Obscured Symmetry Breaking and Low-Lying States in Quantum Many-Body Systems

Tohru Koma

Hal Tasaki

Department of Physics
Gakushuin University
Mejiro, Toshima-ku, Tokyo 171
JAPAN

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. 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 energy per site converges to the ground state energy per site as the system size increases. When the system has a continuous symmetry, we prove that the number of independent low-lying eigenstates grows faster than any given small order of the system size. We show that a translation invariant low-lying state converges to a ground state in the infinite volume limit. We also construct infinite volume ground states with explicit symmetry breaking by taking linear combinations of the (finite-volume) ground state and the low-lying states, and then taking infinite volume limits. We conjecture these infinite volume ground states to be pure. Our general theorems do not only shed light on the nature of symmetry breaking in quantum many-body systems, but provide indispensable information for numerical approaches to these systems. We also discuss applications of our general results to a variety of interesting examples.

KEY WORDS: Symmetry breaking; long range order; finite systems; quantum fluctuation; ground states; low-lying states; pure states.

Contents

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 "classical" points of view. The present paper is devoted to one of such "quantum effects", 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 confusions in the field[1]. We have tried in the present paper not only to present our 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.

The "obscured symmetry breaking" 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 low-lying eigenstates whose energies per site converge to the ground state energy per site as the system size increases.

Although one might be tempted to interpret these low-lying eigenstates as counterparts of excited states in the infinite volume system, they are actually "parts" of the infinite volume ground states. In the infinite volume limit, the low-lying eigenstates and the unique ground state are linearly combined to form a set of *pure* ground states with explicit symmetry breaking.

When a continuous symmetry is broken, there are infinitely many *pure* 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 has been discussed mainly by practitioners of numerical exact diagonalization of quantum spin systems. (It is not easy to list up all the relevant references. See, for example, [17, 23, 8, 7, 28] and the references therein.) But rigorous information has been lacking except in the mean-field model [30, 16, 18]. See also [6] for 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 clarify the relation between the above mentioned two types of manifestations of an "obscured symmetry breaking". In short, our theorems show that, whenever one has a finite volume ground state which does not break symmetry but whose correlation function exhibits a certain long range order, one must also have low-lying

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

eigenstates. The simplest of such results (see Theorem 2.1 below) was proved by Horsch and von der Linden [14]. In general there is a low-lying eigenstate whose excitation energy per site is less than of order N^{-2}, where N is the number of sites in the lattice. Our new results deal with the cases where the long range order is related to a continuous $U(1)$ symmetry. We show that the number of independent low-lying eigenstates increases faster than any given small order of N as the system size N increases. This is the first rigorous (and explicit) demonstration that ever increasing numbers of low-lying states indeed exist. We show that any translation invariant low-lying state converges to a ground state in the infinite volume limit. We also construct infinite volume ground states with explicit symmetry breaking by taking suitable linear combinations of the low-lying states, and then taking infinite volume limits. We conjecture that these ground states are pure, *i.e.*, are physically natural ground states. We also discuss applications of our general results to some concrete examples of interest.

We believe that these results do 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 the 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. The examples include Heisenberg antiferromagnet, the Bose-Einstein condensation in hard core Bose gas on a lattice, the superconductivity in lattice electron models, and the Haldane gap problem in $S = 1$ quantum antiferromagnetic chain. An interesting observation in the application to the Bose gas is that, by following our general discussion in Section 2, we are naturally led to consider ground states which do not conserve the particle number. Sections 4 and 5 are devoted to the proofs of our theorems.

In the 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 a pure infinite volume ground state. In Appendix C, we prove lemmas which characterize the fluctuation 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, we briefly review the notions of ground states in an infinite system, of pure 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 $B \geq 0$, 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 $\Phi_\Lambda(B, B')$ be the normalized ground state of the Hamiltonian $H_\Lambda - B' O_\Lambda$, where O_Λ is the order operator

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

Define the order parameter by

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

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, 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.

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 breaks the up-down symmetry of the Hamiltonian.

When $B > 0$, we encounter "quantum fluctuation". An elementary application of the Perron-Frobenius theorem (as in [30]) implies that the ground state $\Phi_\Lambda(B)$ 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 $\Phi_\Lambda(B)$ 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 $(\Phi_\Lambda(B), S_x^{(3)} \, \Phi_\Lambda(B)) = 0$ for any $B > 0$, we expect (and can prove for sufficiently small B) that

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

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

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

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

holds as $L \uparrow \infty$ with a positive finite constant $\tau(B)$, where $E_\Lambda^{(0)}$ denotes the ground state energy. The sequence of states $\{\Phi_\Lambda^{(1)}(B)\}_\Lambda$ in this situation are typical examples of low-lying eigenstates[2].

