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Physics and Mathematics of Quantum Many-Body Systems

Springer

To my family

Preface

This is a self-contained advanced textbook on quantum many-body systems, which is intended to be accessible to students and researchers in physics, mathematics, quantum information science, and related fields. The prerequisite is undergraduate-level basic knowledge of quantum mechanics, calculus, and linear algebra. We discuss in detail selected topics in quantum spin systems and lattice electron systems, and also describe fundamental concepts and important basic results necessary to understand the advanced topics of the book (and, of course, other related results in the literature).

More specifically, we focus on long-range order and spontaneous symmetry breaking in the antiferromagnetic Heisenberg model in two or higher dimensions (Part I), the Haldane phenomena in antiferromagnetic quantum spin chains and the related notion of symmetry protected topological phase (Part II), and the origin of magnetism in strongly interacting lattice electron systems, namely various versions of the Hubbard model (Part III). Although the selection of the topics is certainly biased by our research interests, we believe that each topic is, by itself, interesting and worth studying. More importantly each of the topics represents certain non-trivial phenomena or features that we universally encounter in a variety of quantum many-body systems, including quantum field theory, condensed matter systems, cold atoms, and artificial quantum systems designed for future quantum computers. In other words, although most of the systems that we treat in the book are models of magnetism in a broad sense, our interest is not limited to magnetism. We are more interested in universal behaviors of quantum many-body systems.

As the title suggests, we here take the point of view of mathematical physics. Our major goal is to discuss mathematically rigorous results which are of essential importance and interest from physicists' point of view. We shall also discuss in depth physical intuitions and pictures behind the mathematical results.

We believe it crucial to insist on mathematically rigorous proofs (when available) since some phenomena in many-body systems are so intricate and subtle that it is not easy for us to reach the right conclusions based only on naive physical intuitions. It is also worth stressing that, in some (but not all) cases, one gets deeper and clearer understanding of "physics" by appreciating a mathematical proof of a certain physical statement. We hope that the reader will have such experiences by studying some of the theorems and proofs in the present book. We have indeed tried to omit proofs which are too technical, but include those which are enlightening and worth studying. Moreover most of the proofs discussed in the book have been considerably reorganized and extended so as to make them as elementary and accessible as possible. To give an example, the famous theorem of Lieb's on the half-filled Hubbard model (Theorem 10.4 in page 343) is among the most significant contributions of modern mathematical physics to the theory of strongly interacting quantum many-body systems. Although the paper containing the theorem has been frequently cited both in theoretical and experimental papers, and the content of the theorem is well-known, it seems that one usually assumes that the proof of the theorem is too difficult to comprehend. We shall however present an elementary and detailed exposition of the complete proof which should be understandable to a sufficiently motivated undergraduate physics student with standard background in mathematics; we do not make use of anything more advanced than diagonalization of Hermitian matrices! (We also should stress that the book is designed in such a manner that one can skip proofs and only appreciate heuristic arguments and rigorous results.)

We do not, on the other hand, go into mathematical formulations which are too advanced, e.g., the operator algebraic formulation of infinitely large quantum many-body systems. Although such sophisticated formalisms have their own merits in deriving stronger results and further extending our physical intuitions, we shall not try to go too much beyond standard formalism of undergraduate quantum mechanics. When treating infinite systems, we try to choose the most elementary formulation, and also carefully introduce and explain necessary notions.

The restriction to non-relativisitc lattice quantum systems has a clear advantage that relatively satisfactory rigorous results are available. One may, for example, study phenomena parallel to those treated in Parts I or II in the framework of quantum field theories, or discuss the origin of magnetism, which is the topic of Part III, starting from the many-body Schrödinger equation for all the electrons and the nuclei that form a magnetic material. But our current (theoretical-physical and mathematical) understanding of these frameworks is so poor that we still have to struggle in obtaining very elementary results (or even defining the system itself) if we insist on mathematical rigor; there is no hope of treating interesting physical phenomena. By concentrating on lattice systems, where conceptual issues are considerably simpler, we are able to concentrate on the essence of interesting "physics" and mathematical mechanisms behind it. We shall discuss this point further in section 1.1.

We assume that the reader is familiar with elementary quantum mechanics including the theory of angular momentum. Some experiences in statistical mechanics and condensed matter physics are welcome but by no means necessary. As for mathematics, we only assume basic calculus and linear algebra. Although some mathematical arguments are motivated from functional analysis, we do not require any familiarity with functional analysis (or any other advanced mathematics). We shall frequently refer to $\mathbb{Z}_2$, U(1), or SU(2) symmetry, but we do not require any knowledge in (continuous) group theory. What one should know is explained.

This means that at least a large part of the present book is accessible to sufficiently motivated undergraduate students. The readers with background in mathematics or quantum information science may notice our heavy use of the theory of quantum mechanical angular momentum. This is nothing but the representation theory of SU(2), but we physicists are so much used to it since undergraduate quantum mechanics classes. For the non-physics-major readers, we have summarized necessary material about angular momentum in the appendix.

