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Symmetry Breaking and Finite-Size Effects in Quantum Many-Body Systems

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We consider a quantum many-body system on a lattice which exhibits a spontaneous symmetry breaking in its infinite-volume ground states, but in which the corresponding order operator does not commute with the Hamiltonian. Typical examples are the Heisenberg antiferromagnet with a Néel order and the Hubbard model with a (superconducting) off-diagonal long-range order. In the corresponding finite system, the symmetry breaking is usually "obscured" by "quantum fluctuation" and one gets a symmetric ground state with a long-range order. In such a situation, Horsch and von der Linden proved that the finite system has a low-lying eigenstate whose excitation energy is not more than of order N^{-1}, where N denotes the number of sites in the lattice. Here we study the situation where the broken symmetry is a continuous one. For a particular set of states (which are orthogonal to the ground state and with each other), we prove bounds for their energy expectation values. The bounds establish that there exist ever-increasing numbers of low-lying eigenstates whose excitation energies are bounded by a constant times N^{-1}. A crucial feature of the particular low-lying states we consider is that they can be regarded as finite-volume counterparts of the infinite-volume ground states. By forming linear combinations of these low-lying states and the (finite-volume) ground state and by taking infinite-volume limits, we construct infinite-volume ground states with explicit symmetry breaking. We conjecture that these infinite-volume ground states are ergodic, i.e., physically natural. Our general theorems not only shed light on the nature of symmetry breaking in quantum many-body systems, but also provide indispensable information for numerical approaches to these systems. We also discuss applications of our general results to a variety of interesting examples. The present paper is intended to be accessible to readers without background in mathematical approaches to quantum many-body systems.

KEY WORDS: Symmetry breaking; long-range order; obscured symmetry breaking; finite-size effects; quantum fluctuation; ground states; low-lying states; ergodic states.

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1. INTRODUCTION

1.1. Motivations

Symmetry breaking in quantum many-body systems is a challenging problem in theoretical physics. In some situations, strong "quantum effects" lead to phenomena which are hard to predict or understand from a "classical" point of view. The present paper is devoted to one such "quantum effect," namely, how a symmetry breaking manifests itself in a *finite* system when the order operator and the Hamiltonian do not commute with each other. The topic reflects subtlety of both quantum mechanics and many-body problems, and indeed has been a source of some confusion in the field.[3] We have tried in the present paper not only to present out new theorems, but also to review (hopefully in an accessible manner) some background materials necessary to understand the nature of the problems.

Suppose that we have a quantum many-body system which exhibits a spontaneous symmetry breaking in its infinite-volume ground states. When the operator that measures the symmetry does not commute with the Hamiltonian, one encounters strong "quantum fluctuation." In the corresponding *finite* system, the symmetry breaking is usually "obscured" by the fluctuation, and one only gets a unique ground state with perfect symmetry.

An "obscured symmetry breaking"[4] usually manifests itself in the following two different ways.

- One observes a long-range order in the ground-state two-point correlation function for the order operators.
- There appear eigenstates of the Hamiltonian with energies "close" to the ground-state energy. We call them "low-lying eigenstates." (See Section 2.1 for precisely how "close" the energies should be, and the motivation for the criterion.)

Although one might be tempted to interpret these "low-lying eigenstates" as counterparts of excited states in the infinite-volume system, some of them are actually "parts" of the infinite-volume ground states. In the infinite-volume limit, some of the "low-lying eigenstates" and the unique

[3] See footnotes in Section 1.2 for what the confusions are.

[4] Even in a classical system or a quantum system with commuting Hamiltonian and order operator one never observes explicit symmetry breaking in a finite system at a *finite temperature*. In this sense, "obscured symmetry breaking" may be regarded as a common phenomenon not necessarily intrinsic to quantum systems. Throughout the present paper, however, we use the term "obscured symmetry breaking" to indicate only the (most interesting and nontrivial) situation where a symmetry breaking in the infinite volume becomes unobservable in a *ground state* of a finite system due to quantum fluctuation.

ground state are linearly combined to form a set of ergodic ground states with explicit symmetry breaking. These ergodic ground states are believed to correspond to physically realizable states in a large system at an extremely low temperature.

When a continuous symmetry is broken, there are infinitely many ergodic ground states in the infinite volume. It is then expected that the number of independent "low-lying eigenstates" in the corresponding finite system increases indefinitely as the system size gets larger. The existence of such ever-increasing numbers of "low-lying states" and the corresponding finite-size scaling behavior of the low-lying spectrum of the Hamiltonian may be regarded as characteristic features of a continuous symmetry breaking in a quantum many-body system. These points have been discussed mainly by practitioners of numerical exact diagonalization of quantum spin systems. (It is not easy to list all the relevant references. See, for example, refs. 18, 24, 8, 7, 29, and 35 and the references therein.) But rigorous information is lacking except in the mean-field model.[32, 17, 19] See also ref. 6 for an early related discussion within the framework of the spin-wave approximation.

The purpose of the present paper is to state general theorems for lattice quantum many-body systems which exhibit "obscured symmetry breaking." Our results can be roughly divided into two parts, which are closely related with each other.

The first set of results clarifies the relation between the above-mentioned two types of manifestations of an "obscured symmetry breaking." Whenever there is a finite-volume ground state which does not break symmetry but whose correlation function exhibits a certain long-range order, we expect that there inevitably appear "low-lying eigenstates." Horsch and von der Linden[15] actually proved that the existence of a long-range order implies the existence of a "low-lying eigenstate" whose excitation energy is less than of order N^{-1}, where N is the number of sites in the lattice. (See Theorem 2.2.) Our new results deal with the cases where the long-range order is related to a continuous $U(1)$ symmetry. We construct a particular set of states which are orthogonal to the ground state and with each other, and prove that they are indeed "low-lying states" in the sense of Definition 2.1. When the system has a higher $U(1) \times \mathbf{Z}_2$ symmetry, we can show that there are ever-increasing numbers of "low-lying eigenstates" whose excitation energies are bounded from above by a constant times N^{-1}. Such finite-size scaling behavior of the low-lying spectrum of the Hamiltonian is characteristic in a system where an "obscured symmetry breaking" related to a continuous symmetry takes place. As far as we know, this is the first rigorous (and explicit) demonstration that ever-increasing numbers of "low-lying states" indeed exist.

A very important problem which we do *not* solve in the present paper is whether such finite-size scaling behavior alone is sufficient to conclude that there is a symmetry breaking in the infinite volume. See refs. 8, 7, and 35 for discussions about this problem. See ref. 26 for a solution of the closely related problem of showing the existence of a symmetry breaking when there is a long-range order in a series of finite systems.

The second set of results of the present paper clarifies the roles played by the "low-lying states" in forming infinite-volume ground states with explicit symmetry breaking. In general we show that any translation-invariant "low-lying states" converge to a ground state in the infinite-volume limit. The particular "low-lying states" we construct have the crucial feature that they can be naturally regarded as "parts" of infinite-volume ground states with explicit symmetry breaking. To demonstrate this fact, we construct [for a general class of models with a $U(1)$ symmetry] infinite-volume ground states with explicit symmetry breaking by taking suitable linear combinations of the low-lying states and the (finite-volume) ground state and then taking infinite-volume limits. We conjecture that these ground states are ergodic, i.e., are physically natural (infinite-volume) ground states.

We also discuss applications of our general results to a variety of concrete examples. The examples include the Heisenberg antiferromagnet, the Bose–Einstein condensation in the hard-core Bose gas on a lattice, the superconductivity in lattice electron models, and the Haldane gap problem in the $S=1$ quantum antiferromagnetic chain. An interesting observation in the application to the Bose gas is that, by following our general discussions, we are naturally led to consider ground states which do not conserve the particle number.

We believe that these results not only clarify the nature of symmetry-breaking phenomena in quantum systems, but also provide indispensable information for numerical approaches to various quantum many-body systems.

The present paper is organized as follows. In the following Section 1.2, we illustrate some of the basic notions by studying a concrete example of the Ising model under a transverse magnetic field. We have tried to make this section accessible to readers who are not familiar with mathematical approaches to quantum many-body problems. In Section 2, we state our theorems in the most general setting and discuss their physical consequences. In Section 3, we discuss applications of our theorems to typical problems. Sections 4 and 5 are devoted to the proofs of our theorems.

In three appendices, we prove and summarize some useful results closely related to the main body of the paper. In Appendix A, we discuss relations between three different definitions of infinite-volume ground states and show that they are all equivalent when restricted to translation-invariant states. In Appendix B, we concentrate on a system with spontaneously broken discrete symmetry and present a theorem which shows how to construct ergodic infinite-volume ground states. In Appendix C, we prove lemmas which characterize fluctuations of bulk quantities.

1.2. "Obscured Symmetry Breaking" and "Low-Lying States" in a Simple Example

Before discussing general theorems, we want to make clear what we mean by "obscured symmetry breaking" and "low-lying states" and how these notions are related to phenomena of symmetry breaking. For this purpose, we shall discuss one of the simplest models in which one observes an "obscured symmetry breaking" and "low-lying states." In the course of the discussion, we briefly review the notions of ground states in an infinite system, of ergodic states, and of symmetry breaking in the absence of a symmetry-breaking field. Although such materials form standard background in mathematical approaches to quantum many-body systems, we have noted that they are not widely appreciated in standard physics literature. Here we will try to explain basic physical ideas rather than developing precise mathematical formalism. Mathematical details will be supplied in the following sections.

Consider the d-dimensional $L\times\cdots\times L$ hypercubic lattice $\Lambda\subset\mathbf{Z}^d$ and impose periodic boundary conditions. We define the $S=1/2$ spin system on Λ with the Hamiltonian

$$H_\Lambda=-\sum_{\langle x,y\rangle} S_x^{(3)}S_y^{(3)}-B\sum_x S_x^{(1)}, \tag{1.1}$$

where the first sum is over nearest-neighbor pairs of sites in Λ, the magnetic field satisfies $B\geqslant 0$, and $\mathbf{S}_x=(S_x^{(1)},S_x^{(2)},S_x^{(3)})$ denote the $S=1/2$ spin operators at site x. The model is known as the Ising model under transverse magnetic field.

The ground state of the Hamiltonian (1.1) is known to exhibit a phase transition as the transverse field B is varied. This is most clearly seen from the following behavior of the order parameter $m(B)$. Let $\Phi_\Lambda^{(0)}(B,B')$ be the normalized ground state of the Hamiltonian $H_\Lambda-B'O_\Lambda$, where O_Λ is the order operator

$$O_\Lambda=\sum_{x\in\Lambda} S_x^{(3)} \tag{1.2}$$

The field B' is usually called the symmetry-breaking field. Define the order parameter by

$$m(B) := \lim_{B' \downarrow 0} \lim_{\Lambda \uparrow \mathbf{Z}^d} \frac{1}{N} (\Phi_\Lambda^{(0)}(B, B'), O_\Lambda \Phi_\Lambda^{(0)}(B, B')) \tag{1.3}$$

where $N = L^d$ is the number of sites in Λ. Throughout the present paper, the symbol $:=$ signifies definition. It can be proved that, for a fixed dimension d ($=1, 2, 3,...$), the order operator satisfies $m(B) = 0$ for sufficiently large B, and $m(B) > 0$ for sufficiently small B. In the latter case, the global up–down symmetry of the system is spontaneously broken in the infinite-volume ground state. [Of course we mean the positive (respectively negative) direction in the third axis by up (respectively down).]

Let us see how this symmetry breaking manifests itself in *finite* systems. When $B = 0$, the model is nothing but the classical Ising model. The Hamiltonian (1.1) has two ground states Φ_Λ^+ and Φ_Λ^-, in which all the spins are pointing up and down, respectively. The ground states are ordered and break the up–down symmetry of the Hamiltoninan.

When $B > 0$, we encounter "quantum fluctuation." By using the Perron–Frobenius theorem, as in Marshall[33] and Lieb and Mattis,[32] one finds that the ground state $\Phi_\Lambda^{(0)}(B)$ of the Hamiltonian (1.1) is unique for an arbitrary finite L. Hence the global up–down symmetry remains unbroken in the finite-volume ground state $\Phi_\Lambda^{(0)}(B)$ for any value of $B > 0$. When $m(B) > 0$, we might say that the symmetry breaking in the infinite-volume limit is "obscured" by "quantum fluctuation" in finite systems.

A sign of the "obscured symmetry breaking" can be found as a long-range order in the two-point correlation functions. Although we have $(\Phi_\Lambda^{(0)}(B), S_x^{(3)} \Phi_\Lambda^{(0)}(B)) = 0$ for any $B > 0$, we expect (and can prove for sufficiently small B) that

$$(\Phi_\Lambda^{(0)}(B), S_x^{(3)} S_y^{(3)} \Phi_\Lambda^{(0)}(B)) \simeq m(B)^2 \tag{1.4}$$

holds for sufficiently large $|x - y|$.

Another sign of the "obscured symmetry breaking" can be found if we consider the first excited (eigen)state $\Phi_\Lambda^{(1)}(B)$ of H_Λ and its energy $E_\Lambda^{(1)}$. When we have $m(B) > 0$, we expect that

$$E_\Lambda^{(1)} - E_\Lambda^{(0)} \approx \exp[-\tau(B) L^d] \tag{1.5}$$

holds as $L \uparrow \infty$ with a positive finite constant $\tau(B)$, where $E_\Lambda^{(0)}$ denotes the ground-state energy. The states $\{\Phi_\Lambda^{(1)}(B)\}_\Lambda$ in this situation are typical examples of "low-lying eigenstates."[5] See Definition 2.1.

[5] A beginner to exact diagonalization might identify $\Phi_\Lambda^{(1)}(B)$ as a finite-size counterpart of an excited state in the infinite system. As will become clear soon, this is totally misleading.

Now we discuss states in the infinite system. A ground state in the infinite system may be defined by the thermodynamic limit

$$\omega_B(A) := \lim_{\Lambda \uparrow \mathbf{Z}^d} (\Phi_\Lambda^{(0)}(B), A\Phi_\Lambda^{(0)}(B)) \tag{1.6}$$

where A is an arbitrary local operator (i.e., a polynomial of spin operators) and $\Phi_\Lambda^{(0)}(B)$ is the unique ground state of H_Λ. The limit is well-defined if one takes suitable subsequence of lattices. (See Section 2.5 and Appendix A for details.) Since the finite-volume ground state $\Phi_\Lambda^{(0)}(B)$ respects the global up–down symmetry, so does the infinite-volume ground state $\omega_B(\cdots)$. In particular we have

$$\omega_B(S_x^{(3)}) = 0 \tag{1.7}$$

for any x.

One might suspect from the above construction and the relation (1.7) that when the symmetry-breaking field B' is vanishing, there is no symmetry breaking even in the infinite-volume limit.[6] From a physical point of view, however, this conclusion is unnatural and misleading. One should recall that there are many situations in nature where we do observe a symmetry breaking in the absence of explicit symmetry-breaking fields.[7] It is indeed possible to develop mathematically sensible definitions of infinite-volume ground states which are capable of describing a symmetry breaking without symmetry-breaking fields. We discuss precise definitions in Section 2.5 (Definition 2.6) and Appendix A. Here we shall see concrete examples.

Before discussing the symmetry breaking, however, let us observe that the above ground state $\omega_B(\cdots)$ indeed has an unnatural property. Let Ω be a hypercubic region in $\mathbf{Z}^d$ and denote by $|\Omega|$ the number of sites in Ω. Consider the bulk physical quantity $M_\Omega := \sum_{x \in \Omega} S_x^{(3)}$. By combining (1.4), (1.7), and Lemma C.1, we find that

$$\frac{1}{|\Omega|^2} \omega_B\{[M_\Omega - \omega_B(M_\Omega)]^2\} \geqslant m(B)^2 \tag{1.8}$$

as $|\Omega| \uparrow \infty$. The relation (1.8) implies that in the state $\omega_B(\cdots)$ the intensive bulk quantity $M_\Omega/|\Omega|$ has a finite fluctuation provided that $m(B) > 0$. This

[6] This is another possible confusion we sometimes encounter.

[7] A typical example is antiferromagnetism, in which a staggered magnetic field plays the role of symmetry-breaking field. No mechanism can generate a real staggered magnetic field in an antiferromagnetic material. A more drastic example is the Bose–Einstein condensation, where the symmetry-breaking field should create and annihilate particles!

is in contrast to the basic requirement in physics that any intensive bulk quantity exhibits essentially no fluctuation in a thermodynamically stable phase. An infinite-volume state in which any intensive bulk quantity has vanishing fluctuation is called an ergodic state. (See Definition 2.7.) It is believed that a physically realizable state in a large system can be well approximated by an ergodic state. (See Remark 1 at the end of the present section for further discussion.) The behavior (1.8) implies that the state $\omega_B(\cdots)$ is not ergodic, and is hence unphysical.

Then there must be some physically natural ground states. Let us note that the ground state $\Phi_\Lambda^{(0)}(B)$ and the first excited state $\Phi_\Lambda^{(1)}(B)$ inherit the existence of symmetry breaking in the infinite-volume limit. We expect that when $m(B) > 0$ these states can be written as

$$\Phi_\Lambda^{(0)}(B) \simeq \frac{1}{\sqrt{2}} [\tilde{\Phi}_\Lambda^+(B) + \tilde{\Phi}_\Lambda^-(B)] \tag{1.9}$$

and

$$\Phi_\Lambda^{(1)}(B) \simeq \frac{1}{\sqrt{2}} [\tilde{\Phi}_\Lambda^+(B) - \tilde{\Phi}_\Lambda^-(B)] \tag{1.10}$$

where $\tilde{\Phi}_\Lambda^+$ and $\tilde{\Phi}_\Lambda^-$ are the states obtained by taking into account local quantum fluctuations into the completely ordered states Φ_Λ^+ and Φ_Λ^-, respectively. Equations (1.9) and (1.10) motivate us to define two states in the infinite system by

$$\begin{aligned} \omega_B^\pm(A) &:= \lim_{\Lambda \uparrow \mathbf{Z}^d} \tfrac{1}{2}([\Phi_\Lambda^{(0)}(B) \pm \Phi_\Lambda^{(1)}(B)], A[\Phi_\Lambda^{(0)}(B) \pm \Phi_\Lambda^{(1)}(B)]) \\ &\simeq \lim_{\Lambda \uparrow \mathbf{Z}^d} (\tilde{\Phi}_\Lambda^\pm(B), A\tilde{\Phi}_\Lambda^\pm(B)) \end{aligned} \tag{1.11}$$

for an arbitrary local operator A. By using (1.5), the translation invariance of the expectation values, and the fact that $(\Phi_\Lambda^{(1)}(B), H_\Lambda \Phi_\Lambda^{(0)}(B)) = 0$, we find that these states satisfy

$$\omega_B^\pm(h_x) = \epsilon_0 := \omega_B(h_x) \tag{1.12}$$

for any $x \in \mathbf{Z}^d$. The local Hamiltonian is $h_x = -\sum_{y;\,|x-y|=1} S_x^{(3)} S_y^{(3)}/2 - BS_x^{(1)}$, where the sum runs over the sites y which are neighboring to x. We call the above ϵ_0 the groud-state energy density. Following Definition 2.6, we shall interpret the relation (1.12) as indicating that the states $\omega_B^\pm(\cdots)$ are infinite-volume ground states.[8] We stress that this is a natural definition

[8] The existence of ground states other than $\omega_B(\cdots)$ apparently contradicts the "uniqueness of the ground state" we mentioned earlier, and has been a source of confusion (especially in much more delicate situations, e.g., in Heisenberg antiferromagnets). Of course there is no contradiction, since the uniqueness (as is proved by the Perron–Frobenius argument[32]) applies only to a finite system.

of ground states. In a bulk (or an infinite) system, it is no longer meaningful to talk about small differences in the total energy. What really count are the expectation values of the local Hamiltonian, and the present definition is designed precisely to look only at them. We shall discuss further the definitions of infinite-volume ground states in Appendix A.

The final expression in (1.11) suggests the existence of an explicit symmetry breaking as

$$\omega_B^{\pm}(S_x^{(3)}) = \pm m(B) \tag{1.13}$$

If we assume the existence of a long-range order as in (1.4) and the existence of a gap above $E_\Lambda^{(1)}$, we can prove the relation (1.13) from (B.7) and Lemma B.4. Under the same assumptions, we can also prove that the infinite-volume ground states $\omega_B^{\pm}(\cdots)$ are ergodic. See Theorem B.1. We conclude that $\omega_B^{\pm}(\cdots)$ constructed by taking linear combinations of $\Phi_\Lambda^{(0)}(B)$ and $\Phi_\Lambda^{(1)}(B)$ are the physically natural ground states in the infinite volume.