The ground state $\Phi_\Lambda(B)$ 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

$$\Phi_\Lambda(B) \simeq \frac{1}{\sqrt{2}}\left(\tilde{\Phi}_\Lambda^+(B) + \tilde{\Phi}_\Lambda^-(B)\right), \tag{1.6}$$

and

$$\Phi_\Lambda^{(1)}(B) \simeq \frac{1}{\sqrt{2}}\left(\tilde{\Phi}_\Lambda^+(B) - \tilde{\Phi}_\Lambda^-(B)\right), \tag{1.7}$$

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.

We can now discuss how the low-lying eigenstates are related to the symmetry breaking in the infinite volume limit. A ground state in the infinite system may be defined by the thermodynamic limit

$$\omega_B(A) := \lim_{\Lambda\uparrow\mathbf{Z}^d} (\Phi_\Lambda(B), A\,\Phi_\Lambda(B)), \tag{1.8}$$

where A is an arbitrary local operator (*i.e.*, a polynomial of spin operators), and $\Phi_\Lambda(B)$ 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.) We shall define the ground state energy density as $\epsilon_0 := \omega_B(h_x)$. Here 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. Since the finite volume ground state $\Phi_\Lambda(B)$ respects the global up-down symmetry, so does the infinite volume ground state $\omega_B(\cdots)$. In particular we have

$$\omega_B(S_x^{(3)}) = 0, \tag{1.9}$$

for any x.

One might suspect from the above construction and the relation (1.9) that, when the symmetry breaking field B' is vanishing, there is no symmetry breaking even in the infinite volume limit[3]. ¿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[4]. It is indeed

[2] A beginner of 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.

[3] This is another possible confusion, to which we sometimes encounter.

[4] A typical example is antiferromagnetism, in which a staggered magnetic field plays the role of a 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!!

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 2.8) 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), (1.9), and Lemma C.1, we find that

$$\frac{1}{|\Omega|^2}\omega_B\left[(M_\Omega-\omega_B(M_\Omega))^2\right]\geq m(B)^2, \tag{1.10}$$

as $|\Omega|\uparrow\infty$. The relation (1.10) implies that, in the state $\omega_B(\cdots)$, the intensive bulk quantity $M_\Omega/|\Omega|$ has a finite fluctuation. This 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 a *pure* state[5]. It is believed that a physically realizable state in a large system can be well approximated by a pure state. The behavior (1.10) implies that the state $\omega_B(\cdots)$ is not pure, and is hence unphysical.

Then there must be some physically natural ground states. Equations (1.6) and (1.7) motivate us to define two states in the infinite system by

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

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

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

for any neighboring x and y, where $\epsilon_0=\omega_B(h_x)$ is the previously defined ground state energy density. Following Definition 2.8, we shall interpret the relation (1.12) as indicating that the states $\omega_B^{\pm}(\cdots)$ are infinite volume ground states[6]. We stress that this is a natural definition of ground states. In a bulk (or an infinite) system, it is no longer meaningful to talk about small difference 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 more about 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

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

[5]The notion of *pure* states in an infinite system is distinct from that in ordinary quantum mechanics. See Definition 2.9 and the remark following it.

[6]The existence of ground states other than $\omega_B(\cdots)$ apparently contradicts with 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 [30]) applies only to a finite system.

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 state $\omega_B^{\pm}(\cdots)$ are pure. See Theorem B.1. We conclude that $\omega_B^{\pm}(\cdots)$ constructed by taking linear combinations of $\Phi_\Lambda(B)$ 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 state.
- The infinite volume ground state defined by a naive infinite volume limit of finite volume ground states is not "pure", i.e., is unphysical.
- A pure ground state may be formed by taking a linear combination of the finite volume ground state and the low-lying 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.

Remark: The reader might wonder about the nature of the ground state $\Phi_\Lambda(B)$ and the first eigenstate $\Phi_\Lambda^{(1)}(B)$ when B is large enough to 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

$$\frac{1}{N}\left(E_\Lambda^{(1)} - E_\Lambda^{(0)}\right) \approx \frac{1}{N}, \tag{1.14}$$

as $N \uparrow \infty$. Although the state $\Phi_\Lambda^{(1)}(B)$ may be again called a low-lying eigenstate, its nature is totally different from that in the case with $m(B) > 0$.