We believe that the material in the present book can be used in several different ways in graduate courses in theoretical or mathematical physics. The author himself has given a half-year course which covers selected topics from Parts I and II, or another course which focuses on topics from Part III. At the time of writing, when many researchers and students are interested in topological phases of matter, a course which covers selected topics from Part II may be attractive.

It is a pleasure to thank Ian Affleck, Takashi Hara, Hosho Katsura, Tom Kennedy, Mahito Kohmoto, Tohru Koma, Elliott Lieb, Andreas Mielke, Yoshiko Ogata, and Akinori Tanaka, who are my collaborators on the subjects related to the topics of the book, for sharing their insights and wisdom with me, and, most of all, for fruitful and enjoyable collaborations. Some of the results from these collaborations are discussed in the present book.

During the preparation of the book, I benefited from useful comments from and discussions with various individuals. I especially wish to thank Hosho Katsura and Akinori Tanaka for their careful readings of the manuscript and for valuable proposals and comments. I also express my gratitude to Ian Affleck, Aron Beekman, Hans Jürgen Briegel, Yuya Dan, Martin Fraas, Yohei Fuji, Keisuke Fujii, Shunsuke Furukawa, Yasuhiro Hatsugai, Takuya Hirano, Chigak Itoi, Tohru Koma, Marius Lemm, Elliott Lieb, Yusuke Masaki, Taku Matsui, Akimasa Miyake, Tadahiro Miyao, Tomonari Mizoguchi, Hisamitsu Mukaida, Bruno Nachtergaele, Fumihiko Nakano, Yoshiko Ogata, Masaki Oshikawa, Glenn Paquette, Louk Rademaker, Robert Raussendorf, Ann Rossilli, Shinsei Ryu, Takahiro Sagawa, Akira Shimizu, Ken Shiozaki, Naoto Shiraishi, Ayumu Sugita, Yuji Tachikawa, Yuhi Tanikawa, Keiji Tasaki, Synge Todo, Masafumi Udagawa, Masahito Ueda, Haruki Watanabe, and Tzu-Chieh Wei for their indispensable contributions.

Last but not least, I wish to thank Mari Okazaki, a renowned Japanese manga artist[1], for providing the book with her fantastic illustrations, one for the cover, and one for each of the three parts. I asked Mari to visualize (admittedly abstract and intangible) ideas developed in the book freely in her own style. I believe that these imaginative illustrations have given an added charm to the book.

Tokyo, *Hal Tasaki*
August 28, 2019

[1] Mari Okazaki's works have been published also in China, France, Italy, Korea, Pórtugal, Spain, Taiwan, and the United States.

Contents

List of Symbols

- ▷ $A := B$ or $B =: A$ means that A is defined in terms of B.
- ▷ $A \simeq B$ means that two quantities A and B are "very close" in a certain sense (usually clear from the context). $A \sim B$ means that A and B are "roughly close" or have the same order of magnitude. We note that this usage may be different from the standard convention in mathematics.
- ▷ $A \cong B$ means that two mathematical objects (such as linear spaces) A and B are isomorphic, which roughly means that A and B have the same structure.
- ▷ For a finite set S, we denote the number of its elements as $|S|$.
- ▷ A condition in a summation (or a product) is specified within brackets as, e.g.,

$$\sum_{\substack{p\in\mathbb{Z} \\ (p \text{ is a prime})}} c_p = c_2 + c_3 + c_5 + c_7 + c_{11} + \cdots .$$

- ▷ c^* denotes the complex conjugate of $c \in \mathbb{C}$.
- ▷ Λ denotes the set of sites of a general lattice (page 21).
- ▷ $\mathscr{B}$ denotes the set of bonds of a general lattice (page 31). A bond is a pair $\{x,y\}$ of two distinct sites $x, y \in \Lambda$. We identify $\{x,y\}$ with $\{y,x\}$.
- ▷ $\mathscr{N}(x) = \{y \in \Lambda \,|\, \{x,y\} \in \mathscr{B}\}$ is the set of sites directly connected to a site $x \in \Lambda$ by a bond.
- ▷ Λ_L is the set of sites of the d-dimensional hyper cubic lattice (page 49):

$$\Lambda_L = \left\{(x_1, x_2, \ldots, x_d) \,\middle|\, x_i \in \mathbb{Z},\ -\frac{L}{2} < x_i \le \frac{L}{2}\right\} \subset \mathbb{Z}^d \tag{3.1.2}$$

- ▷ $\mathscr{B}_L$ is the set of bonds of the d-dimensional hyper cubic lattice with periodic boundary conditions (page 49):

$$\mathscr{B}_L = \left\{ \{x,y\} \,\middle|\, x, y \in \Lambda_L,\ |x-y| = 1 \right\} \tag{3.1.3}$$

- ▷ For $x = (x_1, x_2, \ldots, x_d) \in \mathbb{Z}^d$, we denote the Euclidean norm as $|x| := \sqrt{(x_1)^2 + \cdots + (x_d)^2}$.