Let us summarize what we have learned from the present simple example. When there is an "obscured symmetry breaking," we have the following.

- There inevitably exists a "low-lying eigenstate."
- The infinite-volume ground state defined by a naive infinite-volume limit of finite-volume ground states is not "ergodic," i.e., is unphysical.
- An ergodic ground state may be formed by taking a linear combination of the finite volume ground state and the "low-lying (eigen)-state" and then taking the infinite-volume limit.

In Section 2, we will see that these features are typical when there is an "obscured symmetry breaking." We will mainly concentrate on how the situation is modified when the relevant symmetry is a continuous one.

Remarks. 1. The statement that "a physically realizable state in a large system can be well approximated by an ergodic state" perhaps requires some explanation. Since this is a very delicate problem about observations in quantum many-body systems, we can only give some heuristic ideas.

Consider a large but finite system at an extremely low temperature. (Note that it is impossible to attain the absolute zero temperature as long as observations are done within a finite amount of time.) Suppose that the thermal energy is much larger than the excitation energy of the "low-lying eigenstate," which is quite likely since the thermal energy is proportional to the system size. Then one has a chance to observe not only the ground state, but any linear combination of the ground state and the "low-lying state." Most of these linear combinations, however, suffer from the pathological behavior that some bulk intensive quantities have finite fluctuations as in (1.8). Conventional wisdom suggests that a state with such a pathologically large fluctuation is unstable under perturbations. Small thermal disturbances may well destroy such a state and bring it into a more stable one. We expect that such a mechanism will select only ergodic states out of the infinitely many linear combinations of the ground state and the "low-lying state."

2. The reader might wonder about the nature of the ground state $\Phi_\Lambda^{(0)}(B)$ and the first eigenstate $\Phi_\Lambda^{(1)}(B)$ when B is large enough so that we have $m(B)=0$. In this case, we expect that H_Λ has a finite gap almost uniform in the lattice size N, and thus

$$E_\Lambda^{(1)} - E_\Lambda^{(0)} = O(1) \tag{1.14}$$

as $N \uparrow \infty$. According to Definition 2.1, the state $\Phi_\Lambda^{(1)}(B)$ may be again called a "low-lying eigenstate." However, its nature is totally different from that in the case with $m(B)>0$. (This may be regarded as a disadvantage of our definition of "low-lying states." See the discussion following Definition 2.1.)

Roughly speaking, the first excited state $\Phi_\Lambda^{(1)}(B)$ can be regarded as the state in which a single "magnon" is in the $k=0$ state, i.e.,

$$\Phi_\Lambda^{(1)}(B) \simeq \sum_{x \in \Lambda} \Phi_\Lambda^{(x)}(B) \tag{1.15}$$

where $\Phi_\Lambda^{(x)}(B)$ is the state in which the magnon is localized at site x. When B is extremely large, $\Phi_\Lambda^{(x)}(B)$ may be approximated by the state in which the spin at x is pointing in the direction opposite to the magnetic field and all the other spins are pointing in the direction of the field.

The biggest difference from the case with $m(B)>0$ is that the limit

$$\tilde{\omega}_B(\cdots) := \lim_{\Lambda \uparrow \mathbf{Z}^d} ([\alpha\Phi_\Lambda^{(0)}(B) + \beta\Phi_\Lambda^{(1)}(B)], (\cdots)[\alpha\Phi_\Lambda^{(0)}(B) + \beta\Phi_\Lambda^{(1)}(B)]) \tag{1.16}$$

with any α, β with $|\alpha|^2 + |\beta|^2 = 1$, defines exactly the same state as $\omega_B(\cdots)$ in (1.6). More precisely, we have

$$\omega_B(A) = \tilde{\omega}_B(A) \tag{1.17}$$

for an arbitrary local operator A. The equality (1.17) should be expected since, in an infinite system with only a single magnon, the probability of observing the magnon is vanishing. We expect that in this case the infinite-volume ground state is unique and preserves the global up–down symmetry. Such a result can be proved rigorously for sufficiently large B. See Theorem A.4.

2. RESULTS AND PHYSICAL CONSEQUENCES

In the present section, we describe our main results and their physical consequences in a general setting. One of the goals is the construction of infinite-volume ground states with explicit symmetry breaking presented in Section 2.5. A result on "low-lying eigenstates" which has direct relevance to numerical approaches can be found in Section 2.6.

2.1. Preliminaries

Here we fix some basic notations. We also give a precise definition of "low-lying states" and discuss motivations behind the definition.

We consider a quantum system on a finite lattice Λ with N sites. With each site $x \in \Lambda$ we associate a finite-dimensional Hilbert space $\mathscr{H}_x$. The full Hilbert space is

$$\mathscr{H}_\Lambda := \bigotimes_{x \in \Lambda} \mathscr{H}_x \tag{2.1}$$

We note that a "site" in Λ need not be an atomic site of a quantum many-body system. If necessary, one may call a group of atomic sites a "site" and let $\mathscr{H}_x$ be the corresponding finite-dimensional Hilbert space.

Throughout the present paper, the norm of a state $\Psi_\Lambda \in \mathscr{H}_\Lambda$ is defined as $\| \Psi_\Lambda \| = (\Psi_\Lambda, \Psi_\Lambda)^{1/2}$ and the norm of an operator A on $\mathscr{H}_\Lambda$ as

$$\|A\| := \sup_{\Psi_\Lambda \in \mathscr{H}_\Lambda} \frac{\|A \Psi_\Lambda\|}{\|\Psi_\Lambda\|} \tag{2.2}$$

For a fixed Λ, we take the Hamiltonian

$$H_\Lambda := \sum_{x \in \Lambda} h_x \tag{2.3}$$

where each h_x is a self-adjoint operator on $\mathscr{H}_\Lambda$.

In order to discuss the notion of "low-lying states" we take a sequence $\{\Lambda\}$ of finite lattices which tend to the infinite lattice $\mathbf{Z}^d$. For each Λ (with N sites) we consider a quantum mechanical system on Λ with the Hamiltonian H_Λ and the ground state $\Phi_\Lambda^{(0)}$. The corresponding eigenvalue of H_Λ is denoted as $E_\Lambda^{(0)}$.

Definition 2.1. A sequence of normalized states $\{\Phi'_\Lambda\}_\Lambda$ are called "low-lying states" if

$$\lim_{\Lambda \uparrow \mathbf{Z}^d} \frac{1}{N} [(\Phi'_\Lambda, H_\Lambda \Phi'_\Lambda) - E_\Lambda^{(0)}] = 0 \tag{2.4}$$

holds, and if each Φ'_Λ is orthogonal to the ground state $\Phi^{(0)}_\Lambda$. "Low-lying states" in which each state Φ'_Λ happens to be an eigenstate of the Hamiltonian H_Λ are called "low-lying eigenstates."

The above definition of "low-lying states" is mainly motivated by Theorem 2.8, which says that any translation-invariant "low-lying states" converge to an infinite-volume ground state. We note, however, that the definition is too general to indicate only those "low-lying states" which play crucial roles in forming infinite-volume ground states with symmetry breaking. For example, the "magnon state" (1.15) discussed in the remark of Section 1.2 is also a "low-lying state" according to the definition, but one usually wishes to consider it as an excited state.[9] The reader may regard that the definition is introduced for notational convenience rather than to indicate a physically important notion.[10]

2.2. Theorem of Horsch and von der Linden

Before discussing our own results, we describe the theorem due to Horsch and von der Linden,[15] which was the first rigorous result concerning the existence of a "low-lying state" in the presence of an "obscured symmetry breaking."

We consider a finite lattice Λ with N sites and a quantum many-body system on it as in Section 2.1. Let

$$O_\Lambda := \sum_{x \in \Lambda} o_x \tag{2.5}$$

be the order operator, where each o_x is a self-adjoint operator on $\mathscr{H}_\Lambda$.

Assume that $\|h_x\| \leqslant h$ and $\|o_x\| \leqslant o$ hold for any x with x-independent finite constants h and o. Assume also that $[o_x, o_y] = 0$ holds for any x, y and $[h_x, o_y] = 0$ holds unless the site y belongs to the support set $\mathscr{S}_x$. We require that the number of sites in $\mathscr{S}_x$ is bounded from above by an integer r. Let Φ_Λ be an eigenstate of H_Λ with the eigenvalue E_Λ. We assume that the state Φ_Λ exhibits an "obscured symmetry breaking" in the sense that it satisfies

$$(\Phi_\Lambda, O_\Lambda \Phi_\Lambda) = 0 \tag{2.6}$$

[9] It is worth mentioning, however, that the state with exactly one magnon is never observed as an excited state in actual experiments. One can measure the effects caused by magnons only in the state where magnons have a finite density. Such a state is, of course, not a "low-lying state."

[10] If we recall the discussion in Remark 1 of Section 1.2, however, it is possible to give a physical meaning to the above definition. Equation (2.4) precisely states the condition that the energy gap of the states $\{\Phi'_\Lambda\}$ is dominated by the thermal energy in a sufficiently large system.

and

$$(\Phi_\Lambda, (O_\Lambda)^2 \Phi_\Lambda) \geq (\mu o N)^2 \tag{2.7}$$

with a constant $0 < \mu \leq 1$. We define

$$\Psi_\Lambda := \frac{O_\Lambda \Phi_\Lambda}{\|O_\Lambda \Phi_\Lambda\|} \tag{2.8}$$

which is well-defined since $\|O_\Lambda \Phi_\Lambda\|$ is nonvanishing because of (2.7).

Then the theorem of Horsch and von der Linden is the following. If we set Φ_Λ as the ground state $\Phi_\Lambda^{(0)}$, it shows that there is a sequence of states $\{\Psi_\Lambda^{(1)}\}_\Lambda$ which form "low-lying eigenstates" (in the sense of Definition 2.1), and their excitation energy is less than of order N^{-1}.

Theorem 2.2. The expectation value of the energy in the state Ψ_Λ satisfies

$$\frac{1}{N} |(\Psi_\Lambda, H_\Lambda \Psi_\Lambda) - E_\Lambda| \leq c_0 \frac{1}{N^2} \tag{2.9}$$

with $c_0 = 2r^2 h \mu^{-2}$. When Φ_Λ is the ground state $\Phi_\Lambda^{(0)}$ of H_Λ, there exists an eigenstate $\Phi_\Lambda^{(1)}$ of H_Λ whose energy $E_\Lambda^{(1)}$ satisfies

$$E_\Lambda^{(1)} - E_\Lambda \leq c_0 \frac{1}{N} \tag{2.10}$$

Proof. A crucial observation is that the energy difference can be expressed in terms a double commutator such as the following. Then the first part follows as

$$\begin{aligned}
|(\Psi_\Lambda, H_\Lambda \Psi_\Lambda) - E_\Lambda| &= \frac{|(\Phi_\Lambda, [[O_\Lambda, H_\Lambda], O_\Lambda] \Phi_\Lambda)|}{2\, \|O_\Lambda \Phi_\Lambda\|^2} \\
&\leq \frac{\|[[O_\Lambda, H_\Lambda], O_\Lambda]\|}{2\, \|O_\Lambda \Phi_\Lambda\|^2} \\
&\leq \frac{4r^2 h o^2 N}{2(\mu o N)^2} = c_0 \frac{1}{N}
\end{aligned} \tag{2.11}$$

where we have used the assumed commutation relations and the norm bounds of h_x and o_x as well as (2.7). To prove the second part, we note that the relation (2.6) implies that the state Ψ_Λ is orthogonal to the ground state $\Phi_\Lambda^{(0)}$. Then the statement in the theorem is a simple consequence of the variational principle. ∎

2.3. Main Theorems

Now we shall describe our own theorems about "low-lying states." They apply to a system with a continuous symmetry and establish the existence of ever-increasing numbers of "low-lying eigenstates."

We again consider a finite lattice Λ with N sites and a quantum many-body system on it as in Section 2.1. We further require that the system possesses a global $U(1)$ symmetry whose generator is a self-adjoint operator C_Λ. We assume that

$$[H_\Lambda, C_\Lambda]=0 \tag{2.12}$$

We introduce the order operators

$$O_\Lambda^{(\alpha)} := \sum_{x\in\Lambda} o_x^{(\alpha)} \tag{2.13}$$

where $\alpha=1, 2$, and each $o_x^{(\alpha)}$ is a self-adjoint operator on $\mathscr{H}_\Lambda$. The order operators form two components of a vector $(O_\Lambda^{(1)}, O_\Lambda^{(2)})$ which transforms under the action of $U(1)$ and measure a possible spontaneous breakdown of the $U(1)$ symmetry. They satisfy the standard commutation relations

$$[O_\Lambda^{(1)}, C_\Lambda]=-iO_\Lambda^{(2)}, \qquad [O_\Lambda^{(2)}, C_\Lambda]=iO_\Lambda^{(1)} \tag{2.14}$$

We also introduce

$$O_\Lambda^{\pm} := O_\Lambda^{(1)} \pm iO_\Lambda^{(2)} \tag{2.15}$$

which satisfy the commutation relations

$$[O_\Lambda^{+}, C_\Lambda]=-O_\Lambda^{+}, \qquad [O_\Lambda^{-}, C_\Lambda]=O_\Lambda^{-} \tag{2.16}$$

The operators O_Λ^+ and O_Λ^- are the raising and the lowering operators, respectively, for the quantum number defined by the self-adjoint operator C_Λ.

We assume that these operators satisfy the following three conditions.

(i) $[o_x^{(\alpha)}, o_y^{(\beta)}]=0$ for $x\neq y$ and $\alpha, \beta=1, 2$.

(ii) $[h_x, o_y^{(\alpha)}]=0$ holds for $\alpha=1,2$ unless $y\in\mathscr{S}_x$. The number of sites in the support set $\mathscr{S}_x\subset\Lambda$ is bounded from above by an x-independent integer $r\geqslant 2$.

(iii) There are x-independent finite constants h and o and we have $\|h_x\|\leqslant h$ and $\|o_x^{(\alpha)}\|\leqslant o$ for any $x\in\Lambda$ and $\alpha=1, 2$.

Let Φ_Λ be a normalized simultaneous eigenstate of the Hamiltonian H_Λ and the self-adjoint operator C_Λ. We denote by E_Λ the corresponding eigenvalue of H_Λ. Usually we take Φ_Λ as the ground state $\Phi_\Lambda^{(0)}$ of H_Λ. We assume the following:

(iv) The state Φ_Λ exhibits a long-range order in the sense that

$$(\Phi_\Lambda, (O_\Lambda^{(1)})^2 \Phi_\Lambda) = (\Phi_\Lambda, (O_\Lambda^{(2)})^2 \Phi_\Lambda) \geqslant (\mu o N)^2 \tag{2.17}$$

holds with a constant $0 < \mu \leqslant 1$.

From the commutation relations (2.16) and the fact that Φ_Λ is an eigenstate of C_Λ, we automatically have

$$(\Phi_\Lambda, O_\Lambda^{(1)} \Phi_\Lambda) = (\Phi_\Lambda, O_\Lambda^{(2)} \Phi_\Lambda) = 0 \tag{2.18}$$

In other words, the state Φ_Λ has vanishing order parameters. The relations (2.17) and (2.18) together imply that the state Φ_Λ exhibits an "obscured symmetry breaking."[11]

For a nonvanishing integer M, we consider the state

$$\Psi_\Lambda^{(M)} := \frac{(O_\Lambda^+)^M \Phi_\Lambda}{\|(O_\Lambda^+)^M \Phi_\Lambda\|} \tag{2.19}$$

where we set $(O_\Lambda^+)^M = (O_\Lambda^-)^{-M}$ for a negative M. Although the state (2.19) is ill-defined if $(O_\Lambda^+)^M \Phi_\Lambda = 0$, the following theorems guarantee that this is not the case when certain conditions are met.

The first theorem of the present paper is the following. Although the bound (2.22) for the energy expectation value may not look quite strong, it will turn out to be sufficient for a construction of infinite-volume ground states with symmetry breaking. A better estimate for the energy expectation value will be provided in the second theorem.

Theorem 2.3. When the assumptions (i)–(iv) are valid, and we further have

$$N \geqslant \left(\frac{4r}{\mu}\right)^2 \tag{2.20}$$

and

$$\frac{|M|}{N} \leqslant \frac{\mu^2}{8r} \tag{2.21}$$

[11] In fact (2.17) and (2.18) may well hold in a finite system whose infinite-volume limit does not exhibit a symmetry breaking, in which case the parameter μ vanishes as $\Lambda \uparrow \mathbf{Z}^d$. What we really mean by an "obscured symmetry breaking" is that (2.17) and (2.18) are valid with a Λ-independent $\mu > 0$.

the state $\Psi_\Lambda^{(M)}$ of (2.19) is well-defined. The expectation value of the energy in the state satisfies

$$\frac{1}{N}|(\Psi_\Lambda^{(M)}, H_\Lambda \Psi_\Lambda^{(M)}) - E_\Lambda| \leqslant c_1 \frac{|M|}{N} \tag{2.22}$$

where c_1 is a constant which depends only on h, r, and μ.

By taking Φ_Λ as the ground state $\Phi_\Lambda^{(0)}$ of the Hamiltonian, the theorem implies that $\{\Psi_\Lambda^{(M)}\}_\Lambda$ with a fixed M form "low-lying states" in the sense of Definition 2.1. The theorem will be proved in Section 4.

In order to get a better estimate of the energy difference (at least for small enough $|M|$), we require higher symmetry.

(v) The order operators satisfy the commutation relation

$$[O_\Lambda^{(1)}, O_\Lambda^{(2)}] = i\gamma C_\Lambda \tag{2.23}$$

where γ is a real constant.

In other words, we assume that the vector $(\gamma^{-1/2}O_\Lambda^{(1)}, \gamma^{-1/2}O_\Lambda^{(2)}, C_\Lambda)$ forms generators of $SU(2)$. We do not, however, assume that the system has a full $SU(2)$ symmetry. We only require a partial $U(1)\times \mathbf{Z}_2$ $[\cong O(2)]$ symmetry as follows.

(vi) We have $U_\Lambda H(U_\Lambda)^{-1} = H$ and $U_\Lambda \Phi_\Lambda \propto \Phi_\Lambda$, where $U_\Lambda = \exp[i(\pi/\sqrt{\gamma})\, O_\Lambda^{(1)}]$ represents the π-rotation around the first axis.

Then the second theorem is as follows.

Theorem 2.4. When the assumptions (i)–(vi) are valid and we further have

$$\frac{M^2}{N} \leqslant c_2 \tag{2.24}$$

with $c_2 = \min\{\mu^2/(192r), o\mu/(24\gamma)^{1/2}\}$, the state $\Psi_\Lambda^{(M)}$ of (2.19) is well-defined. The expectation value of the energy in the state satisfies

$$\frac{1}{N}|(\Psi_\Lambda^{(M)}, H_\Lambda \Psi_\Lambda^{(M)}) - E_\Lambda| \leqslant c_3 \left(\frac{M}{N}\right)^2 \tag{2.25}$$

where c_3 is a constant which depends only on h, o, r, μ, and γ.

This theorem has a rather strong implication on the property of the low-lying spectrum of the Hamiltonian H_Λ. See Section 2.6. The theorem will be proved in Section 5.