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 the 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

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

with any α, β with $|\alpha|^2 + |\beta|^2 = 1$, defines exactly the same state as $\omega_B(\cdots)$ in (1.8). 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.

One may form a state distinct from $\omega_B(\cdots)$ by considering, e.g., the limit

$$\omega_B^{(x)}(\cdots) := \lim_{\Lambda\uparrow\mathbf{Z}^d}(\Phi_\Lambda^{(x)}(B), (\cdots)\,\Phi_\Lambda^{(x)}(B)), \tag{1.18}$$

but the resulting state is not translation invariant. We clearly see $\omega_B^{(x)}(h_x) > \epsilon_0$, and hence $\omega_B^{(x)}(\cdots)$ is not an infinite volume ground state. 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.

2.1 Theorem of Horsch and von der Linden

Before discussing our own results, we describe the theorem due to Horsch and von der Linden[14], which is the first rigorous result concerning the existence of a low-lying state in the presence of an obscured symmetry breaking.

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 $\mathcal{H}_x$. The full Hilbert space is

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

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 $\mathcal{H}_x$ be the corresponding finite dimensional Hilbert space.

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

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

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 $\mathcal{H}_\Lambda$. Let

$$O_\Lambda := \sum_{x\in\Lambda} o_x \tag{2.4}$$

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

Assume that $\|h_x\| \le h$ and $\|o_x\| \le o$ hold for any x with 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 $y \in \mathcal{S}_x$. The number of sites in the support set $\mathcal{S}_x$ 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

$$(\Phi_\Lambda, O_\Lambda \Phi_\Lambda) = 0, \tag{2.5}$$

and

$$(\Phi_\Lambda, (O_\Lambda)^2 \Phi_\Lambda) \ge (\mu o N)^2 \tag{2.6}$$

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

$$\Psi_\Lambda := \frac{O_\Lambda \Phi_\Lambda}{\|O_\Lambda \Phi_\Lambda\|}, \tag{2.7}$$

which is well-defined since $\|O_\Lambda \Phi_\Lambda\|$ is nonvanishing because of (2.6).

Then the theorem of Horsch and von der Linden is the following.

Theorem 2.1 *The expectation value of the energy in the state Ψ_Λ satisfies*

$$\frac{1}{N} |(\Psi_\Lambda, H_\Lambda \Psi_\Lambda) - E_\Lambda| \le c_0 \frac{1}{N^2} \tag{2.8}$$

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

$$\frac{1}{N}\left(E_\Lambda^{(1)} - E_\Lambda\right) \le c_0 \frac{1}{N^2}. \tag{2.9}$$

Proof: The first part follows by observing that

$$\begin{aligned} |(\Psi_\Lambda, H_\Lambda \Psi_\Lambda) - E_\Lambda| &= \frac{|(\Phi_\Lambda, [[O_\Lambda, H_\Lambda], O_\Lambda]\ \Phi_\Lambda)|}{2\,\|O_\Lambda \Phi_\Lambda\|^2} \\ &\le \frac{\|[[O_\Lambda, H_\Lambda], O_\Lambda]\|}{2\,\|O_\Lambda \Phi_\Lambda\|^2} \\ &\le \frac{4r^2 h o^2 N}{2(\mu o N)^2} = c_0 \frac{1}{N}, \end{aligned} \tag{2.10}$$

where we have used the assumed commutation relations and the norm bounds of h_x and o_x, as well as (2.6). To prove the second part, we note that the relation (2.5) implies that the state Ψ_Λ is orthogonal to the ground state Φ_Λ. Then the statement in the theorem is a simple consequence of the variational principle. ∎

2.2 Main theorems

Now we shall describe our extensions of the above theorem. Our theorems apply to a system with a continuous symmetry, and establish the existence of ever increasing numbers of low-lying eigenstates.

We again consider the finite lattice Λ with N sites, the Hilbert space $\mathcal{H}_\Lambda$ as in (2.1), and the Hamiltonian H_Λ as in (2.3). We further require that the system possesses a global $U(1)$ symmetry, whose generator is a self-adjoint operator C_Λ. We assume that

$$[H_\Lambda, C_\Lambda] = 0. \tag{2.11}$$

We introduce the order operators

$$O_\Lambda^{(\alpha)} := \sum_{x\in\Lambda} o_x^{(\alpha)}, \tag{2.12}$$

where $\alpha = 1, 2$, and each $o_x^{(\alpha)}$ is a self-adjoint operator on $\mathcal{H}_\Lambda$. 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

$$\left[O_\Lambda^{(1)}, C_\Lambda\right] = -iO_\Lambda^{(2)}, \quad \left[O_\Lambda^{(2)}, C_\Lambda\right] = iO_\Lambda^{(1)}. \tag{2.13}$$