- ▷ $\hat{A}^\dagger$ denotes the Hermitian conjugate of an operator (i.e., a matrix) $\hat{A}$.
- ▷ $\hat{\boldsymbol{S}}_x = (\hat{S}_x^{(1)}, \hat{S}_x^{(2)}, \hat{S}_x^{(3)})$ denotes the spin operator acting on site x (page 21). We have $(\hat{\boldsymbol{S}}_x)^2 = S(S+1)$, where $S = 1/2, 1, 3/2, \ldots$ is the fixed spin quantum number.
- ▷ $\hat{\boldsymbol{S}}_{\text{tot}} = (\hat{S}_{\text{tot}}^{(1)}, \hat{S}_{\text{tot}}^{(2)}, \hat{S}_{\text{tot}}^{(3)})$ denotes the total spin operator (page 22). The eigenvalue of $(\hat{\boldsymbol{S}}_{\text{tot}})^2$ and $\hat{S}_{\text{tot}}^{(3)}$ are denoted as $S_{\text{tot}}(S_{\text{tot}}+1)$ and $S_{\text{tot}}^{(3)}$ (or sometimes as M), respectively.
- ▷ The single-particle Hilbert space (without spin) on lattice Λ is $\mathfrak{h} \cong \mathbb{C}^{|\Lambda|}$. It consists of states $\boldsymbol{\varphi} = (\varphi(x))_{x\in\Lambda}$ with $\varphi(x) \in \mathbb{C}$.
- ▷ The single-particle Hilbert space (with spin) on lattice Λ is $\tilde{\mathfrak{h}} \cong \mathbb{C}^{2|\Lambda|}$. It consists of states $\boldsymbol{\varphi} = (\varphi(x,\sigma))_{x\in\Lambda,\sigma=\uparrow,\downarrow}$ with $\varphi(x,\sigma) \in \mathbb{C}$.
- ▷ $\hat{c}_{x,\sigma}$, $\hat{c}_{x,\sigma}^\dagger$, and $\hat{n}_{x,\sigma}$ are the annihilation, creation and number operators, respectively, of an electron at site $x \in \Lambda$ with spin $\sigma = \uparrow, \downarrow$ (page 310).
- ▷ $\hat{C}_\sigma(\boldsymbol{\varphi})$ and $\hat{C}_\sigma^\dagger(\boldsymbol{\varphi})$ are the annihilation and creation operators, respectively, of an electron in the state $\boldsymbol{\varphi} \in \mathfrak{h}$ with spin $\sigma = \uparrow, \downarrow$ (page 316).
- ▷ $(v_1, \ldots, v_D)^{\text{t}}$ denotes a column vector $\begin{pmatrix} v_1 \\ \vdots \\ v_D \end{pmatrix}$. The symbol t stands for transpose.
- ▷ A bold symbol like $\boldsymbol{v}$ usually stands for a column vector $(v_1, \ldots, v_D)^{\text{t}}$ with $v_j \in \mathbb{C}$. We denote by $(\boldsymbol{v})_j$ the j-th component of $\boldsymbol{v}$.
- ▷ The conjugate of a column vector $\boldsymbol{v} = (v_1, \ldots, v_D)^{\text{t}}$ is the row vector $\boldsymbol{v}^\dagger = (v_1^*, \ldots, v_D^*)$. For column vectors $\boldsymbol{v}$ and $\boldsymbol{u} = (u_1, \ldots, u_D)^{\text{t}}$, we denote by $\langle \boldsymbol{v}, \boldsymbol{u} \rangle = \boldsymbol{v}^\dagger \boldsymbol{u} = \sum_{j=1}^{D} v_j^* u_j$ the inner product, and by $\boldsymbol{u}\boldsymbol{v}\dagger$ (which is the Kronecker product) the matrix such that $(\boldsymbol{u}\boldsymbol{v}\dagger)_{i,j} = u_i v_j^*$.
- ▷ A sans-serif symbol like A usually stands for a square matrix $\mathsf{A} = (a_{i,j})_{i,j=1,\ldots,D}$. We denote by $(\mathsf{A})_{i,j}$ the i, j entry of A. The identity matrix is denoted as I.
- ▷ The determinant of A is denoted as $|\mathsf{A}|$.
- ▷ $\mathsf{A}^\dagger$ and A^{t} denote the Hermitian conjugate and the transpose, respectively, of A. A^* is the matrix obtained by taking the complex conjugate of all the entries of A.
- ▷ For column vectors $\boldsymbol{v}$ and $\boldsymbol{u}$, we write $\langle \boldsymbol{v}, \mathsf{A}\boldsymbol{u} \rangle = \boldsymbol{v}^\dagger \mathsf{A} \boldsymbol{u} = \sum_{i,j=1}^{D} v_i^* a_{i,j} u_j$.