Remark. The condition (vi) for Theorem 2.4 can be weakened to $C_\Lambda \Phi_\Lambda = 0$ if one replaces the definition of the trial state (2.19) by

$$\Psi_\Lambda^{(M)} := \frac{(O_\Lambda^+)^M \Phi_\Lambda + (O_\Lambda^-)^M \Phi_\Lambda}{\|(O_\Lambda^+)^M \Phi_\Lambda + (O_\Lambda^-)^M \Phi_\Lambda\|} \tag{2.26}$$

2.4. States with Explicit Symmetry Breaking

As we have already mentioned in the introduction, the particular set of states $\{\Psi_\Lambda^{(M)}\}$ defined in (2.19) is not introduced as mere candidates of "low-lying states." These states have a special feature that they can be regarded as "parts" of infinite-volume ground states with explicit symmetry breaking. In order to demonstrate this fact, we shall here construct a sequence of "low-lying states" which exhibits symmetry breaking. The basic idea in the present construction appeared already in our earlier publication.[26]

Let us consider a sequence of models which satisfy the conditions (i)–(iv) of Section 2.3 with the state Φ_Λ chosen as the ground state $\Phi_\Lambda^{(0)}$ of the Hamiltonian H_Λ. Note that we are only assuming the $U(1)$ symmetry as is required for Theorem 2.3. For a positive integer k, we take a linear combination of the ground state and the "low-lying states" $\Psi_\Lambda^{(M)}$ as

$$\Xi_\Lambda^{(k)} := \frac{1}{(2k+1)^{1/2}} \left\{ \Phi_\Lambda^{(0)} + \sum_{M=1}^{k} (\Psi_\Lambda^{(M)} + \Psi_\Lambda^{(-M)}) \right\} \tag{2.27}$$

We shall take the lattice Λ sufficiently large so that the bounds (2.20) and (2.21) are valid for any M with $|M| \leqslant k$. By using Theorem 2.3 and the fact that $(\Psi_\Lambda^{(i)}, H_\Lambda \Psi_\Lambda^{(j)}) = 0$ for $i \neq j$, we note that the state $\Xi_\Lambda^{(k)}$ is normalized and satisfies

$$\lim_{\Lambda \uparrow \mathbf{Z}^d} \frac{1}{N} \{ (\Xi_\Lambda^{(k)}, H_\Lambda \Xi_\Lambda^{(k)}) - E_\Lambda \} = 0 \tag{2.28}$$

for any k. Thus $\{\Xi_\Lambda^{(k)}\}_\Lambda$ with a fixed k form "low-lying sates."

These "low-lying states" have the following remarkable properties.

Theorem 2.5. The expectation value of the order operators in the state $\Xi_\Lambda^{(k)}$ satisfies

$$(\Xi_\Lambda^{(k)}, O_\Lambda^{(2)} \Xi_\Lambda^{(k)}) = 0 \tag{2.29}$$

and

$$\lim_{k \uparrow \infty} \lim_{\Lambda \uparrow \mathbf{Z}^d} \frac{1}{N} (\Xi_\Lambda^{(k)}, O_\Lambda^{(1)} \Xi_\Lambda^{(k)}) \geqslant \sqrt{2}\, \mu o \tag{2.30}$$

where the prefactor $\sqrt{2}$ is modified if the model has a higher symmetry. For example, we replace $\sqrt{2}$ with $\sqrt{3}$ when the model has an $SU(2)$ symmetry.

Outline of Proof. We first note that

$$\begin{aligned}(\Xi_\Lambda^{(k)}, O_\Lambda^+ \Xi_\Lambda^{(k)}) &= \frac{1}{2k+1} \sum_{M=-k}^{k} \sum_{M'=-k}^{k} \frac{(\Phi_\Lambda^{(0)}, (O_\Lambda^+)^{-M} O_\Lambda^+ (O_\Lambda^+)^{M'} \Phi_\Lambda^{(0)})}{\|(O_\Lambda^+)^M \Phi_\Lambda^{(0)}\| \cdot \|(O_\Lambda^+)^{M'} \Phi_\Lambda^{(0)}\|} \\ &= \frac{1}{2k+1} \sum_{M=-k+1}^{k} \frac{(\Phi_\Lambda^{(0)}, (O_\Lambda^+)^{-M} O_\Lambda^+ (O_\Lambda^+)^{M-1} \Phi_\Lambda^{(0)})}{\|(O_\Lambda^+)^M \Phi_\Lambda^{(0)}\| \cdot \|(O_\Lambda^+)^{M-1} \Phi_\Lambda^{(0)}\|} \\ &= \frac{1}{2k+1} \sum_{M=1}^{k} \frac{(\Phi_\Lambda^{(0)}, (O_\Lambda^-)^M (O_\Lambda^+)^M \Phi_\Lambda^{(0)})}{\|(O_\Lambda^+)^M \Phi_\Lambda^{(0)}\| \cdot \|(O_\Lambda^+)^{M-1} \Phi_\Lambda^{(0)}\|} \\ &\quad + \frac{1}{2k+1} \sum_{M''=1}^{k} \frac{(\Phi_\Lambda^{(0)}, (O_\Lambda^+)^{M''} (O_\Lambda^-)^{M''} \Phi_\Lambda^{(0)})}{\|(O_\Lambda^-)^{M''-1} \Phi_\Lambda^{(0)}\| \cdot \|(O_\Lambda^-)^{M''} \Phi_\Lambda^{(0)}\|}\end{aligned} \tag{2.31}$$

where we used the shorthand notation $(O_\Lambda^+)^{-M} = (O_\Lambda^-)^M$ for $M > 0$. (It must be noted that O_Λ^- is not the inverse of O_Λ^+.) We have used the facts that Φ_Λ is an eigenstate of C_Λ and $O_\Lambda^\pm$ are the raising and lowering operators for the charge defined by C_Λ to get the second equality. To get the final line, we have set $M'' = 1 - M$. A similar calculation for $(\Xi_\Lambda^{(k)}, O_\Lambda^- \Xi_\Lambda^{(k)})$ shows that $(\Xi_\Lambda^{(k)}, O_\Lambda^+ \Xi_\Lambda^{(k)}) = (\Xi_\Lambda^{(k)}, O_\Lambda^- \Xi_\Lambda^{(k)})$, and hence the desired relation (2.29). Note that we de not have to use the $\mathbf{Z}_2$ symmetry as is assumed in the conditions (v) and (vi) of Section 2.3.

The relation (2.30) is essentially proved in ref. 26. One only has to combine (7.26) of ref. 26 and Theorem 6.1 of ref. 26. Although some estimates in ref. 26 implicitly assume the larger $U(1) \times \mathbf{Z}_2$ symmetry, this is not necessary. A careful treatment (as we did above) shows that all the estimates in ref. 26 are valid for the models with only a global $U(1)$ symmetry.[12] ∎

The theorem establishes that the state $\Xi_\Lambda^{(k)}$ exhibits explicit symmetry breaking. By applying the $U(1)$ rotation $\exp[i\theta C_\Lambda]$ to the state $\Xi_\Lambda^{(k)}$, we also get states in which the order parameter is pointing in different directions.

[12] One can considerably improve the estimates in ref. 26 by using the techniques developed in Section 5 of the present paper.

2.5. Infinite-Volume Ground States

Now we discuss the relation between the "low-lying states" in the sequence of finite systems and the infinite-volume ground states. We again observe that when there is an "obscured symmetry breaking" the naive infinite-volume limit of the finite-volume ground states is not an ergodic state and is hence unphysical. By forming suitable linear combinations of the (finite-volume) ground state and the "low-lying states" and then taking infinite-volume limits, we get infinite-volume ground states with explicit symmetry breaking. We conjecture that these infinite-volume ground states are ergodic, i.e., physically natural.

In order to simplify the discussion, we make several assumptions on the model. We assume that each finite lattice Λ is a d-dimensional hypercubic lattice with periodic boundary conditions. We again denote by N the number of sites in Λ. We assume that the Hamiltonian (2.3) and the order operators (2.13) are translation invariant in the sense that we can write $h_x = \tau_x(h_o)$ and $o_x^{(\alpha)} = \tau_x(o_o^{(\alpha)})$ for any x. Here τ_x is the translation by the lattice vector x (which translation respects the periodic boundary conditions) and the operators h_o and o_o are independent of Λ.

A local operator A is an operator which acts nontrivially only on a finite number of sites [or, more precisely, on a finite-dimensional Hilbert space $\bigotimes_{x \in \mathscr{S}(A)} \mathscr{H}_x$ with a finite support set $\mathscr{S}(A)$]. Let $\rho_\Lambda(\cdots) = \mathrm{Tr}_{\mathscr{H}_\Lambda}[(\cdots)\tilde{\rho}_\Lambda]$ be a state of the system on Λ, where $\tilde{\rho}_\Lambda$ is an arbitrary density matrix on $\mathscr{H}_\Lambda$. Given a sequence of (finite-volume) states $\{\rho_\Lambda(\cdots)\}_\Lambda$, we (formally) define

$$\rho(A) := \lim_{\Lambda \uparrow \mathbf{Z}^d} \rho_\Lambda(A) \tag{2.32}$$

for each local operator A. The above $\rho(\cdots)$ is a linear map from the space of local operators to the set of complex numbers $\mathbf{C}$. We call $\rho(\cdots)$ a *state* of the infinite system. (See Appendix A for the general definition of a state in an infinite system.) It might happen, however, that the limit (2.32) does not exist for all local A. It is known that one can always choose a subsequence of lattices so that the limit is well-defined. See Appendix A for a proof. (An elementary proof can be constructed by using the "diagonal sequence trick" as is illustrated, e.g., in Theorem I.24 of ref. 42.)

We want to describe what we mean by ground states of the infinite system. Since it is meaningless to talk about eigenstates or eigenvalues of the total Hamiltonian H_Λ when $\Lambda \uparrow \mathbf{Z}^d$, a different point of view is necessary. Here we employ probably the simplest definition for ground states of an infinite system. As we discuss in Appendix A, the present definition is equivalent to the other definitions which are standard in the mathematical literature. It simply says that a ground state should minimize the local energy.

Definition 2.6. We define the ground-state energy density ϵ_0 by

$$\epsilon_0 := \lim_{\Lambda \uparrow \mathbf{Z}^d} \inf_{\substack{\Phi_\Lambda \in \mathcal{H}_\Lambda \\ \|\Phi_\Lambda\| = 1}} \frac{1}{N} (\Phi_\Lambda, H_\Lambda \Phi_\Lambda) \tag{2.33}$$

where the limit always exists. An infinite-volume state $\omega(\cdots)$ is said to be a ground state if it satisfies

$$\omega(h_x) = \epsilon_0 \tag{2.34}$$

for any $x \in \mathbf{Z}^d$.

We also introduce the precise notion of ergodic states in an infinite system. In the following, we shall give a simple intuitive definition. See the remark at the end of the present section for the relation between the present definition and other related notions.

In short the definition says that a state is ergodic if and only if any intensive bulk quantity has essentially no fluctuation in the state. Since the requirement is believed to apply to any physically realizable state of a large system, we might say that a translation-invariant state is physically natural if and only if it is ergodic. (See Remark 1 of Section 1.2.) It is also known that a nonergodic translation-invariant state can be decomposed into an "integral" over ergodic states. See the remark at the end of the present section.

Definition 2.7. Let Ω be a hypercubic region in $\mathbf{Z}^d$ and denote the number of sites in Ω by $|\Omega|$. For an arbitrary local self-adjoint operator A, we define the corresponding bulk quantity as $A_\Omega := \sum_{x \in \Omega} \tau_x(A)$, where $\tau_x(A)$ is the translate of A by a lattice vector x. Let $\rho(\cdots)$ be a translation-invariant state, i.e., a state which satisfies $\rho(B) = \rho(\tau_x(B))$ for any local operator B and any $x \in \mathbf{Z}^d$. The state $\rho(\cdots)$ is said to be ergodic if, for any A, the intensive bulk quantity $A_\Omega/|\Omega|$ exhibits vanishing fluctuation in the sense that

$$\lim_{|\Omega| \uparrow \infty} \frac{1}{|\Omega|^2} \rho\{[A_\Omega - \rho(A_\Omega)]^2\} = 0 \tag{2.35}$$

For each finite Λ, let $\Phi_\Lambda^{(0)}$ be a ground state of H_Λ. We can assume $\Phi_\Lambda^{(0)}$ is translation invariant since the Hamiltonian is. Then it is easy to verify that the infinite-volume state defined by

$$\omega(A) := \lim_{\Lambda \uparrow \mathbf{Z}^d} (\Phi_\Lambda^{(0)}, A \Phi_\Lambda^{(0)}) \tag{2.36}$$

for any local operator A (by taking a suitable subsequence) is indeed an infinite-volume ground state in the sense of Definition 2.6.

Assume that each finite-volume ground state $\Phi_\Lambda^{(0)}$ exhibits an "obscured symmetry breaking" in the sense that it satisfies (2.17) and (2.18). Then by using Lemma C.1 we can show that

$$\frac{1}{|\Omega|^2}\,\omega([O_\Omega^{(\alpha)}-\omega(O_\Omega^{(\alpha)})]^2)\geqslant(\mu o)^2 \tag{2.37}$$

for any finite region $\Omega\subset\mathbf{Z}^d$, where $O_\Omega^{(\alpha)}=\sum_{x\in\Omega}o_x^{(\alpha)}$. This implies that the ground state $\omega(\cdots)$ is not an ergodic state, and is hence unphysical.

We still do not know how to construct ergodic ground states in a general setting. In Appendix B, however, we present a general construction of ergodic infinite-volume ground states in a system where a *discrete* symmetry is spontaneously broken and a gap above the first "low-lying eigenstate" is generated. In what follows, we make some observations which suggest that a similar construction as in Appendix B might work in systems with a broken continuous symmetry.

Let us start from a simple but important theorem which summarizes the relation between "low-lying states" and ground states of an infinite system.

Theorem 2.8. Let $\{\Phi'_\Lambda\}_\Lambda$ be "low-lying states" in the sense of Definition 2.1, and assume that each Φ'_Λ defines translation-invariant expectation values, i.e., $(\Phi'_\Lambda, A\Phi'_\Lambda)=(\Phi'_\Lambda, \tau_x(A)\,\Phi'_\Lambda)$ for any $x\in\Lambda$ and for any local operator A. Then the state

$$\omega'(\cdots):=\lim_{\Lambda\uparrow\mathbf{Z}^d}(\Phi'_\Lambda,(\cdots)\,\Phi'_\Lambda) \tag{2.38}$$

defined by taking a suitable subsequence of lattices, is a ground state.

Proof. The translation invariance implies

$$(\Phi'_\Lambda, H_\Lambda\Phi'_\Lambda)=N(\Phi'_\Lambda, h_x\Phi'_\Lambda) \tag{2.39}$$

for any $x\in\Lambda$. Then the condition (2.4) of "low-lying states" reads

$$\lim_{\Lambda\uparrow\mathbf{Z}^d}\{(\Phi'_\Lambda, h_x\Phi'_\Lambda)-(\Phi_\Lambda^{(0)}, h_x\Phi_\Lambda^{(0)})\}=0 \tag{2.40}$$

which reduces to $\omega'(h_x)=\epsilon_0$ for any x. ∎

It should be stressed that in the above the "low-lying states" Φ'_Λ need not be ground states or eigenstates of finite systems.

The states $\Xi_\Lambda^{(k)}$ defined in (2.27) and its $U(1)$ rotations are "low-lying states" with translation-invariant expectation values. By using Theorem 2.8 and Theorem 2.5, we get the following important result, which completes a construction of infinite-volume ground states with explicit symmetry breaking.

Corollary 2.9. For $0 \leqslant \theta \leqslant 2\pi$, define infinite-volume states by

$$\omega_\theta(\cdots) := \lim_{k \uparrow \infty} \lim_{\Lambda \uparrow \mathbf{Z}^d} (e^{i\theta C_\Lambda} \Xi_\Lambda^{(k)}, (\cdots)\, e^{i\theta C_\Lambda} \Xi_\Lambda^{(k)}) \tag{2.41}$$

where we take subsequences if necessary. The states $\omega_\theta(\cdots)$ are infinite-volume ground states. They exhibit explicit symmetry breaking as

$$\omega_\theta[o_x^{(1)}] = m \cos\theta, \qquad \omega_\theta[o_x^{(2)}] = m \sin\theta \tag{2.42}$$

for any x. The order parameter m satisfies

$$m \geqslant \sqrt{2}\, o\mu \tag{2.43}$$

for systems with a $U(1)$ symmetry and $m \geqslant \sqrt{3}\, o\mu$ for systems with an $SU(2)$ symmetry.

It is believed that in a system where a $U(1)$ symmetry is spontaneously broken the nonergodic ground state $\omega(\cdots)$ [defined in (2.36)] is decomposed as

$$\omega(\cdots) = \frac{1}{2\pi} \int_0^{2\pi} d\theta\, \omega_\theta^{\text{ergodic}}(\cdots) \tag{2.44}$$

where $\omega_\theta^{\text{ergodic}}(\cdots)$ is an ergodic ground state which satisfies

$$\omega_\theta^{\text{ergodic}}[o_x^{(1)}] = m_{\max} \cos\theta, \qquad \omega_\theta^{\text{ergodic}}[o_x^{(2)}] = m_{\max} \sin\theta \tag{2.45}$$

where $m_{\max} > 0$ is the maximum possible value of the order parameter within the infinite-volume ground states.

Let us examine how the order parameter $m_{\max}$ is related to the long-range order observed in two-point functions. There are two different ways of defining the long-range order parameter. The first definition deals directly with the infinite-volume state. We define the long-range order parameter μ_1 for the (nonergodic) state $\omega(\cdots)$ by

$$\mu_1 := \lim_{\Omega \uparrow \mathbf{Z}^d} \frac{1}{o\,|\Omega|} [\omega((O_\Omega^{(1)})^2)]^{1/2} \tag{2.46}$$

The other definition deals with a sequence of finite-volume ground states. We define the lang-range order parameter μ_2 as

$$\mu_2 := \limsup_{\Lambda \uparrow \mathbf{Z}^d} \frac{1}{oN} [(\Phi_\Lambda^{(0)}, (O_\Lambda^{(1)})^2 \Phi_\Lambda^{(0)})]^{1/2} \tag{2.47}$$

where $\Phi_\Lambda^{(0)}$ is the ground state on Λ. Note that this definition is motivated by (2.17), one of the basic assumptions of the present paper.

It is quite likely that the above two definitions give the same result for a large class of systems. Unfortunately, we are only able to prove the one-sided inequality $\mu_1 \geqslant \mu_2$. (This follows from Lemma C.1.) Let us proceed by assuming that the equality $\mu_1 = \mu_2$ is valid.

Assuming the decomposition (2.44), we see, for sufficiently large hypercubic region Ω, that

$$\frac{1}{|\Omega|^2} \omega((O_\Omega^{(1)})^2) \simeq \frac{1}{2\pi} \int_0^{2\pi} d\theta \, (m_{\max} \cos\theta)^2 = \frac{(m_{\max})^2}{2} \tag{2.48}$$

where we have used that $\omega_\theta^{\text{ergodic}}(\cdots)$ is ergodic. Then by using (2.46) and (2.48), we observe that $m_{\max} = \sqrt{2}\, o\mu_1$. On the other hand, the inequality (2.43) and the definition (2.47) of the lang-range order parameter immediately imply that $m \geqslant \sqrt{2}\, o\mu_2$. Combining these two equations with the conjectured $\mu_1 = \mu_2$, we get $m \geqslant m_{\max}$. Since $m_{\max}$ is defined as the maximum value of the order parameter, this leads us to the (plausible but nonrigorous) conclusion that we indeed have $m = m_{\max}$.

This observation motivates us to state the following conjecture.

Conjecture 2.10. The infinite-volume ground states $\omega_\theta(\cdots)$ defined in (2.41) are nothing but the desired ergodic (i.e., physically natural) ground states $\omega_\theta^{\text{ergodic}}(\cdots)$.

Unfortunately, we have no direct evidence to support the conjecture. For systems with a discrete symmetry, however, we can prove that the statement corresponding to the above conjecture is in fact valid. See Appendix B.

Remarks. 1. Our Definition 2.7 of ergodic states is actually not exactly the same as the standard one.[9,43,45] For the particular class of systems we are considering here, however, it turns out that our definition is equivalent to the standard definition of $\mathbf{Z}^d$-ergodic states. See, for example, Sections 6.3 and 6.5 of ref. 43. (In fact, our definition is motivated by Lemma 6.5.1 of ref. 43.)

There is a beautiful decomposition theory for $\mathbf{Z}^d$-ergodic states. It states that an arbitrary nonergodic translation-invariant state can be decomposed into a kind of "integral" over ergodic states. See Section I.7 (especially Theorem I.7.10) of ref. 45 or Section 6.4 of ref. 43. A detailed treatment of the decomposition theory can be found in Chapter 4 of ref. 9.

A disadvantage in the notion of ergodic states (as in Definition 2.7) is that one has to *a priori* assume the correct invariance of the states in order to get a physically natural state. Another way of characterizing physically natural states is to make use of the notion of *pure* states. This notion is in some sense more abstract than that of ergodic states, and does not make use of any specific invariance. See refs. 9 and 43 for the definition of *pure* states and for what is known about them. (One should be aware that the notion of pure states for an infinite system is distinct from that for ordinary quantum mechanics with finite degrees of freedom.)