We also introduce

$$O_\Lambda^{\pm} := O_\Lambda^{(1)} \pm iO_\Lambda^{(2)}, \tag{2.14}$$

which satisfy the commutation relations

$$\left[O_\Lambda^{+}, C_\Lambda\right] = -O_\Lambda^{+}, \quad \left[O_\Lambda^{-}, C_\Lambda\right] = O_\Lambda^{-}. \tag{2.15}$$

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 $y \in \mathcal{S}_x$. The number of sites in the support set $\mathcal{S}_x \subset \Lambda$ is bounded from above by an integer $r \geq 2$.

iii) There are finite constants h and o, and we have $\|h_x\| \leq h$ and $\|o_x^{(\alpha)}\| \leq o$ 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 a ground state of H_Λ. We assume that

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

$$(\Phi_\Lambda, (O_\Lambda^{(1)})^2\, \Phi_\Lambda) = (\Phi_\Lambda, (O_\Lambda^{(2)})^2\, \Phi_\Lambda) \geq (\mu o N)^2 \tag{2.16}$$

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

¿From the commutation relations (2.15) and the fact that Φ_Λ is an eigenstate of C_Λ, we automatically have

$$(\Phi_\Lambda, O_\Lambda^{(1)}\,\Phi_\Lambda) = (\Phi_\Lambda, O_\Lambda^{(2)}\,\Phi_\Lambda) = 0. \tag{2.17}$$

In other words, the state Φ_Λ have vanishing order parameters. The relations (2.16) and (2.17) together imply that the state Φ_Λ exhibits an "obscured symmetry breaking"[7].

For a nonvanishing integer M, we consider the state

$$\Psi_\Lambda^{(M)} := \frac{(O_\Lambda^+)^M \Phi_\Lambda}{\left\|(O_\Lambda^+)^M \Phi_\Lambda\right\|}, \tag{2.18}$$

where we set $(O_\Lambda^+)^M = (O_\Lambda^-)^{-M}$ for a negative M. Although the state (2.18) 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.

Theorem 2.2 *When the assumptions i)-iv) are valid, and we further have*

$$N \geq \left(\frac{4r}{\mu}\right)^2, \tag{2.19}$$

and

$$\frac{|M|}{N} \leq \frac{\mu^2}{8r}, \tag{2.20}$$

the state $\Psi_\Lambda^{(M)}$ of (2.18) is well-defined. The expectation value of the energy in the state satisfies

$$\frac{1}{N}\left|(\Psi_\Lambda^{(M)}, H_\Lambda \Psi_\Lambda^{(M)}) - E_\Lambda\right| \leq c_1 \frac{|M|}{N}, \tag{2.21}$$

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

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

$$\left[O_\Lambda^{(1)}, O_\Lambda^{(2)}\right] = i\gamma C_\Lambda, \tag{2.22}$$

where γ is a real constant.

In other words, we assume that the vector $(\gamma^{-1/2} O_\Lambda^{(1)}, \gamma^{-1/2} O_\Lambda^{(2)}, C_\Lambda)$ form 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.

[7]In fact (2.16) and (2.17) 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 (2.16) and (2.17) are valid with a Λ-independent $\mu > 0$.

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 2.3 *When the assumptions i)-vi) are valid, and we further have*

$$\frac{M^2}{N} \le c_2, \tag{2.23}$$

with $c_2 = \min\{\mu^2/(192r), o\mu/\sqrt{24\gamma}\}$, *the state* $\Psi_\Lambda^{(M)}$ *of (2.18) is well-defined. The expectation value of the energy in the state satisfies*

$$\frac{1}{N}\left|(\Psi_\Lambda^{(M)}, H_\Lambda \Psi_\Lambda^{(M)}) - E_\Lambda\right| \le c_3 \left(\frac{M}{N}\right)^2, \tag{2.24}$$

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

The theorem will be proved in Section 5.

Remarks: 1. Theorem 2.3 provides better bound for the energy difference than Theorem 2.2. Theorem 2.2, on the other hand, covers much wider range of low-lying states. We believe each theorem is optimal in each aspect. We still do not know how to prove the optimal theorem which interpolates between the two theorems.