See also Appendix A.1 for a summary of the Dirac notation used throughout the book.

Chapter 1
Introduction

1.1 Universality in macroscopic physics

It is fair to say that one of the goals of physical science is to understand the world around us on the basis of the fundamental laws of physics. However, if we naively consider the task of understanding the properties of, say, a piece of metal sitting in front of us, we may be led to conclude that such an understanding is simply impossible. Of course we know the basic structure of the atoms composing the metal, and we have some knowledge about the crystalline structure of the metal and the basic properties of the electrons in the metal, including the band structure and the interactions between them. But all of this amounts to nothing more than approximate descriptions. How can we have a precise understanding without knowing, for example, the exact form of the many-electron wave function that spreads over the entire crystal? Moreover, an actual, macroscopically large piece of metal under ordinary conditions will generally not be a perfect crystal. Instead, it will contain many impurities and dislocations. Further, it may have a surface with an irregular form and be interacting with an external world that behaves in a complicated, uncontrolled manner. Focusing on more microscopic levels, we know that the nuclei in the metal are composed of quarks, whose behavior should be described by quantum chromodynamics (while a full QCD calculation of even a small nucleus requires a supercomputer). In addition to such comparatively practical problems, there is the essential limitation that we do not possess an ultimate microscopic theory that could provide an exact description of this piece of metal.

Despite the problems raised above, we would like to argue that a nontrivial understanding should be possible. We believe that the possibility for obtaining such an understanding is due to the universality we repeatedly encounter in macroscopic physics. The purpose of this short section is to (attempt to) convince the reader of this point.

One important aspect of universality is robustness. We find that, in many (but, of course, not all) problems of physics, the behavior of an object as a whole is insensitive to many details regarding both its own composition and the environment within which it exists. For example, the center-of-mass motion of a sufficiently heavy rigid body on Earth is very accurately described by the Newton's second law of motion for a point particle under uniform gravitational field, and in many cases, will be almost completely independent of the internal structure of the object and the presence of other objects in its proximity, other than Earth itself. Indeed it may be that the existence of such robustness is a necessary condition for the possibility of constructing an intelligible body of physical science.[1] Returning to our piece of metal, we wish to be optimistic, and we posit that some of its properties can be understood reasonably well without knowing, say, very precise forms of its electronic orbits, the exact locations of its impurities and dislocations, the shape of its surface, what our next-door neighbor is doing, the position of the moon, or the equations of a "theory of everything."

The other important aspect of universality is that, in many cases, we observe the same phenomenon in a variety of physical systems. A notable example is the phenomenon of wave propagation. While wave propagation is found in many forms, the same wave equation describes wave motion in a variety of media, including air, water, and elastic material, and even in vacuum in the case of electromagnetic field. A conceptually deeper example is provided by thermodynamics. We know that the same set of nontrivial (and mathematically beautiful) laws of thermodynamics apply with great accuracy to essentially any macroscopic system in equilibrium [27, 36]. Due to the general validity of the theoretical descriptions provided by the wave equation and the laws of thermodynamics, in either case, we can make definite predictions concerning the actual behavior of individual systems from this general description, without the need to investigate the particular properties of the individual systems themselves.

With regard to the relationship between a physical system and the behavior it exhibits, the conventional thinking is that, in some sense, the system possesses a primary existence, while the behavior it exhibits possesses a derivative existence, dependent on the system. However, the above discussion hints at another interpretation. Considering the cases of wave propagation, thermodynamic behavior, and the many other types of universal structures observed in the world, we are tempted to imagine that these universal structures themselves possess a primary existence, independent of any individual system, while they become "incarnated" in various concrete forms in actual physical systems.[2] But, irrespective to our philosophical point of view, there is no doubt that it is a task of essential importance to discover and understand universal phenomena and universal structures that are independent of the individual systems in which they are observed. Returning again to our piece of metal, our goal, from the point of view of universality, should be to find character-

[1] We can try to imagine a world in which all minute aspects of all elements are strongly interlinked. In such a world, any prediction of the behavior of a given element would be practically impossible, because this would require detailed knowledge of the behavior of all other elements. But this is not the world we live in. (Indeed it would seem quite likely that no intelligence could evolve in such an unpredictable world.)