2. Another way of (formally) defining infinite-volume ground states with explicit symmetry breaking is to apply an infinitesimal symmetry-breaking field to the system. Let $\Phi_\Lambda^{(0)}(B)$ be a ground state of the Hamiltonian $H_\Lambda - BO_\Lambda^{(1)}$, where B is real-valued symmetry-breaking field, and define a state of the infinite system by

$$\tilde{\omega}(\cdots) := \lim_{B \downarrow 0} \lim_{\Lambda \uparrow \mathbf{Z}^d} (\Phi_\Lambda^{(0)}(B), (\cdots)\, \Phi_\Lambda^{(0)}(B)) \tag{2.49}$$

We expect that the state $\tilde{\omega}(\cdots)$ is identical to $\omega_{\theta=0}(\cdots)$ [and to $\omega_{\theta=0}^{\text{ergodic}}(\cdots)$]. The existence of a symmetry breaking in the state $\tilde{\omega}(\cdots)$ (under the assumption that there is a long-range order) was proved in refs. 18 and 26.

2.6. "Low-Lying Eigenstates" in Finite Systems

Let us discuss another implication of our theorem which has direct relevance to numerical diagonalization approaches to quantum many-body systems.

Consider a lattice Λ with N sites and a quantum many-body system on it which satisfies the assumptions (i)–(vi) in Section 2.3. Note that we require the higher $U(1) \times \mathbf{Z}_2$ symmetry. We denote by $E_\Lambda^{(0)}$ the ground-state energy of the Hamiltonian H_Λ. Then we can state the following.

Corollary 2.11. For each nonvanishing integer M which satisfies the bound (2.24), one can find an eigenstate $\Phi_\Lambda^{(M)}$ of the Hamiltonian H_Λ. The state $\Phi_\Lambda^{(M)}$ is orthogonal to the ground state $\Phi_\Lambda^{(0)}$, and the states $\Phi_\Lambda^{(M)}$ with distinct M are orthogonal to each other. The energy eigenvalue $E_\Lambda^{(M)}$ of the state $\Phi_\Lambda^{(M)}$ satisfies the bound

$$E_\Lambda^{(M)} - E_\Lambda^{(0)} \leqslant c_3 \frac{M^2}{N} \tag{2.50}$$

where c_3 is the constant introduced in Theorem 2.4.

Proof. Since the reference state Φ_Λ is an eigenstate of C_Λ, the commutation relations (2.16) imply that the variational states $\Psi_\Lambda^{(M)}$ of (2.19) are orthogonal to the reference state Φ_Λ. Similarly, we see that $\Psi_\Lambda^{(M)}$ with distinct M are orthogonal to each other. The desired result is then a consequence of the variational principle and Theorem 2.4, in which we set $\Phi_\Lambda = \Phi_\Lambda^{(0)}$. ∎

Consider a sequence of finite lattices $\{\Lambda\}$ which tends to $\mathbf{Z}^d$. Suppose that for each Λ we have a quantum many-body system which satisfies the assumptions (i)–(vi) with constants h, o, r, μ, and γ which are independent of Λ. Then the above corollary shows that there exist ever-increasing numbers of "low-lying eigenstates" whose excitation energies are bounded from above by a constant times N^{-1}. Such a finite-size scaling behavior is characteristic for systems with a continuous symmetry breaking and may be regarded as a criterion for detecting the existence of a symmetry breaking from numerical diagonalization in a series of finite systems. Such an approach has been taken in refs. 8, 7, and 35. We stress that this is the first time that the existence of ever-increasing numbers of "low-lying eigenstates" with particular finite-size scaling behavior has been proved.

Nambu–Goldstone excitations associated with the symmetry breaking should also be observed as "low-lying excited states" in finite systems. According to the common wisdom, the excitation energy of a Nambu–Goldstone excitation should be at least of order L^{-2}, where L denotes the linear dimension of the system. Therefore the above corollary guarantees that in three dimensions the "low-lying eigenstates" which are "parts" of infinite-volume ground states have much lower energies than Nambu–Goldstone excitations and can be distinguished from the latter.

Remark. One migth wonder if one can get conclusions similar to Corollary 2.11 from Theorem 2.3, our first theorem on the "low-lying states." By following exactly the same logic as the above, one finds that Theorem 2.3 implies the existence of "low-lying eigenstates" whose excitation energies are (at most) of order 1. Unfortunately, such information alone is not at all meaningful. In any system (with or without symmetry breaking), one can construct excited states with the excitation energy of order 1 by simply locating a finite number of "local defects" into a (finite-volume) ground state. (We wish to thank Tom Kennedy and Bruno Nachtergaele for clarifying this point, which was not properly treated in the earlier version of the present paper.)

In this sense, Theorem 2.3 carries no nontrivial information about the low-lying spectrum of the finite-volume Hamiltonian. As we have stressed before, however, the true value of this theorem is that it establishes that the particular class of states (like $\Psi_\Lambda^{(M)}$ or $\Xi_\Lambda^{(k)}$) are "low-lying" and converge to infinte-volume ground states.

3. EXAMPLES

In this section, we discuss some examples to which our general results apply. Although we only discuss selected models representing typical situations, the reader can easily extend the following analysis to much wider class of quantum many-body problems.

3.1. Ising Model Under Transverse Field

We briefly discuss the Ising model under transverse magnetic field with the Hamiltonian (1.1) considered in Section 1.2. If the field B is smaller than the critical value, the unique ground state $\Phi_\Lambda^{(0)}$ is expected to exhibit an "obscured symmetry breaking" in the sense that the relations $(\Phi_\Lambda^{(0)}, O_\Lambda \Phi_\Lambda^{(0)}) = 0$ and $(\Phi_\Lambda^{(0)}, (O_\Lambda)^2 \Phi_\Lambda^{(0)}) \geqslant (m(B)\,N)^2$ hold, where the order operator O_Λ is defined in (1.2). This can be proved rigorously for sufficiently small B.

Then Horsch and von der Linden's theorem (Theorem 2.2) ensures that there exists a "low-lying eigenstate" whose excitation energy is bounded from above by a constant times N^{-1}. Note that the theorem does not reproduce the expected exponential decay (1.5) of the excitation energy.

3.2. Heisenberg Antiferromagnet with Néel Order

We discuss the Heisenberg quantum antiferromagnetic spin system, which is a typical model with a spontaneously broken continuous symmetry. Let Λ denote the d-dimensional $L \times \cdots \times L$ hypercubic lattice with periodic boundary conditions, where L is an even integer. With each site $x \in \Lambda$ we associate the spin operators $(S_x^{(1)}, S_x^{(2)}, S_x^{(3)})$ for spin $S = 1/2, 1, 3/2, \ldots$. The Hamiltonian (2.3) is defined by the local Hamiltonian

$$h_x = \frac{1}{2} \sum_{y;\, |x-y|=1} (S_x^{(1)} S_y^{(1)} + S_x^{(2)} S_y^{(2)} + \lambda S_x^{(3)} S_y^{(3)}) \tag{3.1}$$

where $0 \leqslant \lambda \leqslant 1$, and the sum is over the sites y neighboring to x. When L is finite, the ground state $\Phi_\Lambda^{(0)}$ of the Hamiltonian (3.1) is rigorously known[33, 32, 3] to be unique and satisfies

$$C_\Lambda \Phi_\Lambda^{(0)} = 0 \tag{3.2}$$

with $C_\Lambda = \sum_{x \in \Lambda} S_x^{(3)}$.

For $\alpha = 1, 2$, we define the order operators (2.13) by the local order operators

$$o_x^{(\alpha)} = \begin{cases} S_x^{(\alpha)} & \text{if} \quad x \in A \\ -S_x^{(\alpha)} & \text{if} \quad x \in B \end{cases} \tag{3.3}$$

where we have decomposed Λ into two sublattices as $\Lambda = A \cup B$, so that for any neighboring sites x, y we have either $x \in A$, $y \in B$ or $x \in B$, $y \in A$.

It is expected, and is partially proved by the Dyson–Lieb–Simon method and its extensions,[10, 16, 21, 22, 27, 28, 39–41] that for any $d \geqslant 2$ and $0 \leqslant \lambda \leqslant 1$ the ground state $\Phi_\Lambda^{(0)}$ exhibits a Néel-type long-range order. We expect that the condition (2.17) is valid with $\mu > 0$ (where μ depends on d and λ, but not on the lattice size N). On the other hand, the absence of explicit symmetry breaking as in (2.18) is obvious from the uniqueness of the ground state. We thus conclude that there is an "obscured symmetry breaking."

Assuming the existence of the Néel order (2.17), we can apply our "low-lying states" theorems. The model has a desired $U(1) \times \mathbf{Z}_2$ symmetry. We can use Theorems 2.3 and 2.4 by noting that the present order operators $O_\Lambda^{(1)}$ and $O_\Lambda^{(2)}$, along with the above-defined C_Λ, satisfy the requirements in the theorems with $\gamma = 1$.

Then we can make use of the general considerations in Section 2.6 and conclude that there are "low-lying eigenstates" with excitation energies not larger than of order N^{-1}. For the $SU(2)$-invariant Heisenberg antiferromagnet with $\lambda = 1$ in (3.1), Momoi[36] constructed some additional "low-lying eigenstates."

In order to apply the general results in Section 2.5, we need extra care. Since the order operators (3.3) do not satisfy the requirement of the translation invariance, we have to redefine what we mean by a "site." We group together 2^d sites forming a $2 \times \cdots \times 2$ hypercubic region (i.e., a unit cell) and call such group a "site." After redefining the local Hilbert space, the local Hamiltonian, and the local order operators according to the new notion of "sites," the model satisfies the assumptions of Section 2.5. We can then construct (presumably ergodic) ground states with explicit symmetry breaking as in (2.41).

We stress that the applicability of our "low-lying states" theorems is not limited to models on the hypercubic lattice. For example, the model on the triangular lattice with the same Hamiltonian (3.1) with $0 \leqslant \lambda \leqslant 1$, where y is summed over nearest neighbor sites of x, has been attracting considerable interest. (See refs. 8, 7, 29, and 35 and many early references therein.) Anticipating the so-called 120° structure, we set the order operators as

$$O_\Lambda^{(1)} = \sum_{x \in A} S_x^{(1)} + \sum_{x \in B} \left(-\frac{1}{2} S_x^{(1)} - \frac{\sqrt{3}}{2} S_x^{(2)} \right) + \sum_{x \in C} \left(-\frac{1}{2} S_x^{(1)} + \frac{\sqrt{3}}{2} S_x^{(2)} \right) \tag{3.4}$$

$$O_\Lambda^{(2)} = \sum_{x \in A} S_x^{(2)} + \sum_{x \in B} \left(\frac{\sqrt{3}}{2} S_x^{(1)} - \frac{1}{2} S_x^{(2)} \right) + \sum_{x \in C} \left(-\frac{\sqrt{3}}{2} S_x^{(1)} - \frac{1}{2} S_x^{(2)} \right) \tag{3.5}$$

where we have divided the triangular lattice into three sublattices A, B, and C so that neighboring sites x, y always belong to different sublattices. These order operators again satisfy the conditions for the theorems with the generator $C_A = \sum_x S_x^{(3)}$. We can then apply the general discussions in Section 2.

3.3. Bose–Einstein Condensation in Hard-Core Bose Gas on a Lattice

We give a brief discussion on the Bose–Einstein condensation problem. It turns out that, by following the general discussions given in Section 2, we are naturally led to consider ground states with unconserved particle number.

Let Λ be the d-dimensional $L \times \cdots \times L$ hypercubic lattice with periodic boundary conditions, where L is an even integer, and $d \geqslant 2$. With each site x we associate the creation operator a_x^* and the annihilation operator a_x of a spinless boson. We consider the Hamiltonian (2.3) defined by

$$h_x = \frac{K}{2} \sum_{y;\, |x-y|=1} (a_x^* a_y + a_y^* a_x) + V n_x(n_x - 1) \tag{3.6}$$

where the sum runs over the sites neighboring to x, and $n_x = a_x^* a_x$ denotes the number operator.

We shall take the limit of infinitely large on-site repulsion $V \uparrow \infty$ before the infinite-volume limit and restrict ourselves to the states with finite energies (in a finite volume). This defines the so-called hard-core Bose gas.

It is well known that the hard-core Bose gas on a lattice is equivalent to the $S = 1/2$ quantum XY model on the same lattice.[34] Based on the equivalence and an extension of the infrared bound method of Dyson *et al.*[10] it was proved by Kennedy *et al.*[22] and Kubo and Kishi[28] that the present model exhibits a Bose–Einstein condensation in the following sense. Let $\Phi_\Lambda^{(0)}$ be the unique ground state of the Hamiltonian (3.6) with the particle number equal to $N = L^d/2$. Define the order operators (2.13) by

$$o_x^{(1)} = \mathscr{P} \frac{a_x^* + a_x}{2} \mathscr{P}, \qquad o_x^{(2)} = \mathscr{P} \frac{a_x^* - a_x}{2i} \mathscr{P} \tag{3.7}$$

where $\mathscr{P}$ is the projection operator onto the space of finite energy states, i.e., Φ such that $n_x(1 - n_x)\Phi = 0$ for any x. Then the result of refs. 22 and 28 is that the condition of the long-range order (2.17) holds with a finite μ which is independent of the lattice size N. On the other hand, the absence of explicit symmetry breaking as in (2.18) is manifest since the state Φ_Λ has a fixed particle number. We see that there is an "obscured symmetry breaking."

It is not hard to see that we can apply our Theorems 2.3 and 2.4 to this situation. For this, we replace the Hamiltonian (3.6) with $\mathscr{P}h_x\mathscr{P}$. Note that the latter is a bounded operator, while the former is unbounded. Since we are only dealing with states with finite energies, this replacement does not change any physics. By using the replaced Hamiltonian and the order operators (3.7), we find that the model has a desired $U(1)\times\mathbf{Z}_2$ symmetry. The relevant $U(1)$ symmetry is that for the quantum mechanical phase generated by $C_\Lambda=\sum_{x\in\Lambda}(n_x-1/2)$, and the $\mathbf{Z}_2$ symmetry is the hole–particle symmetry.

Note that the "low-lying states" in the present model have different particle numbers than the ground state. The "low-lying state" (2.27) with explicit symmetry breaking can be written as

$$\Xi_\Lambda^{(k)}=\frac{1}{(2k+1)^{1/2}}\left\{\Phi_\Lambda^{(0)}+\sum_{M=1}^{k}\left(\frac{\mathscr{P}(\sum_{x\in\Lambda}a_x^*)^M\,\Phi_\Lambda^{(0)}}{\|\mathscr{P}(\sum_{x\in\Lambda}a_x^*)^M\,\Phi_\Lambda^{(0)}\|}+\frac{(\sum_{x\in\Lambda}a_x)^M\,\Phi_\Lambda^{(0)}}{\|(\sum_{x\in\Lambda}a_x)^M\,\Phi_\Lambda^{(0)}\|}\right)\right\} \tag{3.8}$$

Consequently the (presumably ergodic) ground states $\omega_\theta(\cdots)$ have a peculiar feature that they are constructed by summing up the states with different particle numbers as in (3.8). We further find from (2.42) that the state has nonvanishing expectation values of the creation and annihilation operators, for example, as

$$\omega_{\theta=0}(a_x^*)=\omega_{\theta=0}(a_x)\geqslant\sqrt{2}\,o\mu \tag{3.9}$$

for any x.

In a theoretical treatment of the Bose–Einstein condensation, it is standard to consider states without particle number conservation and with nonvanishing expectation values for creation and annihilation operators. Usually such states are introduced within the framework of a certain mean-field theory. We have seen that such states arise naturally if one tries to consider ergodic infinite-volume ground states.

Remark. Since it is physically meaningless to compare the energies of two states with different particle numbers, the existence of "low-lying states" in the present situation has less physical significance. A more important fact is that the states $\omega_\theta(\cdots)$ are really infinite-volume ground states. This point requires further discussion.

A physically natural setup in the present problem is to consider a finite system with a fixed particle number. Then one can add an extra term $\nu\sum_{x\in\Lambda}n_x$ to the Hamiltonian without changing any physics. If we were to consider states without fixed particle numbers, Definition 2.6 is clearly not adequate, since it is sensitive to the value of the "chemical potential" ν. Better definitions in the situations without particle number conservation are those of $\mathscr{G}_1$ or $\mathscr{G}_2$ in Appendix A, with allowed perturbations (local operators A in the former and maps T in the latter) restricted to those that preserve the particle number. This definition is clearly independent of the value of ν. To prove that the above $\omega_\theta(\cdots)$ is a ground state in this sense, it suffices to use the relations between different definitions (Proposition A.2) along with the fact that $\omega_\theta(\cdots)$ is a ground state (in the sense of Definition 2.6 or $\mathscr{G}_3$) when $\nu = 0$.

3.4. Superconductivity in Lattice Electron Systems

We shall discuss applications of our theorems to lattice electron problems. A class of possible applications deals with magnetic ordering in an electron model. Since such problems can be treated in exactly the same manner as the quantum spin systems discussed previously, we leave the details to the interested reader. We concentrate on a symmetry breaking intrinsic to interacting electron systems, namely superconductivity.

Consider an electron system on a finite lattice Λ and denote by $c^*_{x\sigma}$ and $c_{x\sigma}$ the creation and annihilation operators, respectively, of an electron at site x with spin $\sigma = \uparrow, \downarrow$. We consider a Hamiltonian which commutes with the total electron number

$$N_e = \sum_x n_{x\uparrow} + n_{x\downarrow} \tag{3.10}$$

where $n_{x\sigma} = c^*_{x\sigma} c_{x\sigma}$. A typical example is the so-called Hubbard model. (See, for example, refs. 31 and 37.)

A class of Hubbard models with attractive interactions is believed to exhibit superconductivity in their ground states.[13] It is also expected that certain Hubbard models with repulsive interaction also exhibit superconductivity. The latter possibility is interesting not only because of its possible connection with high-T_c superconductivity, but as a new type of collective phenomenon in strongly interacting electron systems.

A standard superconducting phase can be characterized by a condensation of certain electron pairs, which manifests itself as an (off-diagonal) long-range order in the electron pairing correlation function. For example,

[13] As a straightforward consequence of Lieb's theorem,[30] one finds that some attractive Hubbard models exhibit an off-diagonal long-range order.[44] These models, however, do not fit into the present discussion since the order operator (accidentally) commutes with the Hamiltonian. The same comment applies to the solvable models of ref. 11.

the condensation of singlet pairs can be measured as a long-range order (2.17) with respect to the order operators defined by

$$o_x^{(1)} = \frac{1}{2}\,(p_x c_{x\uparrow}^* c_{x\downarrow}^* - \overline{p_x}\, c_{x\uparrow} c_{x\downarrow}) \tag{3.11}$$

$$o_x^{(2)} = \frac{1}{2i}\,(p_x c_{x\uparrow}^* c_{x\downarrow}^* + \overline{p_x}\, c_{x\uparrow} c_{x\downarrow}) \tag{3.12}$$

where p_x (with $|p_x| = 1$) is a certain phase factor. It is easily checked that the model has a $U(1)$ symmetry and satisfies the conditions for Theorem 2.3 with $C_\Lambda = (N_e - N)/2$, where N denotes the number of sites in Λ. We can then follow the general discussions in Section 2 and construct (presumably) ergodic ground states with an explicit $U(1)$ symmetry breaking. As in the Bose–Einstein condensation problem, the ground states do not conserve particle numbers. Except for half-filled models with special Hamiltonians, the models do not have the $U(1) \times \mathbf{Z}_2$ symmetry necessary to apply Theorem 2.4.

We remark that it is possible to treat other types of pairing with some extra care. To treat triplet pairing, for example, we first redefine what we mean by sites of the lattice. We divide the lattice Λ into a disjoint union of nonoverlapping pairs of sites. We then regard each pair $\{x, y\}$ as a "site" of the lattice. The local order parameters to measure a possible condensation of triplet pairs are defined by summing up the following local order operators over all the "sites":

$$o_{\{x,y\}}^{(1)} = \frac{1}{2}\,(c_{x\uparrow}^* c_{y\downarrow}^* + c_{x\downarrow}^* c_{y\uparrow}^* - c_{x\uparrow} c_{y\downarrow} - c_{x\downarrow} c_{y\uparrow}) \tag{3.13}$$

$$o_{\{x,y\}}^{(2)} = \frac{1}{2i}\,(c_{x\uparrow}^* c_{y\downarrow}^* + c_{x\downarrow}^* c_{y\uparrow}^* + c_{x\uparrow} c_{y\downarrow} + c_{x\downarrow} c_{y\uparrow}) \tag{3.14}$$

We again set $C_\Lambda = (N_e - N)/2$ and apply Theorem 2.3 to control "low-lying states."