2. The condition vi) for Theorem 2.3 can be weakened to $C_\Lambda \Phi_\Lambda = 0$ if one replaces the definition of the trial state (2.18) by

$$\Psi_\Lambda^{(M)} := \frac{(O_\Lambda^+)^M \Phi_\Lambda + (O_\Lambda^-)^M \Phi_\Lambda}{\left\|(O_\Lambda^+)^M \Phi_\Lambda + (O_\Lambda^-)^M \Phi_\Lambda\right\|}. \tag{2.25}$$

2.3 Low-lying states

We shall discuss the implications of the above theorems on the problem of low-lying states in a sequence of finite systems. The results for low-lying eigenstates have direct relevance to numerical exact diagonalization approaches to quantum many-body systems.

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, the generator C_Λ, the order operators $(O_\Lambda^{(1)}, O_\Lambda^{(2)})$, and the ground state Φ_Λ. The corresponding eigenvalue of H_Λ is denoted as $E_\Lambda^{(0)}$ (instead of E_Λ) since it is the ground state energy.

Let us now state precisely what we mean by low-lying states and low-lying eigenstates in general.

Definition 2.4 *A sequence of normalized states* $\{\Phi'_\Lambda\}_\Lambda$ *are called low-lying states, if*

$$\lim_{\Lambda\uparrow\mathbf{Z}^d} \frac{1}{N}\left((\Phi'_\Lambda, H_\Lambda\, \Phi'_\Lambda) - E_\Lambda^{(0)}\right) = 0 \tag{2.26}$$

holds, and if each Φ'_Λ *is orthogonal to the ground state* Φ_Λ. *Low-lying states in which each state* Φ'_Λ *happens to be an eigenstate of the Hamiltonian* H_Λ *are called low-lying eigenstates.*

We assume that the sequence of models and the ground states satisfy the assumptions i)-iv) of the previous subsection with constants h, o, r, and μ independent of Λ, or the assumptions i)-vi) with these constants and γ independent of Λ. Then Theorems 2.2 or 2.3 establish that $\{\Psi_\Lambda^{(M)}\}_\Lambda$, constructed as (2.18), with a fixed M form low-lying states.

By combining this observation with the variational argument, we get rigorous control of low-lying eigenstates as follows.

Corollary 2.5 *Suppose that the sequence of models satisfy the assumptions i)-iv) with constants h, o, r, and μ independent of Λ. Fix a lattice Λ whose number of sites N satisfies the bound (2.19). For each nonvanishing integer M which satisfies the bound (2.20), one can find an eigenstate $\Phi_\Lambda^{(M)}$ of the Hamiltonian H_Λ. The state $\Phi_\Lambda^{(M)}$ is orthogonal to the ground state Φ_Λ, 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*

$$\frac{1}{N}(E_\Lambda^{(M)} - E_\Lambda^{(0)}) \le c_1 \frac{M}{N}, \tag{2.27}$$

where c_1 is independent of Λ.

Proof: Since the ground state Φ_Λ is an eigenstate of C_Λ, the commutation relations (2.15) imply that the variational states $\Psi_\Lambda^{(M)}$ are orthogonal to the ground 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 2.2. ∎

The above theorem establishes that the number of low-lying eigenstates increases faster than any given small order of N. As far as we know, this is the first time that the existence of ever increasing numbers of low-lying eigenstates is proved.

We get a similar result from Theorem 2.3.

Corollary 2.6 *Suppose that the sequence of models satisfy the assumptions i)-vi) with constants h, o, r, μ, and γ independent of Λ. Fix a lattice Λ with N sites. For each nonvanishing integer M which satisfies the bound (2.23), one can find an eigenstate $\Phi_\Lambda^{(M)}$ of the Hamiltonian H_Λ. The state $\Phi_\Lambda^{(M)}$ is orthogonal to the ground state Φ_Λ, 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*

$$\frac{1}{N}(E_\Lambda^{(M)} - E_\Lambda^{(0)}) \le c_2 \left(\frac{M}{N}\right)^2, \tag{2.28}$$

where c_2 is independent of Λ.

Proof: The same as the above. ∎

We note that the low-lying eigenstates discussed here have nothing to do with the Nambu-Goldstone excitations. The finite-size counterparts of the Nambu-Goldstone excitations should also have complicated structures, since the (infinite volume) ground states themselves are reorganized into low-lying states in a finite system (as we shall see in Section 2.5).

2.4 States with explicit symmetry breaking

Here we restrict ourselves to models with $U(1) \times \mathbf{Z}_2$ symmetry, and discuss the implications of Theorems 2.2 and 2.3 on the problem of symmetry breaking. We shall see explicitly that, by forming linear combinations of the ground state and the low-lying states $\Psi_\Lambda^{(M)}$, we get states which break the $U(1)$ symmetry explicitly. The results discussed here is based on theorems by Koma and Tasaki [25].