[2] See Chapter 1 of [36] for further discussions of the view based on the notion of universality.

istic and essential phenomena taking place in it, and then to understand the universal structures behind them.[3]

In our pursuit to advance fundamental science, with the manner of thinking described above, we are led to study classes of systems defined by characteristic types of universal phenomena, rather than actual individual systems. Let us call such a class of systems a "universality class."[4] Within a given universality class, we will have not only actual physical systems and faithful theoretical models describing them (which usually have intractable details), but also some idealized theoretical models that appear to be easier to treat. It should be stressed, however, that such idealized models are not simply "made up" to exhibit the desired properties (for some obvious reasons). Rather, they are nontrivial systems that capture only the essence of the phenomena that we wish to understand.[5] By studying such idealized models, we are able to directly confront the problem of elucidating the essential behavior of interest. Perhaps the best example of such an idealized model is the (classical) Ising model. Although the Ising model is now recognized as a model of a ferromagnet, it is too simple to be a faithful model of any actual magnetic system. Nevertheless, we can learn from the Ising model extremely rich essence of phase transitions and critical phenomena associated with the breakdown of $\mathbb{Z}_2$ symmetry, exhibited by various physical systems, including uniaxial ferromagnets and some quantum field theories. It should be pointed out that, despite its relative simplicity, the Ising model is certainly not easy to solve. However, because with this model, one need not treat some of the very complicated problems involved with more realistic models, such as the overlap of electron orbits that determines the exchange interaction and the ultraviolet divergence that must be removed to realize a well-defined field theory, the core problem that we wish to address — that of describing the collective behavior of infinitely many interacting degrees of freedom — is laid bare. This problem is indeed central to understanding the large-scale behavior of a truly vast range of physical systems.

In this book, we treat selected topics in quantum many-body theory that are directly related to important universal phenomena observed mainly in condensed matter systems. We have chosen topics that are of importance from both physical and mathematical points of view. The Heisenberg model and its variants for spin systems and some versions of the Hubbard model for electron systems, which we study in detail throughout the book, are idealized models representing important universality classes in many-body physics. These models play roles in the study of quantum many-body systems analogous to that played by the Ising model in the study of

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[3] Of course we do not argue that this is the only goal. System-dependent properties are important in many applications.

[4] In conventional usage, the term "universality class" refers to a class of statistical mechanical models (or field theories) that exhibit quantitatively identical critical phenomena. Here we are using this terminology in a broader sense.

[5] In most cases, such an idealized model is related to other members of the universality class only through uncontrolled approximations, heuristic arguments, or optimistic hope. It is an extremely challenging problem in theoretical physics to establish firmer connections between complicated and realistic models and simple idealized models. To do so probably requires highly advanced and flexible versions of the renormalization group method.

ferromagnetic systems. We hope that the reader will find the in-depth theoretical studies of these models presented here, which are rooted in our desire to understand a piece of metal sitting in front of us[6], both fruitful and enjoyable.

1.2 Overview of the book

We shall give a brief and informal overview of the topics covered in the present book.[7]

We start from a preparatory chapter (Chapter 2), in which we discuss the basics of quantum spin systems. We encourage the reader to first briefly examine this chapter, no matter what his/her main interest is. The reader may skip the details and come back to them later when necessary.

One of the important results discussed in this chapter is the Marshall-Lieb-Mattis theorem (Theorem 2.2 in page 38) [28, 26]. Consider, for example, the antiferromagnetic Heisenberg model on the d-dimensional $L\times\cdots\times L$ hypercubic lattice with the Hamiltonian

$$\hat{H}=\sum_{x,y}\hat{\boldsymbol{S}}_x\cdot\hat{\boldsymbol{S}}_y, \tag{1.2.1}$$

where x and y are summed over neighboring pairs of sites. (Note that we are using informal notations in this section. We will be more careful in the later sections.) The Marshall-Lieb-Mattis theorem states that, when L is even, the ground state (i.e., the eigenstate with the lowest eigenvalue) of $\hat{H}$ is unique and hence preserves all the symmetry of $\hat{H}$ including, most importantly, the rotational symmetry. We note that in the corresponding ferromagnetic Heisenberg model

$$\hat{H}=-\sum_{x,y}\hat{\boldsymbol{S}}_x\cdot\hat{\boldsymbol{S}}_y, \tag{1.2.2}$$

one gets a large number of ground states in which spins are aligned with each other and pointing in an arbitrarily chosen directions. This comparison already suggests that there is something "more quantum" in antiferromagnets than in ferromagnets, and that the Marshall-Lieb-Mattis theorem touches the essence of this difference.

It may be worth noting that the difference between antiferromagnetic and ferromagnetic systems is apparent even in the simplest possible quantum spin systems, namely, that of two spins with spin quantum number $S=1/2$. It is easily found that the ground state of the antiferromagnetic Hamiltonian $\hat{H}=\hat{\boldsymbol{S}}_1\cdot\hat{\boldsymbol{S}}_2$ is the unique singlet state

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[6] A piece of iron exhibits metallic ferromagnetism, a phenomenon that is still poorly understood theoretically. In the final section of this book, we present a very preliminary attempt at understanding metallic ferromagnetism.