Remark. The lattice fermion problems considered here are different from other examples in that the corresponding Hilbert space is not a simple tensor product of local Hilbert spaces as in (2.1) or (A.1). This difference causes no problem for proving our "low-lying states" theorems since we only make use of some commutation relations between operators in the proof. But some results about infinite-volume states, which are mainly quoted from the literature in Section 2.5 and Appendix A, may not apply.

3.5. $S=1$ Antiferromagnetic Chain

A rather interesting application of the "low-lying states" theorem can be found in the problem related to the so-called Haldane gap. Let Λ be the one-dimensional open chain $\{1, 2,..., N\}$. With each site $x \in \Lambda$ we associate the three-dimensional Hilbert space for an $S=1$ quantum spin and denote by $(S_x^{(1)}, S_x^{(2)}, S_x^{(3)})$ the corresponding spin operators. We consider the Hamiltonian

$$H_\Lambda = \sum_{x=1}^{N-1} (S_x^{(1)} S_{x+1}^{(1)} + S_x^{(2)} S_{x+1}^{(2)} + \lambda S_x^{(3)} S_{x+1}^{(3)}) + D \sum_{x=1}^{N} (S_x^{(3)})^2 \tag{3.15}$$

where λ and D are parameters.

Haldane[14] argued that in a finite range of the parameter space including the Heisenberg point $\lambda = 1$, $D = 0$, the model is in an exotic phase (now called the "Haldane phase") where the unique infinite-volume ground state is accompanied by a finite excitation gap. This was quite surprising since the Heisenberg antiferromagnetic chain with $S = 1/2$ is known to have vanishing gap from the Bethe ansatz solution. (See also ref. 3.) Haldane's prediction was that the gap-containing Haldane phase exists if and only if the spin S is an integer.

The existence of the Haldane phase in $S=1$ chains has been proved rigorously only in the exactly solvable VBS model,[2] its non-$SU(2)$-invariant extensions,[12] and perturbations to the dimerized VBS model.[23] A general treatment of the VBS-type models is given in ref. 12 and the $S=1$ model mentioned here is one of the examples. The $S=1$ model of ref. 12 and the method of constructing the ground state (but not the proof of the existence of a gap) were rediscovered by other authors.[25]

The ground state in the Haldane phase is disordered in the sense that the spin–spin correlation functions decay exponentially. Den Nijs and Rommelse[38] pointed out that the ground state in the Haldane phase of an $S=1$ chain has a "hidden antiferromagnetic order." For $i = 1, 2, 3$, let the string order operator be

$$O_\Lambda^{(i)} := \sum_{x=1}^{N} S_x^{(i)} \exp\left[i\pi \sum_{y=1}^{x-1} S_y^{(i)} \right] \tag{3.16}$$

If we denote the unique normalized ground state for finite Λ with N sites as $\Phi_\Lambda^{(0)}$, we expect to have

$$(\Phi_\Lambda^{(0)}, (O_\Lambda^{(i)})^2 \, \Phi_\Lambda^{(0)}) \geqslant (\sigma^{(i)} N)^2 \tag{3.17}$$

in the Haldane phase with $\sigma^{(1)} = \sigma^{(2)} > 0$ and $\sigma^{(3)} > 0$.

The condition (3.17) corresponds to the antiferromagnetic ordering of spins with $S_x^{(i)} = 1$ and $S_x^{(i)} = -1$, where spins with $S_x^{(i)} = 0$ are inserted randomly in between them.[38, 46] Again the existence of the "hidden antiferromagnetic order" has been established only for special classes of models mentioned above.

Let us consider the following trial states:

$$\Psi_\Lambda^{(i)} = \frac{O_\Lambda^{(i)}\Phi_\Lambda^{(0)}}{\|O_\Lambda^{(i)}\Phi_\Lambda^{(0)}\|} \tag{3.18}$$

for each $i = 1, 2, 3$. We also introduce the operators

$$U_\Lambda^{(i)} = \exp\left[i\pi \sum_{x=1}^{N} S_x^{(i)}\right] \tag{3.19}$$

which rotates all the spins by π around the ith axis. Note that the unique ground state satisfies $U_\Lambda^{(i)}\Phi_\Lambda^{(0)} = \Phi_\Lambda^{(0)}$ for any i and the trial states (3.18) satisfy

$$U_\Lambda^{(i)}\Psi_\Lambda^{(j)} = \begin{cases} \Psi_\Lambda^{(j)} & \text{if} \quad i = j \\ -\Psi_\Lambda^{(j)} & \text{if} \quad i \neq j \end{cases} \tag{3.20}$$

From the difference of parities, we find that the four states $\Phi_\Lambda^{(0)}$, $\Psi_\Lambda^{(1)}$, $\Psi_\Lambda^{(2)}$, and $\Psi_\Lambda^{(3)}$ are orthogonal to each other.

It is not hard to check that we can apply Horsch and von der Linden's theorem (Theorem 2.2) to this situation. We find for each $i = 1, 2, 3$ that the trial states $\Psi_\Lambda^{(i)}$ are "low-lying states." The Hamiltonian (3.15) on a finite open chain should have (at least) three "low-lying eigenstates." (Again the excitation energies of the "low-lying eigenstates" are believed to decay exponentially in N, but the bound in the theorem fails to reproduce this.) These "low-lying eigenstates" are nothing but the so-called "Kennedy triplet" which has been observed in exact solutions,[2] numerical simulations,[20] and actual experiments in impurity-doped samples.[13] The existence of the Kennedy triplet is characteristic in a Haldane gap system on a finite open chain. In a periodic chain, it is believed that the unique ground state is accompanied by a finite excitation gap.

The fundamental connection between the hidden order (3.17) and the existence of the low-lying triplet was discussed by Kennedy and Tasaki[23] from the viewpoint of the "hidden $\mathbf{Z}_2 \times \mathbf{Z}_2$ symmetry breaking." Our remark here is that this connection can be made (formally) explicit at least in one direction.[14]

[14] That the existence of a hidden antiferromagnetic order should imply the existence of the low-lying triplet was pointed out to one of the authors (H.T.) by Ian Affleck in July 1992. The present work initially emerged from an attempt to look for a proof of his claim, although the main interest of the authors has shifted in the long run to problems with continuous symmetry breaking.

The present example is different from the others in that the three "low-lying states" and the unique (finite-volume) ground state converge to a unique infinite-volume ground state. This is related to the nonlocal nature of the order operators. See refs. 2, 20, and 23 for more details.

4. PROOF OF FIRST THEOREM

In the present section, we prove Theorem 2.3 for $M > 0$. Throughout the proof, we drop the subscript Λ from $O_\Lambda^\pm$, H_Λ, E_Λ, Φ_Λ, $\Psi_\Lambda^{(M)}$, etc. Our goal is to bound the quantity

$$\begin{aligned}\Delta^{(M)} &:= \frac{1}{N}\{(\Psi^{(M)}, H\Psi^{(M)}) - E\}\\ &= \frac{(\Phi, (O^-)^M H (O^+)^M \Phi) - (\Phi, (O^-)^M (O^+)^M H\Phi)}{N(\Phi, (O^-)^M (O^+)^M \Phi)}\\ &= \sum_{x\in\Lambda} \frac{(\Phi, (O^-)^M [h_x, (O^+)^M] \Phi)}{N(\Phi, (O^-)^M (O^+)^M \Phi)} \end{aligned} \tag{4.1}$$

The final expression in (4.1) motivates us to decompose the operator O^+ as

$$O^+ = Q_x + R_x \tag{4.2}$$

with

$$Q_x := \sum_{y\notin \mathcal{S}_x} o_y^+, \qquad R_x := \sum_{y\in\mathcal{S}_x} o_y^+ \tag{4.3}$$

Note that we have $[Q_x, h_x] = 0$ and $[Q_x, R_x] = 0$ from the assumptions (ii) and (i), respectively.

Although O^+ does not commute with the local Hamiltonian h_x, Q_x does. This means that it is easier for us to treat Q_x than O^+. A key observation for the proof is that the difference between O^+ and Q_x, which is denoted as R_x, is small compared to O^+. The following useful lemma, for example, makes use of this fact.

Lemma 4.1. Suppose that the conditions (2.20) and (2.21) for N and M are satisfied. Then for $k = 1, 2,..., M$, we have

$$\frac{(\Phi, (Q_x^*)^{M-k} (Q_x)^{M-k} \Phi)}{(\Phi, (Q_x^*)^M (Q_x)^M \Phi)} \leqslant (\mu o N)^{-2k} \tag{4.4}$$

We shall prove the lemma at the end of the present section.

By using the expansion formula

$$(O^+)^M = \sum_{k=0}^{M} \binom{M}{k} (Q_x)^{M-k} (R_x)^k \tag{4.5}$$

we get

$$
\begin{aligned}
&(\Phi, (O^-)^M [h_x, (O^+)^M] \Phi) \\
&\quad = \sum_{k=0}^{M} \sum_{l=0}^{M} \binom{M}{k}\binom{M}{l} (\Phi, (Q_x^*)^{M-k} (R_x^*)^k [h_x, (Q_x)^{M-l} (R_x)^l] \Phi) \\
&\quad = \sum_{k=0}^{M} \sum_{l=1}^{M} \binom{M}{k}\binom{M}{l} (\Phi, (Q_x^*)^{M-k} (R_x^*)^k [h_x, (R_x)^l](Q_x)^{M-l} \Phi)
\end{aligned}
\tag{4.6}
$$

The Schwartz inequality and the definition (2.2) of the operator norm yield the following useful bounds:

$$
\begin{aligned}
|(\Phi, A^*BC\Phi)| &\leqslant [(\Phi, A^*A\Phi)(\Phi, C^*B^*BC\Phi)]^{1/2} \\
&\leqslant \|B\| \, [(\Phi, A^*A\Phi)(\Phi, C^*C\Phi)]^{1/2}
\end{aligned}
\tag{4.7}
$$

for general operators A, B, and C.

By applying (4.7) to (4.6) and noting that (ii) and (iii) imply $\|(R_x^*)^k [h_x, (R_x)^l]\| \leqslant 2h(2ro)^{k+l}$, we get

$$
\begin{aligned}
&\left| \frac{(\Phi, (O^-)^M [h_x, (O^+)^M] \Phi)}{(\Phi, (Q_x^*)^M (Q_x)^M \Phi)} \right| \\
&\quad \leqslant \sum_{k=0}^{M} \sum_{l=1}^{M} \binom{M}{k}\binom{M}{l} 2h(2ro)^{k+l} \\
&\qquad \times \frac{[(\Phi, (Q_x^*)^{M-k} (Q_x)^{M-k} \Phi)(\Phi, (Q_x^*)^{M-l} (Q_x)^{M-l} \Phi)]^{1/2}}{(\Phi, (Q_x^*)^M (Q_x)^M \Phi)} \\
&\quad \leqslant 2h \sum_{k=0}^{M} \sum_{l=1}^{M} \binom{M}{k}\binom{M}{l} (2ro)^{k+l} (\mu o N)^{-(k+l)} \\
&\quad = 2h \left(1 + \frac{2r}{\mu N}\right)^M \left[\left(1 + \frac{2r}{\mu N}\right)^M - 1\right] \\
&\quad \leqslant 2h \exp\left(\frac{2r}{\mu}\frac{M}{N}\right)\left[\exp\left(\frac{2r}{\mu}\frac{M}{N}\right) - 1\right] \\
&\quad \leqslant 2he^{\mu/4} \frac{8r(e^{\mu/4} - 1)}{\mu^2} \frac{M}{N} \\
&\quad = 16rh\mu^{-2}(e^{\mu/2} - e^{\mu/4}) \frac{M}{N}
\end{aligned}
\tag{4.8}
$$

where we have used the bounds (4.4) and (2.21).

Again using (4.5), we get

$$
\begin{aligned}
&(\Phi, (O^-)^M (O^+)^M \Phi) \\
&\quad = (\Phi, (Q_x^*)^M (Q_x)^M \Phi) \\
&\qquad + \sum_{k,l}' \binom{M}{k}\binom{M}{l} (\Phi, (Q_x^*)^{M-k} (R_x^*)^k (R_x)^l (Q_x)^{M-l} \Phi) \qquad (4.9)
\end{aligned}
$$

where the summation on the right-hand side runs over all $k, l = 0, 1, \ldots, M$ except for $k = l = 0$. From (4.7) and (4.4), we get

$$
\begin{aligned}
&\left| \frac{(\Phi, (O^-)^M (O^+)^M \Phi)}{(\Phi, (Q_x^*)^M (Q_x)^M \Phi)} \right| \\
&\quad \geqslant 1 - \sum_{k,l}' \binom{M}{k}\binom{M}{l} (2ro)^{k+l} \\
&\qquad \times \frac{[(\Phi, (Q_x^*)^{M-k} (Q_x)^{M-k} \Phi)(\Phi, (Q_x^*)^{M-l} (Q_x)^{M-l} \Phi)]^{1/2}}{(\Phi, (Q_x^*)^M (Q_x)^M \Phi)} \\
&\quad \geqslant 1 - \left[\left(1 + \frac{2r}{\mu N} \right)^{2M} - 1 \right] \\
&\quad \geqslant 2 - e^{\mu/2} \qquad (4.10)
\end{aligned}
$$

Note that, since $0 \leqslant \mu \leqslant 1$, we have $2 - e^{\mu/2} \geqslant 2 - \sqrt{e} > 0$.

By combining (4.1), (4.8), and (4.10), we finally get

$$
|\Delta^{(M)}| \leqslant 16rh \frac{e^{\mu/2} - e^{\mu/4}}{\mu^2(2 - e^{\mu/2})} \frac{M}{N} = c_1 \frac{M}{N} \qquad (4.11)
$$

Proof of Lemma 4.1. We write $a_m := (\Phi, (Q_x^*)^m (Q_x)^m \Phi)$. We will prove that for $m = 1, 2, \ldots, M$, we have

$$
\frac{a_m}{a_{m-1}} \geqslant (\mu o N)^2 \qquad (4.12)
$$

Then the desired bound (4.4) follows by multiplying (4.12) with $m = M - k + 1, M - k + 2, \ldots, M$.

We start by evaluating a_1 as

$$
\begin{aligned}
a_1 &= (\Phi, (O^- - R_x^*)(O^+ - R_x) \Phi) \\
&\geqslant (\Phi, O^- O^+ \Phi) - 2(2o)^2 rN \\
&= \tfrac{1}{2}\{(\Phi, O^- O^+ \Phi) + (\Phi, O^+ O^- \Phi) + (\Phi, [O^-, O^+] \Phi)\} - 8o^2 rN \\
&\geqslant (\Phi, (O^{(1)})^2 \Phi) + (\Phi, (O^{(2)})^2 \Phi) - 2o^2(1 + 4r^2) N \qquad (4.13)
\end{aligned}
$$

where we have used (i)–(iii) to bound the norm of the commutators.

By substituting the assumption (2.17) on the existence of a long-range order and the bound (2.20) for N, we get

$$
\begin{aligned}
a_1 &\geqslant 2(\mu o N)^2\left(1-\frac{1+4r^2}{\mu^2 N}\right)\\
&\geqslant 2(\mu o N)^2\left(1-\frac{1+4r^2}{16r^2}\right)
\end{aligned}
\tag{4.14}
$$

Since $r \geqslant 2$, we have shown that $a_1 > 0$.

Next we use the Schwartz inequality to get

$$
\begin{aligned}
(a_{m-1})^2 &= (\Phi, (Q_x^*)^{m-2}\, Q_x^*(Q_x)^{m-1}\, \Phi)^2\\
&\leqslant (\Phi, (Q_x^*)^{m-2}\, (Q_x)^{m-2}\, \Phi)(\Phi, (Q_x^*)^{m-1}\, Q_x Q_x^*(Q_x)^{m-1}\, \Phi)\\
&= a_{m-2}\{(\Phi, (Q_x^*)^{m}\, (Q_x)^{m}\, \Phi)\\
&\qquad + (\Phi, (Q_x^*)^{m-1}\, [Q_x, Q_x^*](Q_x)^{m-1}\, \Phi)\}\\
&\leqslant a_{m-2}\{a_m + 4o^2 N a_{m-1}\}
\end{aligned}
\tag{4.15}
$$

where the final inequality follows from (4.7).

Assuming that $a_{m-2} \neq 0$ and $a_{m-1} \neq 0$ (which is true for $m = 2$), we find from (4.15) that

$$
\frac{a_m}{a_{m-1}} \geqslant \frac{a_{m-1}}{a_{m-2}} - 4o^2 N \tag{4.16}
$$

The rest of the proof is easy. Assume that, for a fixed m, $a_{m'} \neq 0$ for all $m' < m \leqslant M$. Then by summing up (4.16) and using the bounds (4.14), (2.21) and $r \leqslant 2$, we see that

$$
\begin{aligned}
\frac{a_m}{a_{m-1}} &\geqslant a_1 - 4o^2 N(m-2)\\
&\geqslant 2(\mu o N)^2\left[1-\frac{1+4r^2}{16r^2}-\frac{2(m-2)}{\mu^2 N}\right]\\
&\geqslant 2(\mu o N)^2\left(1-\frac{1+4r^2}{16r^2}-\frac{1}{4r}\right)\\
&\geqslant (\mu o N)^2
\end{aligned}
\tag{4.17}
$$

and hence $a_m \neq 0$. By proceeding inductively, we see that the desired bound (4.12) holds for $m = 1, 2, \ldots, M$. ▮

5. PROOF OF SECOND THEOREM

In the present section we prove Theorem 2.4. Again we fix Λ and drop the subscript Λ.

Let us define

$$b_m := \frac{2^{2m}(m!)^2}{(2m)!} (\Phi, (O^{(1)})^{2m} \Phi) \tag{5.1}$$

which satisfies the following useful inequalities.

Lemma 5.1. We have

$$\frac{1}{2(oN)^2} \leqslant \frac{b_{m-1}}{b_m} \leqslant \frac{1}{(\mu o N)^2} \tag{5.2}$$

Proof. By using the Schwartz inequality we get

$$\begin{aligned}(\Phi, (O^{(1)})^{2m-2} \Phi)^2 &= (\Phi, (O^{(1)})^m (O^{(1)})^{m-2} \Phi)^2 \\ &\leqslant (\Phi, (O^{(1)})^{2m} \Phi)(\Phi, (O^{(1)})^{2m-4} \Phi)\end{aligned} \tag{5.3}$$

which, with $(\Phi, (O^{(1)})^2 \Phi) > 0$, proves inductively $(\Phi, (O^{(1)})^{2m} \Phi) > 0$ for any m. By rearranging (5.3), we get

$$\begin{aligned}\frac{(\Phi, (O^{(1)})^{2(m-1)} \Phi)}{(\Phi, (O^{(1)})^{2m} \Phi)} &\leqslant \frac{(\Phi, (O^{(1)})^{2(m-2)} \Phi)}{(\Phi, (O^{(1)})^{2(m-1)} \Phi)} \leqslant \cdots \leqslant \frac{1}{(\Phi, (O^{(1)})^2 \Phi)} \\ &\leqslant \frac{1}{(\mu o N)^2}\end{aligned} \tag{5.4}$$

where we used (2.17). We also note that the definition (2.2) implies

$$(\Phi, (O^{(1)})^{2m} \Phi) \leqslant \|O^{(1)}\|^2 (\Phi, (O^{(1)})^{2(m-1)} \Phi) \leqslant (oN)^2 (\Phi, (O^{(1)})^{2(m-1)} \Phi) \tag{5.5}$$

By substituting (5.3) and (5.5) into

$$\frac{b_{m-1}}{b_m} = \frac{2m(2m-1)}{(2m)^2} \frac{(\Phi, (O^{(1)})^{2(m-1)} \Phi)}{(\Phi, (O^{(1)})^{2m} \Phi)} \tag{5.6}$$

which follows from the definition (5.1), we get (5.2). ∎

In the present proof, we bound various quantities in terms of b_m. One of the main ingredients in the proof is the following lemma, which allows us to approximate expectation values including $O^{\pm}$ with those including the self-adjoint operator $O^{(1)}$. See Eq. (5.14) for a typical situation to which we apply the lemma.

