. In this situation, we expect rigorous results to provide certain checks and standards to verify approximate theories.

The large-U limit of the Hubbard model at half filling is written as the spin-1/2 Heisenberg antiferromagnet. In this limit, as we have discussed in Section 2.3, rigorous arguments and numerical studies arrive at the consistent conclusion that the ground state has the antiferromagnetic long-range order in two- and higher-dimensional systems. In these systems, the spin-wave theory [5, 77] and rigorous results [135, 104] show that the spin-wave excitations have gapless k-linear modes (see Section 4.2), and experimental results [46] on La_2CuO_4 also insist that the magnon excitations have the same dispersion as given by the conventional spin-wave theory. However the situations become quite complicated, when holes (or electrons) are doped in the system. For doped systems, stability of the antiferromagnetic order and the incommensurate order has been discussed in the literature [131, 151, 59, 39, 63]. Furthermore, many authors, motivated by Nagaoka's theorem [113, 140], expected ferromagnetism in the strong-coupling region. (It is not easy to list all the relevant references. See, for example, Refs. [125, 123] and the references therein.)

Since high-T_c superconductivity was discovered in a material with the CuO_2 planes, the superconducting phases have also been expected to appear in the two- or three-dimensional Hubbard model. According to numerical studies, there is no evidence for superconductivity in the ground state [57, 56, 111]. However, this issue is not settled yet. On the other hand, several authors reported that superconductivity may appear in the t-J model, which effectively describes the Hubbard model in the strong-coupling region. (For a review, see [24].)

Here, we discuss the short-range repulsive Hubbard model. The Hamiltonian is given by

$$H_\Lambda = -t \sum_{\langle i,j\rangle \in \Lambda} \sum_{\sigma=\uparrow,\downarrow} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_{i\in\Lambda} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\in\Lambda} (n_{i\uparrow} + n_{i\downarrow}), \tag{5.38}$$

where $c_{i\sigma}^\dagger$ is the creation operator of an electron at site i with spin σ and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The summation of the hopping term runs over all nearest-neighbor sites. For simplicity, we use the hypercubic lattice $\Lambda \subset \mathbf{Z}^d$ for $d \geq 2$, but the following analyses can be generalized to arbitrary lattices. Moreover, the arguments in the present section can be easily extended to the t-J model.

The purpose of the present section is to obtain rigorous upper bounds of the excitation spectra in various phases in which continuous symmetries are spontaneously broken.

[2]The contents of this section were published in [107].

Assuming the breakdown of a continuous symmetry, we extend the arguments given in Section 4.2 to the Hubbard model, and thereby estimate the excitation spectra of the Goldstone modes in the magnetically ordered phases and in the superconducting phases. We concentrate on the density excitations created by operation of the Fourier transforms of the density operators. We use S_k^x and $(n_{k\uparrow} + n_{k\downarrow})$ to discuss spin and charge excitations, respectively.

Let us introduce the system under an infinitesimally small field which is conjugate to the order parameter. The Hamiltonian is written as

$$H_\Lambda(B) = H_\Lambda - B\mathcal{O}_\Lambda, \tag{5.39}$$

where $\mathcal{O}_\Lambda$ denotes the order-parameter operator. We define the equilibrium state using the grand canonical ensemble. Taking the thermodynamic limit at $T = 0$, we obtain the ground state with broken symmetry as

$$\langle \cdots \rangle = \lim_{B\searrow 0} \lim_{\Lambda \nearrow \mathbf{Z}^d} \lim_{\beta\nearrow\infty} \frac{\mathrm{Tr} \cdots \exp\{-\beta H_\Lambda(B)\}}{\mathrm{Tr} \exp\{-\beta H_\Lambda(B)\}}. \tag{5.40}$$

To bound the lowest frequency $\omega(k)$, we use the inequality (4.30),

$$\omega(k) \leq \frac{\langle [A_k, [H, A_{-k}^\dagger]]\rangle^{1/2} \langle [B_k, [H, B_{-k}^\dagger]]\rangle^{1/2}}{|\langle [A_k, B_k]\rangle|}. \tag{5.41}$$

As shown in Section 4.A, the right-hand side of (5.41) gives an upper bound for the lowest frequency of the excited states created by an operator $A_k = |\Omega|^{-1/2} \sum_{j\in\Omega} A_j \exp(ikr_j)$. Setting A_k as $S_k^x - \langle S_k^x \rangle$ and $n_k - \langle n_k \rangle$, we discuss the spin and charge excitations, respectively. Choosing B_k that satisfies $[A_k, B_k] = \mathcal{O}_\Omega$, we can obtain an upper bound for the energy spectrum from (5.41). This upper bound gives the Goldstone theorem. Note that (5.41) is invariant under the exchange of A_k and B_k, and consequently (5.41) gives an upper bound for the lowest frequency of the excited states $B_k|0\rangle$ as well.