[7] To the reader interested in the connection of our mathematical-physical approach to the standard condensed matter physics, we recommend the book by Fazekas [11].

$$|\Phi_{0,0}\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\big), \tag{1.2.3}$$

which is rotationally invariant, while the ground states of the ferromagnetic Hamiltonian $\hat{H} = -\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2$ are the triplet states

$$|\Phi_{1,1}\rangle = |\uparrow\rangle_1|\uparrow\rangle_2, \quad |\Phi_{1,0}\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\big), \quad |\Phi_{1,-1}\rangle = |\downarrow\rangle_1|\downarrow\rangle_2, \tag{1.2.4}$$

and their linear combinations. (The reader who is not familiar with these notions should not be discouraged; they will be explained in the later sections.)

In Part I of this book, we focus on the problem of spontaneous symmetry breaking and long-range order, which are among the most universal phenomena encountered in physical systems with large degrees of freedom.

A prototypical model is the antiferromagnetic Heisenberg model (1.2.1). It is known that the ground state of the model in two or higher dimensions has antiferromagnetic long-range order (LRO), in the sense that spins separated far away on the lattice are still correlated because of the antiferromagnetic interaction. The proof of the existence of LRO, based on the reflection positivity method due to Dyson, Lieb, and Simon [8], is one of the most important achievements of mathematical physics for quantum-many body systems. We shall carefully describe the proof of the theorem by Kennedy, Lieb, and Shastry (Theorem 4.1 in page 73) [21]. We hope that our detailed account of the method of reflection positivity in quantum spin systems is accessible to a wide range of readers.

Given the existence of LRO, one naively expects that the ground state resembles the Néel state, in which spins are pointing in the alternating directions. See Figure 3.1 (page 48). Such a ground state can only appear as a result of spontaneous symmetry breaking (SSB) because the directions of spins should be chosen arbitrarily. However this picture is in conflict with the aforementioned Marshall-Lieb-Mattis theorem. The unique ground state must have complete rotational invariance, and it is impossible for a spin to point in a certain fixed direction. Thus the exact ground state of (1.2.1) does exhibit LRO, but does not exhibit SSB. This conclusion is physically rather mystifying since states with Néel order are observed experimentally at very low temperatures.

This "mystery", which was already known in 1950's, has been almost completely resolved by now. It turns out that the ground state with LRO but without SSB is accompanied by a series of excited states, known as "Anderson's tower", which have very low excitation energies [3, 5]. A physical ground state with both LRO and SSB, which should be observed experimentally at very low temperatures, is not an exact energy eigenstate but is a superposition of the exact ground state and a large number of the low-lying excited states. This in turn means that the exact ground state is a kind of Schrödinger's cat, in the sense that it is a superposition of various physical ground states.

The above picture has been confirmed rigorously by Koma and Tasaki [24], whose works are based on earlier pioneering works on discrete symmetry breaking by Horsch and von der Linden [16] and Kaplan, Horsch, and von der Linden [19].

We shall discuss these rigorous results carefully, starting from an elementary but important example, namely, the quantum Ising model, and proceed to the difficult case of the Heisenberg model, where one encounters an ever-increasing number of low-lying excited states which form the "tower". We also briefly discuss how LRO naturally leads to SSB in the ground states of infinitely large systems. Although we do not go deeply into operator algebraic formulation of quantum many-body systems, which provides a sophisticated description of infinite systems, we shall discuss some essential points so that the reader can appreciate the flavor of the advanced formulation. In the course of discussion, we also give an important remark about the role of symmetry in the notion of phases. See Figures 3.5 and 3.6 (page 61).

One encounters "LRO without SSB" in ground states of various quantum many-body systems in which the order operator and the Hamiltonian do not commute. Examples include not only quantum antiferromagnets, but superconductivity, Bose-Einstein condensation, and a variety of quantum field theories. Since there is a fundamental difference between spin systems and particle systems, we shall discuss in detail the phenomenon of Bose-Einstein condensation in the Bosonic Hubbard model, placing main emphasis on LRO and SSB.

In this part we also give a quick overview of LRO and SSB in quantum Heisenberg model at nonzero temperatures. This includes (probably the first) proof of a stronger version of the famous Hohenberg-Mermin-Wagner theorem about the absence of symmetry breaking in two dimensions.

The topic of Part II, topological phases of matter in quantum spin chains, is no doubt the most fashionable among the subjects treated in this book. As mentioned already, the reader may directly start from this part, after taking a glance at Chapter 2.

The main theme of the study is still the antiferromagnetic Heisenberg model (1.2.1), but the one defined on the one-dimensional lattice (which is often called the chain). It has been known for quite a long time that, unlike in higher dimensions, the ground state of the one-dimensional model does not exhibit any long-range order. The nature of the ground state for the most basic model with $S = 1/2$ had been studied by using the Bethe ansatz method. (Here S denotes the spin quantum number, which takes the values $S = 1/2, 1, 3/2, 2, \ldots$.) It was found that the ground state is critical, i.e., the correlation functions decay with power law, and there are gapless excitations immediately above the ground state.