Let A be an operator written as $A = \sum_{x \in \Lambda} a_x$, where $[a_x, o_y^{(\alpha)}] = 0$ for $\alpha = 1, 2$ if $y \notin \mathscr{S}_x$, and $\|a_x\| \leqslant a$ for any x with an x-independent finite constant a. The support set $\mathscr{S}_x$ is the same for that of h_x. In the following we set $O^\sigma = O^+$ or O^-, depending on $\sigma = +1$ or -1.

Lemma 5.2. Let K, L be nonnegative integers which satisfy

$$\frac{48r}{\mu^2}\frac{K+L}{N} + \frac{3\gamma}{2o^2\mu^2}\frac{(K+L)^3}{N^2} \leqslant 1 \tag{5.7}$$

We assume that A satisfies

$$[C, (O^+)^{K-L} A] = 0 \tag{5.8}$$

where C is the generator of the $U(1)$ symmetry. [For $K - L < 0$, we set $(O^+)^{K-L} = (O^-)^{L-K}$.] The relation (5.8) essentially means that A consists of $(K-L)$ lowering operators. Let $\{\sigma_i\}_{i=1,\dots,K+L}$ be such that $\sigma_i = \pm 1$ and $\sum_{i=1}^{K+L} \sigma_i = K - L$. Then for any integer k with $0 \leqslant k \leqslant K + L$, we have

$$\begin{aligned} &\left| \left(\Phi, \left(\prod_{i=1}^{k} O^{\sigma_i} \right) A \left(\prod_{i=k+1}^{K+L} O^{\sigma_i} \right) \Phi \right) \right. \\ &\qquad \left. - \frac{2^{2J}(J!)^2}{(2J)!} (\Phi, (O^{(1)})^J \{A(O^+)^{(K-L)}\}(O^{(1)})^J \Phi) \right| \\ &\leqslant \delta(A; K, L) \end{aligned} \tag{5.9}$$

where $J = \min\{K, L\}$ and

$$\left| \left(\Phi, \left(\prod_{i=1}^{k} O^{\sigma_i} \right) A \left(\prod_{i=k+1}^{K+L} O^{\sigma_i} \right) \Phi \right) \right| \leqslant 3\delta(A; K, L) \tag{5.10}$$

Here $\delta(A; K, L)$ is given by

$$\delta(A; K, L) := \tfrac{1}{2}(aN)(2oN)^{|K-L|}\, b_J \tag{5.11}$$

for general A. For $A = 1$, in which case only $K = L$ is allowed, we can set

$$\delta(1; K, K) = \tfrac{1}{2} b_K \tag{5.12}$$

The lemma will be proved after completing the proof of the main theorem.

We again want to control the quantity $\Delta^{(M)}$ in (4.1). By using the relation $UO^\sigma U^{-1} = -O^{-\sigma}$ [which follows from (2.23)], we find that $\Delta^{(M)}$ can be written in terms of a double commutator as follows [this is reminiscent of the similar representation (2.11) used in the proof of the simplest "low-lying states" theorem of Section 2.2]:

$$
\begin{aligned}
&2N\,\|\Psi^{(M)}\|^2\,\Delta^{(M)}\\
&\quad=2(\Phi,(O^-)^M H(O^+)^M\Phi)-2E(\Phi,(O^-)^M(O^+)^M\Phi)\\
&\quad=(\Phi,(O^-)^M H(O^+)^M\Phi)+(\Phi,(O^+)^M H(O^-)^M\Phi)\\
&\qquad-(\Phi,(O^-)^M(O^+)^M H\Phi)-(\Phi,H(O^+)^M(O^-)^M\Phi)\\
&\quad=(\Phi,[(O^-)^M,[H,(O^+)^M]]\Phi)\\
&\quad=\sum_{m=0}^{M-1}(\Phi,[(O^-)^M,(O^+)^m[H,O^+](O^+)^{M-m-1}]\Phi)\\
&\quad=\sum_{m=1}^{M-1}\sum_{l=0}^{M-1}\sum_{n=0}^{m-1}(\Phi,(O^-)^l(O^+)^n\\
&\qquad\times[O^-,O^+](O^+)^{m-n-1}[H,O^+](O^+)^{M-m-1}(O^-)^{M-l-1}\Phi)\\
&\qquad+\sum_{m=0}^{M-1}\sum_{l=0}^{M-1}(\Phi,(O^-)^l(O^+)^m\\
&\qquad\times[O^-,[H,O^+]](O^+)^{M-m-1}(O^-)^{M-l-1}\Phi)\\
&\qquad+\sum_{m=0}^{M-2}\sum_{l=0}^{M-1}\sum_{n=0}^{M-m-2}(\Phi,(O^-)^l(O^+)^m\\
&\qquad\times[H,O^+](O^+)^n[O^-,O^+]\\
&\qquad\times(O^+)^{M-m-n-2}(O^-)^{M-l-1}\Phi)
\end{aligned}
\tag{5.13}
$$

Note that the symmetry (vi), along with the relation $UCU^{-1}=-C$ [which follows from (2.14) and (2.23)], implies that $C\Phi=0$. By also using the relation $[O^-,O^+]=-2\gamma C$ and the fact that $O^\pm$ are the raising and the lowering operators, we can bound the above quantity as

$$
\begin{aligned}
&|2N\,\|\Psi^{(M)}\|^2\,\Delta^{(M)}|\\
&\quad\leqslant\sum_{m=1}^{M-1}\sum_{l=0}^{M-1}\sum_{n=0}^{m-1}2\gamma M\\
&\qquad\times|(\Phi,(O^-)^l(O^+)^{m-1}[H,O^+](O^+)^{M-m-1}(O^-)^{M-l-1}\Phi)|\\
&\qquad+\sum_{m=0}^{M-1}\sum_{l=0}^{M-1}|(\Phi,(O^-)^l(O^+)^m\\
&\qquad\times[O^-,[H,O^+]](O^+)^{M-m-1}(O^-)^{M-l-1}\Phi)|\\
&\qquad+\sum_{m=0}^{M-2}\sum_{l=0}^{M-1}\sum_{n=0}^{M-m-2}2\gamma M\\
&\qquad\times|(\Phi,(O^-)^l(O^+)^m[H,O^+](O^-)^{M-m-2}(O^-)^{M-l-1}\Phi)|
\end{aligned}
$$

$$\leqslant 6\gamma M^4\,\delta([H, O^+]; M-2, M-1)$$
$$+3M^2\,\delta([O^-, [H, O^+]]; M-1, M-1) \tag{5.14}$$

where we have used (5.10). The use of Lemma 5.2 is justified since M satisfies (2.24), which (with $K+L \leqslant 2M$) guarantees the condition (5.7).

By using (5.11) in Lemma 5.2, we get

$$|2N\,\|\Psi^{(M)}\|^2\,\Delta^{(M)}|$$
$$\leqslant 3\gamma M^4(4r\dot{o}hN)(2oN)\,b_{M-2}+\frac{3}{2}\,M^2(16r^2o^2hN)\,b_{M-1}$$
$$\leqslant \left(\frac{24\gamma rh}{o^2\mu^4}\frac{M^4}{N^2}+\frac{24r^2h}{\mu^2}\frac{M^2}{N}\right)b_M \tag{5.15}$$

where we have used the bound (5.2) in Lemma 5.1 to relate b_M with different M.

On the other hand, from (5.9) and (5.12), we find

$$\|\Psi^{(M)}\|^2=(\Phi, (O^-)^M\,(O^+)^M\,\Phi)\geqslant \tfrac{1}{2}b_M \tag{5.16}$$

By combining (5.15) and (5.16) and substituting the assumed bound (2.24), we finally get

$$|\Delta^{(M)}|\leqslant \frac{24r^2h}{\mu^2}\left(1+\frac{\gamma}{o^2\mu^2r}\frac{M^2}{N}\right)\left(\frac{M}{N}\right)^2$$
$$\leqslant c_3\left(\frac{M}{N}\right)^2 \tag{5.17}$$

with $c_3=24r^2h\mu^{-2}(1+\gamma o^{-2}\mu^{-2}r^{-1}c_2)$.

It remains to prove Lemma 5.2. We prepare the following.

Lemma 5.3. Let K, L be nonnegative integers which satisfy (5.7). We assume that the operator A satisfies the conditions of Lemma 5.2. Let $\{\sigma_i\}_{i=1,\dots,K+L}$, $\{\tau_i\}_{i=1,\dots,K+L}$ be such that $\sigma_i=\pm 1$, $\tau_i=\pm 1$, and $\sum_{i=1}^{K+L}\sigma_i=\sum_{i=1}^{K+L}\tau_i=K-L$. Then for any integers k, l with $0\leqslant k, l\leqslant K+L$, we have

$$\left|\left(\Phi, \left(\prod_{i=1}^{k} O^{\sigma_i}\right) A\left(\prod_{i=k+1}^{K+L} O^{\sigma_i}\right)\Phi\right)-\left(\Phi, \left(\prod_{i=1}^{l} O^{\tau_i}\right) A\left(\prod_{i=l+1}^{K+L} O^{\tau_i}\right)\Phi\right)\right|$$
$$\leqslant \delta(A; K, L) \tag{5.18}$$

with the same $\delta(A; K, L)$ as in (5.11) and (5.12).

Proof of Lemma 5.2 Given Lemma 5.3. Let B be an arbitrary operator which satisfies $[B, C]=0$. Then

$$
\begin{aligned}
&(\Phi, (O^{(1)})^J B(O^{(1)})^J \Phi) \\
&= \left(\Phi, \left(\frac{O^+ + O^-}{2}\right)^J B\left(\frac{O^+ + O^-}{2}\right)^J \Phi\right) \\
&= \sum_{\tau_1 = \pm 1} \cdots \sum_{\tau_{2J} = \pm 1} 2^{-2J}\left(\Phi, \left(\prod_{i=1}^{J} O^{\tau_i}\right) B\left(\prod_{i=J+1}^{2J} O^{\tau_i}\right)\Phi\right) \\
&= \sum_{\{\tau_i\};\, \sum \tau_i = 0} 2^{-2J}\left(\Phi, \left(\prod_{i=1}^{J} O^{\tau_i}\right) B\left(\prod_{i=J+1}^{2J} O^{\tau_i}\right)\Phi\right)
\end{aligned}
\tag{5.19}
$$

where the final sum is over all $\tau_i = \pm 1$ with $\sum_{i=1}^{2J} \tau_i = 0$. The constraint comes from the fact that Φ is an eigenstate of the $U(1)$ generator C. Since the number of distinct combinations $\{\tau_i\}$ which satisfy the constraint is equal to $\binom{2J}{J} = (2J)!/(J!)^2$, we can rewrite (5.19) as

$$
\begin{aligned}
&\binom{2J}{J}^{-1} \sum_{\{\tau_i\};\, \sum \tau_i = 0} \left(\Phi, \left(\prod_{i=1}^{J} O^{\tau_i}\right) B\left(\prod_{i=J+1}^{2J} O^{\tau_i}\right)\Phi\right) \\
&\quad = \frac{2^{2J}(J!)^2}{(2J)!} (\Phi, (O^{(1)})^J B(O^{(1)})^J \Phi)
\end{aligned}
\tag{5.20}
$$

To prove (5.9), we set $B = A(O^+)^{K-L}$ and substitute (5.20) into the left-hand side of (5.9) to get

$$
\begin{aligned}
&\left|\left(\Phi, \left(\prod_{i=1}^{k} O^{\sigma_i}\right) A\left(\prod_{i=k+1}^{K+L} O^{\sigma_i}\right)\Phi\right)\right. \\
&\qquad \left. - \frac{2^{2J}(J!)^2}{(2J)!} (\Phi, (O^{(1)})^J A(O^+)^{K-L} (O^{(1)})^J \Phi)\right| \\
&\leqslant \binom{2J}{J}^{-1} \sum_{\{\tau_i\};\, \sum \tau_i = 0} \left|\left(\Phi, \left(\prod_{i=1}^{k} O^{\sigma_i}\right) A\left(\prod_{i=k+1}^{K+L} O^{\sigma_i}\right)\Phi\right)\right. \\
&\qquad \left. - \left(\Phi, \left(\prod_{i=1}^{J} O^{\tau_i}\right) A(O^+)^{K-L}\left(\prod_{i=J+1}^{2J} O^{\tau_i}\right)\Phi\right)\right| \\
&\leqslant \binom{2J}{J}^{-1} \sum_{\{\tau_i\};\, \sum \tau_i = 0} \delta(A; K, L) \\
&= \delta(A; K, L)
\end{aligned}
\tag{5.21}
$$

where we have used (5.18).

To prove (5.10), we simply substitute the estimate

$$\left|\frac{2^{2J}(J!)^2}{(2J)!}(\Phi,(O^{(1)})^J A(O^+)^{K-L}(O^{(1)})^J\Phi)\right|$$
$$\leqslant \|A(O^+)^{K-L}\| \frac{2^{2J}(J!)^2}{(2J)!}(\Phi,(O^{(1)})^{2J}\Phi) \leqslant 2\delta(A;K,L) \quad (5.22)$$

which follows from the definition of norm (2.2), into the bound (5.9). ∎

Proof of Lemma 5.3. The desired bound (5.18) is trivial if $K=L=0$. We shall prove the bound inductively in $K+L$.

Fix K, L with $K \geqslant L$ (the bounds for $K<L$ follow from the symmetry), and assume (5.18) for any nonnegative integers K', L' with $K'+L'<K+L$. Note that we are also allowed to use the resulting bounds (5.9) and (5.10) for the same K', L'.

We first assume $A \neq 1$. We denote by D the left-hand side of (5.18), and bound it as

$$\begin{aligned} D \leqslant & \left|\left(\Phi,\left(\prod_{i=1}^{k} O^{\sigma_i}\right) A\left(\prod_{i=k+1}^{K+L} O^{\sigma_i}\right)\Phi\right)-\left(\Phi, A\left(\prod_{i=1}^{K+L} O^{\sigma_i}\right)\Phi\right)\right| \\ & +\left|\left(\Phi, A\left(\prod_{i=1}^{K+L} O^{\sigma_i}\right)\Phi\right)-\left(\Phi, A\left(\prod_{i=1}^{K+L} O^{\tau_i}\right)\Phi\right)\right| \\ & +\left|\left(\Phi, A\left(\prod_{i=1}^{K+L} O^{\tau_i}\right)\Phi\right)-\left(\Phi,\left(\prod_{i=1}^{l} O^{\tau_i}\right) A\left(\prod_{i=l+1}^{K+L} O^{\tau_i}\right)\Phi\right)\right| \\ =: & \; D_1+D_2+D_3 \end{aligned} \quad (5.23)$$

The quantity D_1 in (5.23) can be bounded as

$$D_1 \leqslant \sum_{j=1}^{k}\left|\left(\Phi,\left(\prod_{i=1}^{j-1} O^{\sigma_i}\right)[O^{\sigma_j}, A]\left(\prod_{i=j+1}^{K+L} O^{\sigma_i}\right)\Phi\right)\right| \quad (5.24)$$

Each term in the sum of (5.24) can be bounded by using (5.10), where we identify $[O^\pm, A]$ as the operator A in (5.10). The condition (5.8) is clearly satisfied if we properly replace $K-L$ by $K-L\mp 1$. To apply (5.10), we rewrite the operator as $[O^\pm, A]=\sum_{x\in\Lambda}[\sum_{y\in\mathscr{S}_x} o_y^\pm, a_x]$ and note that $\|[\sum_{y\in\mathscr{S}_x} o_y^\pm, a_x]\| \leqslant 4rao$. When $\sigma_j=+1$, we get

$$\begin{aligned}
&\left|\left(\Phi, \left(\prod_{i=1}^{j-1} O^{\sigma_i}\right)[O^+, A]\left(\prod_{i=j+1}^{K+L} O^{\sigma_i}\right)\Phi\right)\right| \\
&\quad \leqslant 3\delta([O^+, A]; K-1, L) \\
&\quad \leqslant \begin{cases} \frac{3}{2}(4raoN)(2oN)^{K-L-1}\, b_L & \text{if} \quad K>L \\ \frac{3}{2}(4raoN)(2oN)\, b_{L-1} & \text{if} \quad K=L \end{cases} \\
&\quad \leqslant \tfrac{3}{2}(4raoN)(2oN)^{K-L+1}\, b_{L-1}
\end{aligned} \tag{5.25}$$

for $K \geqslant L$, where we used the bound (5.2) in the case $K > L$.

When $\sigma_j = -1$, we also get

$$\begin{aligned}
&\left|\left(\Phi, \left(\prod_{i=1}^{j-1} O^{\sigma_i}\right)[O^-, A]\left(\prod_{i=j+1}^{K+L} O^{\sigma_i}\right)\Phi\right)\right| \\
&\quad \leqslant 3\delta([O^-, A]; K, L-1) \\
&\quad \leqslant \tfrac{3}{2}(4raoN)(2oN)^{K-L+1}\, b_{L-1}
\end{aligned} \tag{5.26}$$

Since there are at most $(K+L)$ terms in the sum in (5.24), we find that

$$D_1 \leqslant (K+L)\, \tfrac{3}{2}(4raoN)(2oN)^{K-L+1}\, b_{L-1} \tag{5.27}$$

It is obvious that the quantity D_3 satisfies the same bound as (5.27).

To evaluate the quantity D_2 in (5.23), we transform $\{\sigma_i\}_{i=1,\ldots,K+L}$ into $\{\tau_i\}_{i=1,\ldots,K+L}$ by successively exchanging neighboring indices. We then get

$$D_2 \leqslant \sum_{\{\kappa_i\}} \left|\left(\Phi, A\left(\prod_{i=1}^{j-1} O^{\kappa_i}\right)[O^{\kappa_j}, O^{\kappa_{j+1}}]\left(\prod_{i=j+2}^{K+L} O^{\kappa_i}\right)\Phi\right)\right| \tag{5.28}$$

where $\{\kappa_i\}_{i=1,\ldots,K+L}$ is summed over the sequence of configurations which interpolates between $\{\sigma_i\}_{i=1,\ldots,K+L}$ and $\{\tau_i\}_{i=1,\ldots,K+L}$, and j (which depends on $\{\kappa_i\}_{i=1,\ldots,K+L}$) indicates where the indices are exchanged.

By using the commutation relation (2.23) and $C\Phi = 0$, we can further bound D_2 as

$$\begin{aligned}
D_2 &\leqslant \sum_{\{\kappa_i\}} 2\gamma(K+L)\left|\left(\Phi, A\left(\prod_{i=1}^{j-1} O^{\kappa_i}\right)\left(\prod_{i=j+2}^{K+L} O^{\kappa_i}\right)\Phi\right)\right| \\
&\leqslant \sum_{\{\kappa_i\}} 6\gamma(K+L)\,\delta(A; K-1, L-1) \\
&\leqslant 3\gamma KL(K+L)(aN)(2oN)^{K-L}\, b_{L-1}
\end{aligned} \tag{5.29}$$

where we have used the fact that at most KL exchanges are necessary to get $\{\tau\}_{i=1,\ldots,K+L}$ from $\{\sigma_i\}_{i=1,\ldots,K+L}$ and the bound (5.10).

By substituting the bounds (5.27) and (5.29) into the decomposition (5.23) and using the bounds (5.2) and (5.11), we finally get

$$\begin{aligned} D &\leqslant \{24(K+L)\, ro^2N + 3\gamma KL(K+L)\}(aN)(2oN)^{K-L}\, b_{L-1} \\ &\leqslant \left\{\frac{48r}{\mu^2}\frac{K+L}{N} + \frac{6\gamma}{o^2\mu^2}\frac{KL(K+L)}{N^2}\right\}\delta(A;K,L) \\ &\leqslant \delta(A;K,L) \end{aligned} \tag{5.30}$$

where we used the assumption (5.7) and $KL \leqslant (K+L)^2/4$. This proves the desired (5.18) for $A \neq 1$.