The contents of this section is as follows: In Section 5.2.2, we obtain rigorous upper bounds of the spin-wave excitations in the magnetically ordered phases. They show gapless spectra. The antiferromagnetic, ferromagnetic and incommensurate orders are considered. In Section 5.2.3, we discuss the charge excitations in the superconducting phase. It is shown that the charge excitations have gapless modes, and furthermore the particle excitations of the Cooper pairs become gapless. Finally, Section 5.2.4 contains summary and discussions.

5.2.2 Magnetic phases

Here, we discuss the spin-wave spectrum in magnetically ordered phases. To create the spin-wave excitations, we set A_k as $|\Omega|^{-1/2} \sum_{j\in\Omega} S_j^x \exp(ikr_j)$. As shown in Chapter 4, the excited states created by S_k^x give a precise spin-wave spectrum in the Heisenberg antiferromagnets [48, 135, 104]. Moreover, for the one-dimensional Hubbard model, we know that they are concentrated near the lowest frequency of the spin excitations in many parameter regions, although some of them have much larger frequency in the low-density limit or in the strong coupling limit of doped systems [106].

First we consider the magnetically ordered state whose order-parameter operator is given by

$$\mathcal{O}_\Omega = \sum_{j\in\Omega} \{S_j^z \cos(\boldsymbol{q}\cdot\boldsymbol{r}_j) + S_j^x \sin(\boldsymbol{q}\cdot\boldsymbol{r}_j)\}. \tag{5.42}$$

The ground state is defined by (5.40). We assume that the ground state has the magnetic order,

$$m \equiv \frac{1}{|\Omega|}\langle \mathcal{O}_\Omega \rangle > 0. \tag{5.43}$$

Setting the operators as $A_k = |\Omega|^{-1/2}\sum_{j\in\Omega} S_j^y \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_j)$ and $B_k = |\Omega|^{-1/2}\sum_{j\in\Omega} S_j^x \exp[i(\boldsymbol{q}-\boldsymbol{k})\cdot\boldsymbol{r}_j]$, we have

$$\begin{aligned} |\langle [A_k, B_k]\rangle| \geq \mathrm{Im}\langle [A_k, B_k]\rangle &= \frac{1}{|\Omega|}\sum_{j\in\Omega}\langle S_j^z \cos(\boldsymbol{q}\cdot\boldsymbol{r}_j)\rangle \\ &= \frac{m}{|\Omega|}\sum_{j\in\Omega}\cos^2(\boldsymbol{q}\cdot\boldsymbol{r}_j). \end{aligned} \tag{5.44}$$

In the infinite limit $\Omega \nearrow \mathbf{Z}^d$, we have

$$\lim_{\Omega\nearrow\mathbf{Z}^d} |\langle [A_k, B_k]\rangle| \geq m\cdot f_c(q), \tag{5.45}$$

where

$$f_c(q) = \lim_{\Omega\nearrow\mathbf{Z}^d}\frac{1}{|\Omega|}\sum_{j\in\Omega}\cos^2(\boldsymbol{q}\cdot\boldsymbol{r}_i). \tag{5.46}$$

Furthermore, the double commutator of (5.41) become

$$\lim_{\Omega\nearrow\mathbf{Z}^d}\langle [A_{-k}^\dagger, [H, A_k]]\rangle = \frac{dtK}{2}(1-\gamma_k), \tag{5.47}$$

$$\lim_{\Omega\nearrow\mathbf{Z}^d}\langle [B_{-k}^\dagger, [H, B_k]]\rangle = \frac{dtK}{2}(1-\gamma_{k-q}), \tag{5.48}$$

where

$$K = \lim_{\Omega\nearrow\mathbf{Z}^d}\frac{1}{d|\Omega|}\sum_{\langle i,j\rangle\in\Omega}\sum_\sigma \langle c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}\rangle, \tag{5.49}$$

$$\gamma_k = \frac{1}{d}\sum_{i=1}^d \cos k_i. \tag{5.50}$$

Inserting (5.45), (5.47) and (5.48) into (5.41), we obtain an upper bound of the spin-wave spectrum in the form

$$\omega_{\mathrm{s}}(\boldsymbol{k}) \leq \frac{dtK}{2mf_c(q)}\sqrt{(1-\gamma_k)(1-\gamma_{k-q})}. \tag{5.51}$$