In 1983, Duncan Haldane, who received the 2016 Nobel prize in physics mainly for this contribution, discovered that there is a qualitative difference between the low energy properties of the models with a half-odd-integral spin and an integral spin [14, 15]. According to Haldane, properties of the spin S Heisenberg antiferromagnetic chain are basically the same as those for $S = 1/2$ when S is a half-odd-integer, such as 3/2 or 5/2. However, when S is an integer, low energy properties are completely different. The correlation functions decay exponentially, and there is a nonvanishing energy gap (now known as the Haldane gap) above the ground state energy. One can say that the ground state of an integer spin chain is disordered.

It seems that Haldane's conclusion was totally against common beliefs of experts of the day. This may be the reason why people referred to his conclusion as the “Haldane conjecture” in the1980’s.[8] The validity of Haldane’s conclusion was gradually established through a series of experimental, numerical, theoretical, and mathematical works.

A strong theoretical (and mathematical) support to Haldane’s conclusion was provided by Affleck, Kennedy, Lieb, and Tasaki in 1987 [1, 2]. They proposed a model of $S = 1$ antiferromagnetic spin chain whose ground state can be written down explicitly. The Hamiltonian of the model, now called the AKLT model, is given by

$$\hat{H}_{\mathrm{AKLT}} = \sum_{x=1}^{L} \bigl\{ \hat{\boldsymbol{S}}_x \cdot \hat{\boldsymbol{S}}_{x+1} + \frac{1}{3} (\hat{\boldsymbol{S}}_x \cdot \hat{\boldsymbol{S}}_{x+1})^2 \bigr\}, \tag{1.2.5}$$

which has extra biquadratic terms when compared to the original Heisenberg Hamiltonian (1.2.1). As we shall discuss in detail in Chapter 7, it was proved that the model possesses the precise properties that Haldane had predicted for integer spin chains, i.e., the ground state is unique, accompanied by a gap, and has exponentially decaying correlations. It is now believed that the AKLT model represents the universality class of models exhibiting Haldane phenomena.

It also turned out that the ground state of the AKLT model is an example of a class of states called the matrix product states (MPS) proposed and formulated by Fannes, Nachtergaele, and Werner in 1989 [9, 10]. The formulation of MPS provides an extremely efficient way of approximately describing a large class of states in one-dimensional quantum many-body systems, and has been playing indispensable roles in condensed matter physics, mathematical physics, and quantum information science. Section 7.2.2 of this book can be read as a tutorial introduction to MPS motivated by the AKLT model.

The ground state of the AKLT model is not only disordered but has two unexpected exotic properties, namely, the hidden antiferromagnetic order and the effective $S = 1/2$ degrees of freedom at the edge of an open chain. It was later pointed out by den Nijs and Rommelses [7] and by Kennedy [20] that these exotic properties are shared by a class of models which includes the Heisenberg model. Kennedy and Tasaki noted that these properties can be interpreted as consequences of spontaneous breakdown of the hidden $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry [22].

All these observations suggest that the $S = 1$ antiferromagnetic Heisenberg chain and the AKLT model, which have exotic disordered ground states, belong to a new quantum phase which should be called the “Haldane phase”. The true nature of the new phase remained unclear until Gu and Wen pointed out in 2009 that the Haldane phase should be identified as a symmetry protected topological (SPT) phase [13]. Pollmann, Turner, Berg, and Oshikawa soon determined the complete set of symmetry necessary to protect the Haldane phase, and also defined indices (within the MPS formulation) that characterize the topological phases [33]. We present in

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[8] In mathematics a plausible statement is called a conjecture until it is finally proved and becomes a theorem. It is rather unusual to call a statement in theoretical physics a conjecture, since most of “established facts” in theoretical physics are conjectures from mathematicians’ point of view. Mathematically speaking, Haldane’s conclusions for the Heisenberg chain (1.2.1) is still a conjecture. (But nobody calls it the “Haldane conjecture” any more).

sections 8.3.3 and 8.3.4 a detailed account of their index theory. Finally, in 2018 and 2019, by using sophisticated notions in operator algebraic approach to quantum many-body systems, Ogata developed fully rigorous index theorems, which essentially solves the problem of SPT phases in quantum spin chains [31, 32].

In this part, we also discuss two topics from quantum information science which are closely related to the main theme of the part, namely, the Briegel-Raussendorf state (cluster state) [6] and its generalizations (section 7.3.3) and Kitaev's toric code model (section 8.4) [23]. The latter is of considerable interest as a simple model exhibiting topological order, which is distinct from (and probably more important than) symmetry protected topological order.