The case $A = 1$ is much easier. One notes that only D_2 is nonvanishing in the decomposition (5.23). A similar estimate as the above proves the desired result. ▮

APPENDIX A: GROUND STATES OF INFINITE SYSTEMS

In the present appendix we give mathematically precise definitions of ground states in an infinite system and discuss relations between different definitions. The contents of the present appendix might be well known to experts, but they have not been written down explicitly as far as we know. We think it would be convenient for the reader to have them included in the present paper.

We start by briefly reviewing basic setups in the operator-algebraic approach to quantum systems with infinitely many degrees of freedom.[9, 43, 45] For simplicity we consider a quantum many-body system defined on the d-dimensional hypercubic lattice $\mathbf{Z}^d$. With each site $x \in \mathbf{Z}^d$ we associate a finite-dimensional Hilbert space $\mathscr{H}_x$ which is assumed to be identical to $\mathscr{H}_0$, where o is a fixed site (the origin) of $\mathbf{Z}^d$. The Hilbert space corresponding to a finite subset $\Omega \subset \mathbf{Z}^d$ is

$$\mathscr{H}_\Omega := \bigotimes_{x \in \Omega} \mathscr{H}_x \tag{A.1}$$

Let $\mathscr{A}_\Omega$ denote the set of all the operators on $\mathscr{H}_\Omega$. The basic object in the operator-algebraic approach is the algebra of quasilocal operators defined as

$$\mathscr{A} := \overline{\bigcup_{\Omega} \mathscr{A}_\Omega} \tag{A.2}$$

where the union is over all the finite subsets $\Omega \subset \mathbf{Z}^d$ and the completion is taken with respect to the norm (2.2) for local operators. Note that we have made $\mathscr{A}$ into a Banach space.

A state $\rho(\cdots)$ is a linear map from $\mathscr{A}$ to $\mathbf{C}$ which satisfies $\rho(1)=1$ and $\rho(A^*A)\geqslant 0$ for any $A\in\mathscr{A}$. It can be shown[9] that it automatically holds that $|\rho(A)|\leqslant\|A\|$ and $\rho(A^*)=\rho(A)^*$. We denote by $\mathscr{E}$ the set of all states on $\mathscr{A}$. Since $\mathscr{E}$ is the intersection of the unit sphere of the dual space $\mathscr{A}^*$ and the cone of positive functionals, the Banach–Alaoglu theorem[42] implies that $\mathscr{E}$ is compact in the weak-$*$ topology.

The compactness provides us with a useful way of constructing states on $\mathscr{A}$. Let $\{\Omega_i\}_{i=1,2,\ldots}$ be an arbitrary sequence of finite subsets of $\mathbf{Z}^d$ which tends to $\mathbf{Z}^d$ in the sense of van Hove[47, 43] as $i\uparrow\infty$. For each i we take a state (density matrix) $\rho_i(\cdots)$ on the algebra $\mathscr{A}_{\Omega_i}$. Since $\rho_i(\cdots)$ can be naturally regarded[15] as an element of $\mathscr{E}$, the compactness ensures that one can take a subsequence $\{i(j)\}_{j=1,2,\ldots}\subset\{1,2,\ldots\}$ such that the weak-$*$ limit

$$\rho(\cdots):=\lim_{j\uparrow\infty}\rho_{i(j)}(\cdots) \tag{A.3}$$

exists. In the physicists' language, (A.3) should be read

$$\rho(A)=\lim_{j\uparrow\infty}\rho_{i(j)}(A) \tag{A.4}$$

for each $A\in\mathscr{A}$.

As in Section 2, we let h_0 be the local Hamiltonian at the origin $o\in\mathbf{Z}^d$, which acts on the finite-dimensional Hilbert space $\bigotimes_{x\in\mathscr{S}_o}\mathscr{H}_x$ with the support set $\mathscr{S}_o$ containing r sites. We also set $h_x=\tau_x(h_o)$ and for any finite set $\Omega\in\mathbf{Z}^d$,

$$H_\Omega:=\sum_{x\in\Omega}h_x \tag{A.5}$$

where τ_x denotes the translation by the lattice vector x.

We now describe three different definitions of the set of *ground states*. The first definition is standard in mathematical literature, and is

$$\mathscr{G}_1:=\{\omega\in\mathscr{E}\,|\,\omega(A^*[H_{\bar\Omega},A])\geqslant 0\text{ for any }A\in\mathscr{A}_\Omega\text{ and for any finite }\Omega\subset\mathbf{Z}^d\} \tag{A.6}$$

Here we introduced

$$\bar\Omega:=\{x\,|\,\mathscr{S}_x\cap\Omega\neq\varnothing\} \tag{A.7}$$

[15] For $A\in\mathscr{A}_{\Omega_i}$ and $B\in\mathscr{A}_{\Omega_i^c}$ (where $\Omega_i^c=\mathbf{Z}^d\backslash\Omega_i$), we set $\tilde\rho_i(AB)=\rho_i(A)\,\sigma_i(B)$, where $\sigma_i(\cdots)$ is an arbitrary state on $\mathscr{A}_{\Omega_i^c}$. By using linearlity, $\tilde\rho_i(\cdots)$ extends over the whole $\mathscr{A}$. The state $\sigma_i(\cdots)$ may be chosen, for example, as the trace state defined by $\sigma_i(\cdots)=\lim_{\Gamma\uparrow\Omega_i^c}\mathrm{Tr}_{\mathscr{H}_\Gamma}[\cdots]/\mathrm{Tr}_{\mathscr{H}_\Gamma}[1]$. This choice corresponds to the so-called free boundary conditions.

where $\mathscr{S}_x = \tau_x(\mathscr{S}_o)$ is the support set for h_x. (We use the same symbol τ_x to denote the translation operators for subsets of $\mathbf{Z}^d$ and that for operators.)

The second definition is due to Aizenman and Lieb[5] (see also ref. 4). The definition is useful because of its similarity to "classical" definitions of ground states. It is

$$\mathscr{G}_2 := \{\omega \in \mathscr{E} \mid \omega(H_\Omega) \leqslant \omega(T(H_\Omega)) \text{ for any } T \in \mathscr{P}_\Omega \text{ and for any finite } \Omega \subset \mathbf{Z}^d\} \tag{A.8}$$

where $\mathscr{P}_\Omega$ is the set of all local perturbations on Ω. A local perturbation T on Ω is a linear mapping $T: \mathscr{A} \to \mathscr{A}$ which satisfies $T(A) \geqslant 0$ for any $A \geqslant 0$, and $T(A) = A$ for any $A \in \mathscr{A}_{\Omega^c}$, where $\mathscr{A}_{\Omega^c} := \overline{\bigcup_{\Omega'} \mathscr{A}_{\Omega' \setminus \Omega}}$ is the operator outside of Ω.

The third definition already appeared in Sections 1.2 and 2.5, and is probably the simplest among the three definitions. (Essentially the same definition can be found in ref. 2.) It is

$$\mathscr{G}_3 := \{\omega \in \mathscr{E} \mid \omega(h_x) = \epsilon_0 \text{ for any } x \in \mathbf{Z}^d\} \tag{A.9}$$

where the ground-state energy density ϵ_0 is defined as follows. Let Λ be the d-dimensional $L \times \cdots \times L$ hypercubic lattice. We define the corresponding Hamiltonian with periodic boundary conditions as

$$H_\Lambda^{\text{p.b.c.}} = \sum_{x \in \Lambda} h_x \tag{A.10}$$

where for a site x close to the boundary of Λ we identify h_x in (A.10) as an operator in $\mathscr{A}_\Lambda$ by imposing periodic boundary conditions. Note that in the present paper a Hamiltonian with periodic boundary conditions is simply denoted as H_Λ except in the present appendix. Then we define ϵ_0 by

$$\epsilon_0 := \lim_{\Lambda \uparrow \mathbf{Z}^d} \inf_{\rho_\Lambda \in \mathscr{A}_\Lambda} \frac{1}{|\Lambda|} \rho_\Lambda(H_\Lambda^{\text{p.b.c.}}) \tag{A.11}$$

where $|\Lambda|$ is the number of sites in Λ and the existence of the limit can be proved by a standard argument.

For each $i = 1, 2, 3$, we denote by $\hat{\mathscr{G}}_i$ the set of $\omega \in \mathscr{G}_i$ which is translation invariant, i.e., $\omega(\tau_x(A)) = \omega(A)$ for any $A \in \mathscr{A}$ and any $x \in \mathbf{Z}^d$.

Now we discuss the relations between these different definitions. We first note the following.

Proposition A.1. We have $\mathscr{G}_1 = \mathscr{G}_2$.

Outline of Proof. Nontrivial parts of the proof are worked out in the literature, and we only have to make some formal observations. We make use of the results summarized as Theorem 6.2.52 in ref. 9.

To prove $\mathscr{G}_1 \subset \mathscr{G}_2$, we note that the above-mentioned theorem in ref. 9 says that $\omega \in \mathscr{G}_1$ if and only if

$$\omega(H_{\bar{\Omega}}) \leqslant \omega'(H_{\bar{\Omega}}) \tag{A.12}$$

for any $\omega' \in \mathscr{E}$ such that $\omega(B) = \omega'(B)$ for all $B \in \mathscr{A}_{\Omega^c}$ and for any finite $\Omega \in \mathbf{Z}^d$. By choosing the perturbed state $\omega'(\cdots)$ in a special form $\omega(T(\cdots))$ as in the definition of $\mathscr{G}_2$, we see that $\omega \in \mathscr{G}_2$.

To prove $\mathscr{G}_2 \subset \mathscr{G}_1$, we can follow the part $(1) \Rightarrow (2)$ of the proof of the above-mentioned theorem in ref. 9 without any essential modifications. ▮

Next we note the following.

Proposition A.2. We have $\mathscr{G}_1 = \mathscr{G}_2 \supset \mathscr{G}_3$.

Proof. Because of Proposition A.1, it suffices to show $\mathscr{G}_3 \subset \mathscr{G}_2$. The proof is elementary.

We want to get a contradiction out of the assumption that there is a state ω such that $\omega \in \mathscr{G}_3$ and $\omega \notin \mathscr{G}_2$. From the assumption, there exists a finite set $\Omega \subset \mathbf{Z}^d$, a local perturbation $T \in \mathscr{P}_\Omega$, and a constant $\varepsilon > 0$ such that

$$\omega(H_{\bar{\Omega}}) - \omega(T(H_{\bar{\Omega}})) \geqslant \varepsilon \tag{A.13}$$

Let l be an integer such that $\bar{\Omega}$ is contained in a suitable d-dimensional $l \times \cdots \times l$ hypercubic lattice Λ_0. For an integer n, let Λ be the d-dimensional $(nl) \times \cdots \times (nl)$ hypercubic lattice. There are translation operators τ_i with $i = 1, 2, \ldots, n^d$ such that

$$\Lambda = \bigcup_{i=1}^{n^d} \tau_i(\Lambda_0) \tag{A.14}$$

Let ω_Λ be the state obtained by simply restricting ω onto $\mathscr{A}_\Lambda$. We further define

$$\omega'_\Lambda(A) := \omega_\Lambda(\tilde{T}(A)) \tag{A.15}$$

for a suitable $A \in \mathscr{A}_\Lambda$, where

$$\tilde{T} = \prod_{i=1}^{n^d} \tau_i^{-1} T \tau_i \tag{A.16}$$

By using (A.13) and the properties of local perturbations, we observe that

$$\omega_\Lambda(H_\Lambda^{\text{p.b.c.}}) - \omega'_\Lambda(H_\Lambda^{\text{p.b.c.}}) = \sum_{i=1}^{n^d} \{\omega_\Lambda(H_{\tau_i(\bar{\Omega})}) - \omega_\Lambda(T(H_{\tau_i(\bar{\Omega})}))\} \geqslant n^d \varepsilon \tag{A.17}$$

On the other hand, since we have $\omega(h_x) = \epsilon_0$, we get

$$\omega_\Lambda(H_\Lambda^{\text{p.b.c.}}) \leqslant (nl)^d \epsilon_0 + \beta(nl)^{d-1} \tag{A.18}$$

where β is a finite constant which takes care of the boundary effects. By combining the bounds (A.17) and (A.18), we get

$$(nl)^{-d} \omega'_\Lambda(H_\Lambda^{\text{p.b.c.}}) - \epsilon_0 \leqslant -l^{-d}\varepsilon + \beta(nl)^{-1} \tag{A.19}$$

which contradicts the definition (A.11) of ϵ_0 by taking n sufficiently large. ∎

It should be noted that we do not have $\mathscr{G}_1 = \mathscr{G}_2 = \mathscr{G}_3$. For example, a state with a single domain wall in the Ising model belongs to $\mathscr{G}_1 = \mathscr{G}_2$ but not to $\mathscr{G}_3$. It is a delicate problem to decide which definition is more "realistic."

As for the translation-invariant ground states, however, we have the following rather satisfactory result.

Proposition A.3. We have $\hat{\mathscr{G}}_1 = \hat{\mathscr{G}}_2 = \hat{\mathscr{G}}_3$.

Proof. Because of Propositions A.1 and A.2, it suffices to show that $\hat{\mathscr{G}}_1 \subset \mathscr{G}_3$. Again the most essential part can be found in the literature. In Theorem 6.2.58 of ref. 9 it is proved that a translation-invariant state ω belongs to $\mathscr{G}_1$ if and only if $\omega(h_x) = \tilde{\epsilon}_0$ for any $x \in \mathbf{Z}^d$. The ground-state energy density is defined as

$$\tilde{\epsilon}_0 := \inf_{\omega' \in \mathscr{E}_{\text{inv}}} \omega'(h_x) \tag{A.20}$$

where $\mathscr{E}_{\text{inv}}$ is the set of translation-invariant states in $\mathscr{E}$. We only have to show that $\epsilon_0 = \tilde{\epsilon}_0$, and this may be done in several ways. Here we offer a simple constructive proof. For each Λ, we can take a ground state $\Phi_\Lambda^{(0)} \in \mathscr{H}_\Lambda$ of the Hamiltonian $H_\Lambda^{\text{p.b.c.}}$, whose expectation values are invariant under translations that take into account the periodic boundary conditions imposed on Λ. Define a state $\omega \in \mathscr{E}$ by the (weak-*) limiting procedure (2.36). By construction, we see that $\omega \in \hat{\mathscr{G}}_1$. The above-mentioned theorem of ref. 9 then implies that $\omega(h_x) = \tilde{\epsilon}_0$. On the other hand, our definition (A.11) of ϵ_0 implies that $\omega(h_x) = \epsilon_0$. ∎

One might be interested to know if there is any general theorem which tells us exactly what are the elements of the above sets of ground states. The following is an example of such general theorems. It establishes uniqueness of the ground state when there is a decoupled Hamiltonian with a unique ground state, and then one adds a weak (but completely arbitrary) translation-invariant perturbation to the model.

Suppose that the Hamiltonian at the origin can be written as

$$h_o = v_o + \delta p_o \tag{A.21}$$

The main part v_o acts only on the space $\mathscr{H}_o$ and its lowest eigenvalue is simple. The perturbation p_o is an arbitrary self-adjoint operator on $\bigotimes_{x \in \mathscr{S}_o} \mathscr{H}_x$ and δ is a constant. By using a rigorous perturbation technique, the following was proved in ref. 23.

Theorem A.4. There exists a finite constant $\delta_0 > 0$ which depends on the dimension d and on the operators v_o and p_o. For $|\delta| \leqslant \delta_0$, the set of ground states $\hat{\mathscr{G}}_1 = \hat{\mathscr{G}}_2 = \hat{\mathscr{G}}_3$ consists of a unique element.

For example, the Ising model under sufficiently large transverse magnetic field (1.1) is covered by the above theorem by setting $h_o = S_o^{(1)}$.

APPENDIX B. ERGODIC INFINITE-VOLUME GROUND STATE IN SYSTEMS WITH DISCRETE SYMMETRY BREAKING

In the present appendix we concentrate on a system in which a discrete symmetry is spontaneously broken. We assume for each finite system the existence of an "obscured symmetry breaking" and the existence of an energy gap above the first "low-lying eigenstate." Then we can prove that, by forming a linear combination of the (finite-volume) ground state and the "low-lying state" and then taking an infinite-volume limit, one indeed gets an ergodic infinite-volume ground state.

As far as we know, this is the first rigorous and general result which explicitly tells one how to construct an ergodic infinite-volume ground state when there is a symmetry breaking. The theorem is desirable in this sense, but we have to note that the assumption on the existence of a gap is a rather strong one, which is not at all easy to verify even in relatively simple problems.[16] We also stress that the techniques involved here crucially depend on the fact that there is only one "low-lying eigenstate." To prove the corresponding conjecture (stated in Section 2.5) for the models with broken continuous symmetry seems formidably difficult at present.

We study the situation basically identical to that in Section 2.2, but with additional assumptions on the translation invariance. The translation invariance is by no means essential in proving the main theorem, but the

[16] Even in models (like the transverse Ising model of Section 1.2) where one has a convergent cluster expansion, it may not be easy to verify the existence of the gap. As for the transverse Ising model in one dimension, one can make use of the mapping to the free fermion problem to control the gap.

implication of the theorem is interesting only in translation-invariant systems.

Let Λ be a d-dimensional hypercubic lattice with periodic boundary conditions and denote by N the number of sites in Λ. We consider a quantum many-body system on Λ as in Sections 2.1 and 2.2. The Hilbert space is constructed as in (2.1), the Hamiltonian as in (2.3), and the order operator as in (2.5). The additional assumptions are that we have $h_x = \tau_x(h_o)$ and $o_x = \tau_x(o_o)$, where τ_x is the translation operator that takes into account the periodic boundary conditions. We also require that each o_x acts only on the local Hilbert space $\mathscr{H}_x$. In some situations, one might need to redefine the notion of "sites" to satisfy the translation invariance. See Section 3.2.

Let $E_\Lambda^{(0)}$, $E_\Lambda^{(1)}$ with $E_\Lambda^{(0)} < E_\Lambda^{(1)}$ be the two lowest eigenvalues of H_Λ, and $\Phi_\Lambda^{(0)}$, $\Phi_\Lambda^{(1)}$ be the corresponding normalized eigenstates. We assume that if E'_Λ is any other eigenvalue of H_Λ, we have

$$E'_\Lambda - E_\Lambda^{(1)} \geqslant E_{\mathrm{G}} \tag{B.1}$$

with a (Λ-independent) constant $E_{\mathrm{G}} > 0$. We also assume that the ground state $\Phi_\Lambda^{(0)}$ exhibits an "obscured symmetry breaking" as

$$(\Phi_\Lambda^{(0)}, O_\Lambda \Phi_\Lambda^{(0)}) = 0 \tag{B.2}$$

$$(\Phi_\Lambda^{(0)}, (O_\Lambda)^2 \Phi_\Lambda^{(0)}) \geqslant (\mu o N)^2 \tag{B.3}$$

with a constant $\mu > 0$ and

$$(\Phi_\Lambda^{(0)}, (O_\Lambda)^3 \Phi_\Lambda^{(0)}) = 0 \tag{B.4}$$

Although we did not assume the condition (B.4) in Section 1.2, it is valid in most situations.

We shall again consider the "low-lying state" of Horsch and von der Linden,[15]

$$\Psi_\Lambda := \frac{O_\Lambda \Phi_\Lambda^{(0)}}{\|O_\Lambda \Phi_\Lambda^{(0)}\|} \tag{B.5}$$

and its linear combination with the ground state

$$\Xi_\Lambda := \frac{1}{\sqrt{2}} (\Phi_\Lambda^{(0)} + \Psi_\Lambda) \tag{B.6}$$

which was first considered by Kaplan *et al.*[18] From a straightforward calculation using the definitions (B.5), (B.6), and the assumed (B.2), (B.3), and (B.4), we find[18] that the above state (B.6) exhibits a symmetry breaking as

$$(\Xi_\Lambda, O_\Lambda \Xi_\Lambda) = \frac{1}{2}\left\{(\Phi_\Lambda^{(0)}, O_\Lambda \Phi_\Lambda^{(0)}) + \frac{2(\Phi_\Lambda^{(0)}, (O_\Lambda)^2 \Phi_\Lambda^{(0)})}{\|O_\Lambda \Phi_\Lambda^{(0)}\|} + \frac{(\Phi_\Lambda^{(0)}, (O_\Lambda)^3 \Phi_\Lambda^{(0)})}{\|O_\Lambda \Phi_\Lambda^{(0)}\|^2}\right\}$$
$$= [(\Phi_\Lambda^{(0)}, (O_\Lambda)^2 \Phi_\Lambda^{(0)})]^{1/2} \geqslant \mu o N \tag{B.7}$$

Let A be a local self-adjoint operator which acts on $\bigotimes_{x \in \mathcal{S}'} \mathcal{H}_x$, where the number of sites in the support set $\mathcal{S}'$ is bounded by a constant r'. For a subset $\Omega \subset \Lambda$, we set

$$A_\Omega := \sum_{x \in \Omega} \tau_x(A) \tag{B.8}$$

where $\tau_x(A)$ is a translate of A by a lattice vector x. Then the main result of the present appendix is the following.