Let us consider a sequence of models which satisfy the conditions i)-vi). For a positive integer k, consider the state

$$\Xi_\Lambda^{(k)} := \frac{1}{\sqrt{2k+1}} \left\{ \Phi_\Lambda + \sum_{M=1}^{k} \left(\Psi_\Lambda^{(M)} + \Psi_\Lambda^{(-M)} \right) \right\}, \tag{2.29}$$

where Λ is taken sufficiently large so that the bounds (2.19), (2.23) are valid for any M with $|M| \le k$. By using Theorem 2.2 or 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

$$\lim_{\Lambda \uparrow \mathbf{Z}^d} \frac{1}{N} \left\{ (\Xi_\Lambda^{(k)}, H_\Lambda \, \Xi_\Lambda^{(k)}) - E_\Lambda \right\} = 0, \tag{2.30}$$

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

A remarkable properties of these low-lying states are the following.

Theorem 2.7 *The expectation value of the order operators in the state $\Xi_\Lambda^{(k)}$ satisfy*

$$(\Xi_\Lambda^{(k)}, O_\Lambda^{(2)} \, \Xi_\Lambda^{(k)}) = 0, \tag{2.31}$$

and

$$\lim_{k \uparrow \infty} \lim_{\Lambda \uparrow \mathbf{Z}^d} \frac{1}{N} (\Xi_\Lambda^{(k)}, O_\Lambda^{(1)} \, \Xi_\Lambda^{(k)}) \ge \sqrt{2} \mu o, \tag{2.32}$$

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: The relation (2.31) follows by symmetry. The relation (2.32) is essentially proved in [25]. One only has to combine (7.26) of [25] and Theorem 6.1 of [25]. respectively. ■

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 different directions.

2.5 Infinite volume ground states

Finally we shall discuss the relation between the low-lying states in the sequence of finite systems and the infinite volume ground states. We again observe that the naive infinite volume limit of the finite volume ground states is not a pure state (hence is unphysical) when there is an obscured symmetry breaking. By forming a linear combination of the (finite-volume) ground state and the low-lying states, and then taking an in finite volume limit, we get an infinite volume ground state with explicit symmetry breaking, which state we conjecture to be pure.

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 assume that the Hamiltonian (2.3) and the order operators (2.12) 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 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 $\bigotimes_{x\in\mathcal{S}(A)}\mathcal{H}_x$ with a finite support set $\mathcal{S}(A)$). Let $\rho_\Lambda(\cdots) = \mathrm{Tr}_{\mathcal{H}_\Lambda}[(\cdots)\widetilde{\rho}_\Lambda]$ be a state of the system on Λ, where $\widetilde{\rho}_\Lambda$ is an arbitrary density matrix on $\mathcal{H}_\Lambda$. Given a sequence of (finite-volume) states $\{\rho_\Lambda(\cdots)\}_\Lambda$, we (formally) define

$$\rho(A) := \lim_{\Lambda\uparrow\mathbf{Z}^d} \rho_\Lambda(A) \tag{2.33}$$

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 (2.33) 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 [39].)

We want to describe what we mean by a ground state 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 possibly 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 mathematical literature. It simply says that a ground state should minimize the local energy.

Definition 2.8 *We define the ground state energy density ϵ_0 by*

$$\epsilon_0 := \lim_{\Lambda\uparrow\mathbf{Z}^d} \inf_{\Phi_\Lambda\in\mathcal{H}_\Lambda} \frac{1}{N}(\Phi_\Lambda, H_\Lambda\,\Phi_\Lambda), \tag{2.34}$$

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

$$\omega(h_x) = \epsilon_0, \tag{2.35}$$

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

We also introduce the precise notion of *pure* states in an infinite system. We shall follow a physically natural definition which can be found in Ruelle's textbook [40]. In short it says that a state in which any intensive bulk quantity shows essentially no fluctuation is pure. 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 pure in the following sense. See also the remark at the end of the present section for the limitation of the definition.