In Part III of the book, we turn our attention to the origin of interactions between spins which we see, e.g., in the Hamiltonians (1.2.1) and (1.2.2). We therefore need to take one step further down to the microscopic level, and study the problem of interacting electrons. Such a study was first made back in 1928 by Heisenberg, who argued, based on a simple perturbation theory for a two-electron system, that the Coulomb interaction between electrons and quantum many-body dynamics of fermions lead to ferromagnetic exchange interaction as in (1.2.2). (This is the reason for calling the model the Heisenberg model.)

The Hubbard model was introduced in the 1960's independently by Kanamori [18], Gutzwiller [12], and Hubbard [17] in order to study the origin of ferromagnetism in many-electron systems. It is a tight-binding model with the simple Hamiltonian

$$\hat{H} = \sum_{\substack{x,y \\ \sigma=\uparrow,\downarrow}} t_{x,y}\, \hat{c}^\dagger_{x,\sigma} \hat{c}_{y,\sigma} + U \sum_x \hat{n}_{x,\uparrow} \hat{n}_{x,\downarrow}\,, \tag{1.2.6}$$

where the first term represents quantum mechanical hopping of electrons, and the second term describes the on-site Coulomb interaction. We stress that the model is not designed to be a faithful model of realistic systems. It should be regarded as an idealized model that is designed to capture universal phenomena and mechanisms taking place in interacting many-electron systems.

We do not assume that the reader is familiar with the Hubbard model. We shall carefully explain in chapter 9.2 the description (also known as the "second quantization" formalism) of many-electron systems in terms of creation and annihilation operators, the motivations behind the definition of the Hamiltonian (1.2.6), and the basics about non-interacting fermion systems.

As we see in Chapter 10, the origin of antiferromagnetic interaction (1.2.1) is easily understood, at least heuristically, from Anderson's perturbative argument for half-filled Hubbard models [4]. In 1989, Elliott Lieb proved an important and nontrivial theorem for the Hubbard model at half-filling, which partially confirms the above perturbative picture [25]. Lieb's theorem on the Hubbard model is one of the most important achievements in mathematical physics for quantum many-body systems. For certain classes of models, the theorem also establishes the emergence of ferrimagnetism and superconductivity. We shall discuss in detail the statement, applications, and the proof of Lieb's theorem. As we have already stressed, a detailed (and hopefully readable) account of the proof of the theorem is one of the main contributions of the present book.

The long final chapter, Chapter 11, is devoted to the emergence of ferromagnetism in the Hubbard model. The first rigorous example of ferromagnetism in the Hubbard model was discovered by Nagaoka in 1966 [30]. Nagaoka's ferromagnetism takes place in a rather singular situation where the number of electrons is one less than the number of lattice sites, and the on-site Coulomb interaction is infinitely large. Then there appears a single "hole" in the configuration, and the motion of the hole generates ferromagnetic coupling of the whole electrons. Although Nagaoka's ferromagnetism is interesting and nontrivial from a theoretical point of view, it is nowadays believed that the mechanism leading to the ferromagnetism does not work in less singular situations with finite interaction and multiple holes.

Almost for a quarter of a century, Nagaoka's ferromagnetism was the only rigorous example of ferromagnetism in the Hubbard model. The situation changed drastically in the early 1990's when first Mielke [29] and then Tasaki [34] proposed essentially different rigorous examples. They considered special classes of tight-binding models in which the corresponding single-electron spectra have a flat lowest band. It was proved that the ground states of the model exhibit ferromagnetism for any nonzero Coulomb interaction when the number of electrons is exactly the same as the degeneracy of the flat band. These examples are now called the flat-band ferromagnetism. The elegant construction Mielke's flat-band models makes use of the notion of line graphs.

It should be noted that all the above rigorous examples of ferromagnetism are singular in some aspects. Nagaoka's ferromagnetism requires infinitely large interaction and exactly one "hole". Flat-band ferromagnetism takes place only when one has a singular band structure with infinitely large density of states. Rigorous examples of ferromagnetism which are free from any such singularities were finally discovered by Tasaki in 1995 [35]. The models were obtained by perturbing Tasaki's flat-band models to make the lowest band dispersive. Then the emergence of ferromagnetism in the ground states was proved for sufficiently large but finite interaction when the width of the lowest band is sufficiently narrow. Tasaki also proved that the model has spin-wave excitations whose dispersion relation precisely recovers the form expected in an insulating ferromagnet. Thus, starting from a well-defined non-singular model of strongly interacting itinerant electron system, it was established that the low energy properties of the model coincide with what are expected in a "healthy" ferromagnetic system. We believe that this is the most satisfactory answer (for the moment) to the problem raised by Heisenberg, i.e., to explain the origin of ferromagnetism in terms of many-body quantum mechanics.

Of course all these are very special examples of ferromagnetic insulators. The problem of the origin of ferromagnetism is still widely open. We end the chapter by discussing our own very preliminary attempts at constructing rigorous examples of metallic ferromagnetism.

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