Theorem B.1. We have

$$\lim_{|\Omega| \uparrow \infty} \lim_{N \uparrow \infty} \frac{1}{|\Omega|^2} \{(\Xi_\Lambda, (A_\Omega)^2 \Xi_\Lambda) - (\Xi_\Lambda, A_\Omega \Xi_\Lambda)^2\} = 0 \tag{B.9}$$

for any local operator A.

From the Definition 2.7 of ergodic state, we get the following interesting conclusion.

Corollary B.2. The infinite-volume ground state

$$\omega_+(\cdots) = \lim_{N \uparrow \infty} (\Xi_\Lambda, (\cdots) \Xi_\Lambda) \tag{B.10}$$

defined by taking a suitable subsequence is an ergodic translation-invariant ground state.

It is obvious that the same is true for the infinite-volume ground state $\omega_-(\cdots)$ constructed from $(\Phi_\Lambda^{(0)} - \Psi_\Lambda)/\sqrt{2}$ instead of (B.6).

In the following we prove Theorem B.1. For simplicity, we drop the subscript Λ from $\Phi_\Lambda^{(0)}$, $\Phi_\Lambda^{(1)}$, Ψ_Λ, H_Λ, O_Λ, etc.

We start from the following lemma, which provides us with the basic tool in the proof. In short the lemma says that the set of two states $\{\Phi^{(0)}, \Phi^{(1)}\}$ can be used almost as a "complete basis" in some situations.

Lemma B.3. Let B and C be arbitrary self-adjoint operators. Then for $i, j = 0$ or 1, we have

$$\begin{aligned}\left|(\Phi^{(i)}, BC\Phi^{(j)}) - \sum_{k=0,1} (\Phi^{(i)}, B\Phi^{(k)})(\Phi^{(k)}, C\Phi^{(j)})\right| \\ = |(\Phi^{(i)}, B\mathscr{P}C\Phi^{(j)})| \\ \leqslant \frac{(\|[B, [H, B]]\| \cdot \|[C, [H, C]]\|)^{1/2}}{2E_G}\end{aligned} \tag{B.11}$$

where $\mathscr{P}$ is the projection operator onto the space orthogonal to both $\Phi^{(0)}$ and $\Phi^{(1)}$.

Proof. From the existence of a gap as in (B.1), we get the operator inequality $\mathscr{P} \leqslant (H - E_i)/E_G$ for $i = 0, 1$. By using the Schwartz inequality, we have

$$\begin{aligned}&|(\Phi^{(i)}, B\mathscr{P}C\Phi^{(j)})|^2 \\ &\leqslant (\Phi^{(i)}, B\mathscr{P}B\Phi^{(i)})(\Phi^{(j)}, C\mathscr{P}C\Phi^{(j)}) \\ &\leqslant \left(\Phi^{(i)}, B\frac{H-E_i}{E_G} B\Phi^{(i)}\right)\left(\Phi^{(j)}, C\frac{H-E_i}{E_G} C\Phi^{(j)}\right) \\ &= (2E_G)^{-2} (\Phi^{(i)}, [B, [H, B]]\Phi^{(i)})(\Phi^{(j)}, [C, [H, C]]\Phi^{(j)}) \\ &\leqslant (2E_G)^{-2} \|[B, [H, B]]\| \cdot \|[C, [H, C]]\|\end{aligned} \tag{B.12}$$

which is the desired bound. ∎

As the first application of the lemma, we state the following result, which is both useful and important. The lemma says that the "low-lying state" (B.5) is indeed a very good approximation of the first excited state $\Phi^{(1)}$.

Lemma B.4. One can redefine the (quantum mechanical) phase of the first excited state $\Phi^{(1)}$ so that the bound

$$\|\Phi^{(1)} - \Psi\|^2 \leqslant \frac{4hr^2}{E_G \mu^2} \frac{1}{N} \tag{B.13}$$

holds.

Proof. Since $(\Phi^{(0)}, \Psi) = 0$, we can write $\Psi = \alpha\Phi^{(1)} + \Psi'$, where $\Psi' = \mathscr{P}\Psi$. By redefining the phase of $\Phi^{(1)}$, we can choose $\alpha \geqslant 0$. First note that

$$\begin{aligned}\|\Phi^{(1)} - \Psi\|^2 &= \|(1-\alpha)\Phi^{(1)} - \Psi'\|^2 \\ &= (1-\alpha)^2 + \|\Psi'\|^2 \leqslant 2\,\|\Psi'\|^2\end{aligned} \tag{B.14}$$

where we have used $(1-\alpha)^2 \leqslant 1-\alpha \leqslant 1-\alpha^2 = \|\Psi'\|^2$. To bound $\|\Psi'\|$, we use (B.11) to get

$$\begin{aligned}
\|\Psi'\|^2 = (\Psi, \mathscr{P}\Psi) &= \frac{(\Phi^{(0)}, O\mathscr{P}O\Phi^{(0)})}{(\Phi^{(0)}, O^2\Phi^{(0)})} \\
&\leqslant \frac{\|[O[H, O]]\|}{2E_{\mathrm{G}}(\Phi^{(0)}, O^2\Phi^{(0)})} \\
&\leqslant \frac{4o^2r^2N}{2E_{\mathrm{G}}(o\mu N)^2} = \frac{2hr^2}{E_{\mathrm{G}}\mu^2}\frac{1}{N}
\end{aligned} \tag{B.15}$$

where we used (B.3). ∎

We now turn to the estimate of the left-hand side of (B.9). Note that we can assume

$$(\Phi^{(0)}, A_\Omega \Phi^{(0)}) = 0 \tag{B.16}$$

since otherwise we can redefine $A - (\Phi^{(0)}, A\Phi^{(0)})$ as a new A. Let

$$\Xi' := \frac{1}{\sqrt{2}}(\Phi^{(0)} + \Phi^{(1)}) \tag{B.17}$$

which is essentially the same as Ξ according to the definition (B.6) and the relation (B.13). In particular, we have

$$\begin{aligned}
&|\{(\Xi, (A_\Omega)^2\,\Xi) - (\Xi, A_\Omega\Xi)^2\} - \{(\Xi', (A_\Omega)^2\,\Xi') - (\Xi', A_\Omega\Xi')^2\}| \\
&\quad\leqslant \frac{a_1\,\|A\|^2}{\sqrt{N}}\,|\Omega|^2
\end{aligned} \tag{B.18}$$

Throughout the present proof, a_i denote constants which depend only on h, r, μ, and E_{G}. By using the definition (B.17) and the requirement (B.16), we observe that

$$\begin{aligned}
&(\Xi', (A_\Omega)^2\,\Xi') - (\Xi', A_\Omega\Xi')^2 \\
&\quad= \tfrac{1}{2}\{(\Phi^{(0)}, (A_\Omega)^2\,\Phi^{(0)}) + (\Phi^{(0)}, (A_\Omega)^2\,\Phi^{(1)}) + (\Phi^{(1)}, (A_\Omega)^2\,\Phi^{(0)}) \\
&\qquad+ (\Phi^{(1)}, (A_\Omega)^2\,\Phi^{(1)})\} \\
&\qquad- \tfrac{1}{4}\{(\Phi^{(0)}, A_\Omega\Phi^{(1)}) + (\Phi^{(1)}, A_\Omega\Phi^{(0)}) + (\Phi^{(1)}, A_\Omega\Phi^{(1)})\}^2 \\
&\quad= \tfrac{1}{2}\{(\Phi^{(0)}, (A_\Omega)^2\,\Phi^{(0)}) - (\Phi^{(0)}, A_\Omega\Phi^{(1)})(\Phi^{(1)}, A_\Omega\Phi^{(0)})\} \\
&\qquad+ \tfrac{1}{2}\{(\Phi^{(0)}, (A_\Omega)^2\,\Phi^{(1)}) - (\Phi^{(0)}, A_\Omega\Phi^{(1)})(\Phi^{(1)}, A_\Omega\Phi^{(1)})\} \\
&\qquad+ \tfrac{1}{2}\{(\Phi^{(1)}, (A_\Omega)^2\,\Phi^{(0)}) - (\Phi^{(1)}, A_\Omega\Phi^{(1)})(\Phi^{(1)}, A_\Omega\Phi^{(0)})\} + R
\end{aligned} \tag{B.19}$$

The remaining term R can be further rewritten as

$$
\begin{aligned}
R &= \tfrac{1}{2}(\Phi^{(1)}, (A_\Omega)^2\, \Phi^{(1)}) - \tfrac{1}{4}\{(\Phi^{(0)}, A_\Omega \Phi^{(1)})^2 \\
&\quad + (\Phi^{(1)}, A_\Omega \Phi^{(0)})^2 + (\Phi^{(1)}, A_\Omega \Phi^{(1)})^2\} \\
&= \tfrac{1}{2}\left\{(\Phi^{(1)}, (A_\Omega)^2\, \Phi^{(1)}) - \sum_{i=0,1} (\Phi^{(1)}, A_\Omega \Phi^{(i)})(\Phi^{(i)}, A_\Omega \Phi^{(1)})\right\} \\
&\quad + \tfrac{1}{4}\{(\Phi^{(1)}, A_\Omega \Phi^{(0)})(\Phi^{(0)}, A_\Omega \Phi^{(1)}) - (\Phi^{(1)}, A_\Omega \Phi^{(0)})^2\} \\
&\quad + \tfrac{1}{4}\{(\Phi^{(1)}, A_\Omega \Phi^{(0)})(\Phi^{(0)}, A_\Omega \Phi^{(1)}) - (\Phi^{(0)}, A_\Omega \Phi^{(1)})^2\} \\
&\quad + \tfrac{1}{4}(\Phi^{(1)}, A_\Omega \Phi^{(1)})^2
\end{aligned}
\tag{B.20}
$$

By using the "completeness" relations (B.11) and (B.16) to bound the right-hand sides of (B.19) and (B.20), we have

$$
\begin{aligned}
&|(\Xi', (A_\Omega)^2\, \Xi') - (\Xi', A_\Omega \Xi')^2| \\
&\quad \leqslant \frac{1}{2}\, |(\Phi^{(1)}, A_\Omega \Phi^{(0)})(\Phi^{(0)}, A_\Omega \Phi^{(1)}) - (\Phi^{(1)}, A_\Omega \Phi^{(0)})^2| \\
&\quad\quad + \frac{1}{4}\, (\Phi^{(1)}, A_\Omega \Phi^{(1)})^2 + \frac{1}{E_G}\, \|[A_\Omega, [H, A_\Omega]]\|
\end{aligned}
\tag{B.21}
$$

We shall bound each term in the right-hand side of (B.21). To bound the first term, we use (B.13) to get

$$
\begin{aligned}
&|(\Phi^{(1)}, A_\Omega \Phi^{(0)})(\Phi^{(0)}, A_\Omega \Phi^{(1)}) - (\Phi^{(1)}, A_\Omega \Phi^{(0)})^2| \\
&\quad \leqslant \|A_\Omega\|\; |(\Phi^{(0)}, A_\Omega \Phi^{(1)}) - (\Phi^{(1)}, A_\Omega \Phi^{(0)})| \\
&\quad \leqslant \|A_\Omega\| \left\{ \left| \frac{(\Phi^{(0)}, (AO - OA)\Phi^{(0)})}{(\Phi^{(0)}, O^2 \Phi^{(0)})^{1/2}} \right| + \frac{a_2\, \|A_\Omega\|}{\sqrt{N}} \right\} \\
&\quad \leqslant \frac{\|A_\Omega\| \cdot \|[A_\Omega, O]\|}{(\Phi^{(0)}, O\Phi^{(0)})^{1/2}} + \frac{a_2\, \|A_\Omega\|^2}{\sqrt{N}} \\
&\quad \leqslant \frac{2\, \|A\|^2\, r'\, |\Omega|^2}{\mu N} + \frac{a_2\, \|A\|^2\, |\Omega|^2}{\sqrt{N}}
\end{aligned}
\tag{B.22}
$$

where we have used the lower bound (B.3) and the bound $\|[A_\Omega, O]\| \leqslant 2\, \|A\|\, or'\, |\Omega|$.

To bound the second term, we first use (B.13) and (B.3) to get

$$
\begin{aligned}
(\Phi^{(1)}, A_\Omega \Phi^{(1)}) &\leqslant \frac{(\Phi^{(0)}, OA_\Omega O\Phi^{(0)})}{(\Phi^{(0)}, O^2 \Phi^{(0)})} + \frac{a_3\, \|A_\Omega\|}{\sqrt{N}} \\
&\leqslant \frac{(\Phi^{(0)}, OA_\Omega O\Phi^{(0)})}{(\mu o N)^2} + \frac{a_3\, \|A\| \cdot |\Omega|}{\sqrt{N}}
\end{aligned}
\tag{B.23}
$$

To bound the right-hand side of (B.23), we use the "completeness" relations (B.11) and (B.16) to get

$$\begin{aligned}
&|(\Phi^{(0)}, OA_\Omega O\Phi^{(0)})| \\
&\quad \leqslant |(\Phi^{(0)}, O^2 A_\Omega \Phi^{(0)})| + |(\Phi^{(0)}, O[A_\Omega, O]\Phi^{(0)})| \\
&\quad \leqslant |(\Phi^{(0)}, O^2\Phi^{(1)})(\Phi^{(1)}, A_\Omega \Phi^{(0)})| \\
&\qquad + \frac{(\|[O^2, [H, O^2]]\| \cdot \|[A_\Omega, [H, A_\Omega]]\|)^{1/2}}{2E_G} + \|O[A_\Omega, O]\| \\
&\quad \leqslant |(\Phi^{(0)}, O^2\Phi^{(1)}) \, \|A_\Omega\| \, | \\
&\qquad + \frac{(16 o^4 h^2 r N^3 \times 4 \, \|A\|^2 \, hrr'^2 \, |\Omega|)^{1/2}}{2E_G} + \|A\| \, o^2 r' \, |\Omega| \, N
\end{aligned} \tag{B.24}$$

We further use (B.13) to see

$$\begin{aligned}
|(\Phi^{(0)}, O^2\Phi^{(1)})| &\leqslant \frac{|(\Phi^{(0)}, O^2 O \Phi^{(0)})|}{(\Phi^{(0)}, O^2\Phi^{(0)})^{1/2}} + \frac{a_2 \, \|O^2\|}{\sqrt{N}} \\
&\leqslant o^2 a_2 N^{3/2}
\end{aligned} \tag{B.25}$$

where we used (B.4). By substituting (B.24) and (B.25) into (B.23), we get

$$(\Phi^{(1)}, A_\Omega \Phi^{(1)})^2 \leqslant c \, \frac{|\Omega|^2}{N} \tag{B.26}$$

where c is an N-independent constant.

In order to control the third term on the right-hand side of (B.21), we note that $\|[A_\Omega, [H, A_\Omega]]\| \leqslant 4 \, \|A\|^2 \, hrr'^2 \, |\Omega|$. By putting (B.18), (B.21), (B.22), and (B.26) together, we finally see that

$$\frac{1}{|\Omega|^2} \, |(\Xi, (A_\Omega)^2 \, \Xi) - (\Xi, A_\Omega \Xi)^2| \leqslant \frac{4 \, \|A\|^2 \, hrr'^2}{E_G} \, \frac{1}{|\Omega|} + O(N^{-1/2}) \tag{B.27}$$

APPENDIX C. LOWER BOUND FOR FLUCTUATION OF BULK QUANTITIES

In the present appendix we prove simple lemmas which characterize the behavior of the fluctuation of bulk quantities in a translation-invariant state. The lemma was used in Sections 1.2 and 2.5 to demonstrate that the infinite-volume ground state obtained as a limit of finite-volume ground states is not ergodic.

Let Λ be a d-dimensional hypercubic lattice with N sites and with periodic boundary conditions. We consider a quantum many-body system on Λ with the Hilbert space (2.1). We do not make any specific assumption about the system. We denote by τ_x the translation which acts on the operators and which respects the periodic boundary conditions.

Let B be an arbitrary local operator. For a subset $\Omega \subset \Lambda$, we set

$$B_\Omega := \sum_{x \in \Omega} \tau_x(B) \tag{C.1}$$

Lemma C.1. Let Φ_Λ be an arbitrary state which defines a translation-invariant expectation values, i.e., $(\Phi_\Lambda, \tau_x(A)\Phi_\Lambda) = (\Phi_\Lambda, A\Phi_\Lambda)$ for any local operator A. Then for any local operator B, we have

$$\frac{1}{|\Omega|^2}(\Phi_\Lambda, B_\Omega^* B_\Omega \Phi_\Lambda) \geqslant \frac{1}{N^2}(\Phi_\Lambda, B_\Lambda^* B_\Lambda \Phi_\Lambda) \tag{C.2}$$

Although we only apply the inequality to ground states in the present paper, we note that it has a trivial extension to finite-temperature Gibbs states as follows. We note that the following result has been (implicitly) quoted in the introduction of our previous publication,[26] when we mentioned that the naive infinite-volume limit of the Gibbs states without symmetry breaking is not ergodic.

Lemma C.2. Let H_Λ be a translation-invariant Hamiltonian. Then for any local operator B, we have

$$\frac{1}{|\Omega|^2} Z(\beta)^{-1} \operatorname{Tr}(B_\Omega^* B_\Omega e^{-\beta H_\Lambda}) \geqslant \frac{1}{N^2} Z(\beta)^{-1} \operatorname{Tr}(B_\Lambda^* B_\Lambda e^{-\beta H_\Lambda}) \tag{C.3}$$

where the partition function is $Z(\beta) = \operatorname{Tr}[\exp(-\beta H_\Lambda)]$.

We now prove Lemma C.1. Let $\mathscr{P}_B$ be the projection operator onto the state $B_\Lambda \Phi_\Lambda / \|B_\Lambda \Phi_\Lambda\|$. If the state is vanishing, we set $\mathscr{P}_B = 0$. Since $1 - \mathscr{P}_B$ is nonnegative, we see that

$$\begin{aligned}(\Phi_\Lambda, B_\Omega^* B_\Omega \Phi_\Lambda) \geqslant (\Phi_\Lambda, B_\Omega^* \mathscr{P}_B B_\Omega \Phi_\Lambda) &= \frac{(\Phi_\Lambda, B_\Omega^* B_\Lambda \Phi_\Lambda)(\Phi_\Lambda, B_\Lambda^* B_\Omega \Phi_\Lambda)}{(\Phi_\Lambda, B_\Lambda^* B_\Lambda \Phi_\Lambda)} \\ &= \frac{|\Omega|^2}{N^2}(\Phi_\Lambda, B_\Lambda^* B_\Lambda \Phi_\Lambda)\end{aligned} \tag{C.4}$$

where we used the translation invariance and the periodic boundary conditions to get the final line. If $\mathscr{P}_B = 0$, the inequality is trivial since the final expression is vanishing. This proves the lemma.

In order to prove Lemma C.2, we let $\{\Phi^{(n)}\}$ be a complete basis where each basis state $\Phi^{(n)}$ is an eigenstate of H_Λ with the eigenvalue E_n and also defines translation-invariant expectation values. By using the bound (C.2), we get

$$\begin{aligned} Z(\beta)^{-1}\operatorname{Tr}(B_\Omega^* B_\Omega e^{-\beta H_\Lambda}) &= Z(\beta)^{-1}\sum_n (\Phi^{(n)}, B_\Omega^* B_\Omega \Phi^{(n)}) e^{-\beta E_n} \\ &\geqslant \frac{|\Omega|^2}{N^2} Z(\beta)^{-1}\sum_n (\Phi^{(n)}, B_\Lambda^* B_\Lambda \Phi^{(n)}) e^{-\beta E_n} \\ &= \frac{|\Omega|^2}{N^2} Z(\beta)^{-1}\operatorname{Tr}(B_\Lambda^* B_\Lambda e^{-\beta H_\Lambda}) \end{aligned} \tag{C.5}$$

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