Definition 2.9 *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. A translation invariant state $\rho(\cdots)$ is said to be* pure *if, for any A, the intensive bulk quantity $A_\Omega/|\Omega|$ exhibits vanishing fluctuation in the sense that*

$$\lim_{|\Omega|\uparrow\infty} \frac{1}{|\Omega|^2}\rho\left[(A_\Omega - \rho(A_\Omega))^2\right] = 0. \tag{2.36}$$

For each finite Λ, let Φ_Λ be a ground state of H_Λ. We can assume Φ_Λ is translation invariant. Then it is easy to verify that the infinite volume state defined by

$$\omega(A) := \lim_{\Lambda\uparrow\mathbf{Z}^d} (\Phi_\Lambda, A\,\Phi_\Lambda), \tag{2.37}$$

for any local operator A (by taking a suitable subsequence), is indeed an infinite-volume ground state in the sense of Definition 2.8.

Assume that each finite volume ground state Φ_Λ exhibits an obscured symmetry breaking in the sense that it satisfies (2.16) and (2.17). Then by using Lemma C.1, we can show that

$$\frac{1}{|\Omega|^2}\omega\left((O_\Omega^{(\alpha)} - \omega(O_\Omega^{(\alpha)}))^2\right) \geq (\mu o)^2, \tag{2.38}$$

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 a pure state, and is hence unphysical.

We still do not know how to construct a pure ground state in general. In Appendix B, however, we present a general construction of a pure infinite volume ground state in a model 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 the similar construction as in Appendix B might work in models 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 2.10 *Let $\{\Phi'_\Lambda\}_\Lambda$ be low-lying states, 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*

$$\omega'(\cdots) := \lim_{\Lambda\uparrow\mathbf{Z}^d} (\Phi'_\Lambda, (\cdots)\,\Phi'_\Lambda), \tag{2.39}$$

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

Proof: The translation invariance implies

$$(\Phi'_\Lambda, H_\Lambda\,\Phi'_\Lambda) = N(\Phi'_\Lambda, h_x\,\Phi'_\Lambda), \tag{2.40}$$

for any $x \in \Lambda$. Then the condition (2.26) of low-lying states reads

$$\lim_{\Lambda\uparrow\mathbf{Z}^d} \{(\Phi'_\Lambda, h_x\,\Phi'_\Lambda) - (\Phi_\Lambda, h_x\,\Phi_\Lambda)\} = 0, \tag{2.41}$$

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 (2.29), and its $U(1)$ rotations are low-lying states with translation invariant expectation values. Therefore Theorem 2.10 implies that the limiting infinite volume states

$$\omega_\theta(\cdots) := \lim_{k\uparrow\infty} \lim_{\Lambda\uparrow\mathbf{Z}^d} (e^{i\theta C_\Lambda}\,\Xi_\Lambda^{(k)}, (\cdots)\, e^{i\theta C_\Lambda}\,\Xi_\Lambda^{(k)}), \tag{2.42}$$

defined by taking suitable subsequences, are ground states. Theorem 2.7, on the other hand, implies that

$$\omega_\theta\left[o_x^{(1)}\right] = m\cos\theta, \quad \omega_\theta\left[o_x^{(2)}\right] = m\sin\theta, \tag{2.43}$$

for any x, where $m \ge \sqrt{2}o\mu$ (or $m \ge \sqrt{3}o\mu$ if the system has an $SU(2)$ symmetry). The states $\omega_\theta(\cdots)$ are infinite volume ground states that explicitly shows a symmetry breaking.

It is believed that, in a system where a $U(1)$ symmetry is spontaneously broken, the non-pure ground state $\omega(\cdots)$ (defined in (2.37)) is decomposed as

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

where $\omega_\theta^{\mathrm{pure}}(\cdots)$ is a pure ground state which satisfies (2.43) with m replaced with some m_{pure}. Assuming the decomposition (2.44), we see, for sufficiently large hypercubic region Ω, that

$$\frac{1}{|\Omega|^2}\omega((O_\Omega^{(1)})^2) \simeq \frac{1}{2\pi}\int_0^\theta d\theta\,(m_{\mathrm{pure}}\cos\theta)^2 = \frac{(m_{\mathrm{pure}})^2}{2}, \tag{2.45}$$

where we have used that $\omega_\theta^{\mathrm{pure}}(\cdots)$ is pure.

Define the long range order parameter $\tilde{\mu} \ge 0$ for the state $\omega(\cdots)$ by

$$(\tilde{\mu}o)^2 = \frac{1}{|\Omega|^2}\lim_{\Lambda\uparrow\mathbf{Z}^d}\omega((O_\Omega^{(1)})^2). \tag{2.46}$$

Then (2.45) implies the relation $m_{\mathrm{pure}} = \sqrt{2}o\tilde{\mu}$.