We discuss the excitation spectrum for various values of $\boldsymbol{q}$. The order (5.43) corresponds to the antiferromagnetic order when $\boldsymbol{q} = (\pi,\cdots,\pi)$, and to the ferromagnetic order when $\boldsymbol{q} = \mathbf{0}$. Otherwise, the order (5.43) means the incommensurate order (or the spiral order).

Antiferromagnetic order

In the antiferromagnetic phase, the order-parameter operator is given by (5.42) with $\boldsymbol{q} = (\pi, \cdots, \pi)$. We have $f_c(q) = 1$ and hence we obtain the bound

$$\omega_{\mathrm{s}}(\boldsymbol{k}) \leq \frac{dtK}{2m_{\mathrm{s}}} \sqrt{(1-\gamma_k)(1+\gamma_k)}, \tag{5.52}$$

where m_{s} denotes the staggered magnetization per site. Thus, in the Néel ordered phase, the lowest frequency of the spin excitations is bounded from above by a gapless k-linear dispersion relation. The momentum dependence of our bound is exactly equal to that of the Heisenberg antiferromagnet [135, 104]. The spin-wave velocity is bounded from above by $\sqrt{d}tK/2m_{\mathrm{s}}$. Note that this upper bound is applicable to arbitrary values of the parameter U/t and the filling n, if and only if $m_{\mathrm{s}} > 0$.

In the large-U limit of the Hubbard model at half filling, it is expected that the kinetic energy behaves as $K \propto t/U$. In the one-dimensional system, the kinetic energy was exactly evaluated and it indeed behaves as $K \propto t/U$ in the large U-limit at half filling [11]. In this limit, hence the upper bound of the spin-wave velocity depends on parameters in the form t^2/U. This result is consistent with the fact that the large-U limit with the half filling is described by the Heisenberg antiferromagnet with exchange coupling $4t^2/U$.

Ferromagnetic order

Next we discuss the ferromagnetic order, setting $\boldsymbol{q} = \boldsymbol{0}$. In this case, we have $f_c(q) = 1$ and hence we obtain an upper bound of the spin-wave spectrum in the form

$$\omega_{\mathrm{s}}(\boldsymbol{k}) \leq \frac{dtK}{2m_z}(1-\gamma_k), \tag{5.53}$$

where m_z denotes the uniform magnetization per site.

Thus the spin-wave spectrum is bounded from above by a gapless k-quadratic form. If the ground state has the saturated (fully ordered) magnetization, one can easily obtain a similar bound. It should be remarked that (5.53) holds in the imperfect-ferromagnetic-order phase as well.

Incommensurate order

Finally we discuss the incommensurate order, in which $\boldsymbol{q} \neq \boldsymbol{0}$, $(\pi, \cdots, \pi)$. In this case, equation (5.51) again gives an upper bound of the spin-wave spectrum, but the value of $f_c(q)$ depends on q. To determine the upper bound more explicitly, we consider other upper bounds. Setting $A_k = |\Omega|^{-1/2} \sum_{j\in\Omega} S_j^y \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_j)$ and $B_k = |\Omega|^{-1/2} \sum_{j\in\Omega} S_j^z \exp[i(\boldsymbol{q}-\boldsymbol{k})\cdot\boldsymbol{r}_j]$, and then taking the infinite limit $\Omega \nearrow \mathbf{Z}^d$, we obtain another upper bound

$$\omega_{\mathrm{s}}(\boldsymbol{k}) \leq \frac{dtK}{2mf_s(q)} \sqrt{(1-\gamma_k)(1-\gamma_{k-q})}, \tag{5.54}$$

where

$$f_s(q) = \lim_{\Omega \nearrow \mathbf{Z}^d} \frac{1}{|\Omega|} \sum_{j\in\Omega} \sin^2(\boldsymbol{q}\cdot\boldsymbol{r}_i). \tag{5.55}$$

Note that $f_c(q) + f_s(q) = 1$ and hence one of $f_c(q)$ and $f_s(q)$ is larger than 1/2. Then we have

$$\omega_{\mathrm{s}}(\boldsymbol{k}) \le \frac{dtK}{m}\sqrt{(1-\gamma_k)(1-\gamma_{k-q})}. \tag{5.56}$$

These bounds are not symmetric with k and hence they are still incomplete. To estimate another bound, we use $B_k = |\Omega|^{-1/2}\sum_{j\in\Omega} S_j^x \exp[-i(\boldsymbol{q}+\boldsymbol{k})\cdot\boldsymbol{r}_j]$. Then we obtain the upper bound that is given from (5.51) by changing $\boldsymbol{q}$ to $-\boldsymbol{q}$. In the same way, setting $B_k = |\Omega|^{-1/2}\sum_{j\in\Omega} S_j^z \exp[-i(\boldsymbol{q}+\boldsymbol{k})\cdot\boldsymbol{r}_j]$, we obtain another bound that is given from (5.54) by changing $\boldsymbol{q}$ to $-\boldsymbol{q}$. Using these bounds and the fact $f_c(q) + f_s(q) = 1$, we have

$$\omega_{\mathrm{s}}(\boldsymbol{k}) \le \frac{dtK}{m}\sqrt{(1-\gamma_k)(1-\gamma_{k+q})}, \tag{5.57}$$

which is nothing but the momentum-reversed form of (5.56). In (5.57), the energy spectrum is estimated better than in (5.56) in the region $\gamma_{k+q} > \gamma_{k-q}$.

To summarize, the lowest frequency of the spin-wave spectrum in the incommensurate-order phase is bounded from above; $\omega_{\mathrm{s}}(\boldsymbol{k}) \le (dtK/m)\sqrt{(1-\gamma_k)(1-\gamma_{k+q})}$ for $\boldsymbol{k}$ satisfying the inequality $\gamma_{k+q} \le \gamma_{k-q}$, and $\omega_{\mathrm{s}}(\boldsymbol{k}) \le (dtK/m)\sqrt{(1-\gamma_k)(1-\gamma_{k-q})}$ for $\boldsymbol{k}$ satisfying the inequality $\gamma_{k+q} \ge \gamma_{k-q}$. This upper bound has a finite gap at $\boldsymbol{k} = (\pi, \cdots, \pi)$, while the points $\boldsymbol{k} = \boldsymbol{0}$ and $\boldsymbol{k} = \pm\boldsymbol{q}$ are gapless. The spin-wave spectrum $\omega_{\mathrm{s}}(k)$ is bounded from above by a gapless k-linear form around $\boldsymbol{k} = \boldsymbol{0}$ and $\pm\boldsymbol{q}$, which is consistent with the energy spectrum derived by Shraiman and Siggia [131]. Upper bounds of the spin-wave velocities are given by $tK\sqrt{d(1-\gamma_q)}/\sqrt{2}m$ for both of the modes at $\boldsymbol{k} \simeq \boldsymbol{0}$ and $\boldsymbol{k} \simeq \pm\boldsymbol{q}$. Finally, we remark that these bounds may not be the optimal ones, since there remain possibilities of better choices of B_k, and moreover we have not estimated $f_c(q)$ properly.

5.2.3 Superconducting phase

Next, we discuss the charge-fluctuation spectrum above a superconducting ground state, taking the operator A_k as $(n_{k\uparrow} + n_{k\downarrow}) - \langle (n_{k\uparrow} + n_{k\downarrow}) \rangle$. From the study of one-dimensional Hubbard model [105], we found that the excited states given by the operator n_k concentrate near the lowest charge excitation in fairly doped systems, though these states contain a number of higher excitations in the vicinity of half-filling.

Here we discuss the superconductivity of the on-site Cooper pairs, whose order-parameter operator is defined by

$$\mathcal{O}_\Omega = \sum_{i\in\Omega}(c_{i\uparrow}c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger) \tag{5.58}$$

and whose ground state is given by (5.40). We consider the phase in which the ground state has the superconductivity

$$O_{\mathrm{Cooper}} \equiv \frac{1}{|\Omega|}\langle \mathcal{O}_\Omega \rangle > 0. \tag{5.59}$$

We set the operators as

$$A_k = n_k - \langle n_k \rangle, \tag{5.60}$$

$$B_k = |\Omega|^{-1/2}\sum_{j\in\Omega}(c_{j\uparrow}c_{j\downarrow} + c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger)\exp(-i\boldsymbol{k}\cdot\boldsymbol{r}_j), \tag{5.61}$$

where $n_k = |\Omega|^{-1/2} \sum_{j\in\Omega}(n_{j\uparrow} + n_{j\downarrow}) \exp(ik \cdot r_j)$, and then we obtain

$$\lim_{\Omega\nearrow\mathbf{Z}^d} \langle [A^\dagger_{-k}, [H, A_k]] \rangle = 2dtK(1 - \gamma_k), \tag{5.62}$$

$$\lim_{\Omega\nearrow\mathbf{Z}^d} \langle [B^\dagger_{-k}, [H, B_k]] \rangle = 2dtK(1 + \gamma_k) + 2(2\mu - U)(n - 1) \tag{5.63}$$

and

$$\lim_{\Omega\nearrow\mathbf{Z}^d} |\langle [A_k, B_k] \rangle| = \lim_{\Omega\nearrow\mathbf{Z}^d} \frac{2}{|\Omega|} \langle \mathcal{O}_\Omega \rangle = 2O_{\text{Cooper}}, \tag{5.64}$$

where K denotes the kinetic energy per bond defined by (5.49) and n denotes the electron filling per site. Inserting (5.62)–(5.64) into (5.41), we obtain an upper bound for the lowest frequency of the charge-excitation spectrum

$$\omega_{\mathrm{c}}(\boldsymbol{k}) \leq \frac{dtK}{O_{\text{Cooper}}} \sqrt{(1 - \gamma_k)(1 + g + \gamma_k)}, \tag{5.65}$$

where $g = (2\mu - U)(n - 1)/dtK \geq 0$. One can obtain similar bounds in superconducting phases of other types, e.g. nearest-neighbor s-wave or p-wave.

Equation (5.65) shows that, in the superconducting phase, the lowest frequency of the charge excitations is bounded from above by a gapless k-linear dispersion relation. Owing to breakdown of the global $U(1)$ gauge-symmetry of electrons, the charge excitations have a gapless mode. These excitations correspond to the collective modes first discussed by Anderson [6]. It should be remarked that (5.65) also gives an upper bound of the excitations created by B_k, which are particle excitations of the Cooper pairs with a finite momentum. Equation (5.65) thus shows that creation of the Cooper pairs does not require energy. Similar relations between particle excitations and density excitations were discussed for the Bose superfluids in [134] and references therein.

Finally we give a remark that these results hold for the negative-U Hubbard model as well, in which superconductivity is widely believed to occur. They also can be easily extended to a wide class of electron systems with short-range interactions. Furthermore, the present result does not depend on the mechanism of symmetry breaking.

5.2.4 Summary and discussion

To summarize, we have estimated the energy spectra of the Hubbard model in the magnetic-order phases and in the superconducting phase. The spin-wave spectrum in the antiferromagnetic phase is bounded from above by a gapless k-linear form and in the ferromagnetic phase by a k-quadratic form. We have also discussed the magnetic phase with an incommensurate wave number $\boldsymbol{q}$ and found that the energy spectra of the modes at $\boldsymbol{k} \simeq \mathbf{0}$ and $\boldsymbol{k} \simeq \pm\boldsymbol{q}$ are bounded by gapless k-linear forms.

Moreover, it has been shown for the superconducting phase that the charge excitations and the Cooper-pair excitations are gapless. It is known, however, that, if the interactions of the charge are correctly included in a more realistic model, these gapless excitations disappear by the Anderson-Higgs mechanism [6]. Hence these gapless modes will not exist in real superconductors.

Concerning the two-dimensional Hubbard model, it has been proved [40, 72] that there is no symmetry breaking at finite temperatures and on the other hand, ground states may have long-range orders. This phenomenon occurs as a result of the existence of these gapless modes: Since the excitation spectrum has gapless modes, elementary excitations of macroscopic numbers appear in the two-dimensional system at finite temperatures and hence the order disappears.

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