Let us assume that the above $\tilde{\mu}$ is equal to the largest μ which satisfies (2.16) for sufficiently large N. (Unfortunately we can only prove the one-side bound $\tilde{\mu} \ge \mu$ in general. See Lemma C.1.) Then the relation $m_{\mathrm{pure}} = \sqrt{2}o\tilde{\mu}$ and the inequality $m \ge \sqrt{2}o\mu$ reduces to the bound $m \ge m_{\mathrm{pure}}$. Since the translation invariant pure ground states are believed to have the largest order parameter among all the ground states, this suggests that we indeed have $m = m_{\mathrm{pure}}$. This motivates us to further conjecture that the states $\omega_\theta(\cdots)$ are nothing but the desired *pure* ground states $\omega_\theta^{\mathrm{pure}}(\cdots)$. (It is trivial to extend the present discussion to the case with a general symmetry group.) Unfortunately we have no direct evidences which support the conjecture.

Remark: 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. (The two notions, of course, are closely related, especially if one concentrates on the geometry of the space of all the states.)

¿From Definition 2.9, one finds, among other things, that pure states can be also characterized as $\mathbf{Z}^d$-ergodic states (see sections 6.3 and 6.5 of [40]), and that a non-pure translation invariant state can be uniquely expressed as an "integral" over pure states (see section 6.4 of [40]).

A disadvantage in the above definition is that one has to a priori assume the correct invariance of the states in order to get a physically natural pure states. See [9, 40] for the notion of pure states which does not rely on any invariance.

3 Examples

In this section, we shall 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 shall 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 Φ_Λ is expected to exhibit an "obscured symmetry breaking" in the sense that the relations $(\Phi_\Lambda, O_\Lambda\,\Phi_\Lambda) = 0$ and $(\Phi_\Lambda, (O_\Lambda)^2\,\Phi_\Lambda) \geq (m(B)N)^2$ 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 2.1) ensures that there exists a low-lying eigenstate whose excitation energy per site is bounded from above by a constant times N^{-2}. Note that the theorem does not reproduce the expected exponential decay (1.5) of the energy difference.

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

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

where $0 \leq \lambda \leq 1$, and the sum is over the sites y neighboring to x. When L is finite, the ground state Φ_Λ of the Hamiltonian (3.1) is rigorously known [31, 30, 3] to be unique and satisfies

$$C_\Lambda \Phi_\Lambda = 0, \tag{3.2}$$

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

For $\alpha = 1, 2$, we define the order operators (2.12) by the local order operators

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

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, 15, 20, 21, 26, 27, 36, 37, 38] that, for any $d \geq 2$ and $0 \leq \lambda \leq 1$, the ground state Φ_Λ exhibits a Néel-type long range order. We expect that the condition (2.16) is valid with $\mu > 0$ (where μ depends on d and λ). On the other hand, the absence of explicit symmetry breaking as in (2.17) 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 (2.16), we can apply our low-lying states theorems. The model has a desired $U(1) \times \mathbf{Z}_2$ symmetry. We can use Theorems 2.2 and 2.3 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 2.3, and conclude that the number of independent low-lying eigenstates increases faster than any given small order of N. For the $SU(2)$ invariant Heisenberg antiferromagnet with $\lambda = 1$ in (3.1), Momoi [33] recently succeeded in improving the present result.

In order to apply the general results in Section 2.5, we need an 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 the 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 form (presumably pure) ground states with explicit symmetry breaking as in (2.42).

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 $0 \leq \lambda \leq 1$, where y is summed over nearest neighbor sites of x, has been attracting considerable interest. (See [8, 7, 28] 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 $C_\Lambda = \sum_x S_x^{(3)}$, and Theorems 2.2 and 2.3 are applicable.

3.3 Bose-Einstein condensation in hard core Bose gas on lattice

We shall give a brief discussion on the Bose-Einstein condensation problem. It turns out that, by following the general discussions given in the previous section, 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 $d \geq 2$. 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 [32]. Based on the equivalence and an extension of the infrared bound method of Dyson, Lieb and Simon [10], it was proved by Kennedy, Lieb and Shastry [21], and by Kubo and Kishi [27] that the present model exhibits a Bose-Einstein condensation in the following sense. Let Φ_Λ be the unique ground state of the Hamiltonian (3.6) with the particle number equal to $N = L^d/2$. Define the order operators (2.12) by

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

where $\mathcal{P}$ 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 [21, 27] is that the condition of the long range order (2.16) holds with a finite μ. On the other hand the absence of explicit symmetry breaking as in (2.17) 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 2.2 and 2.3 to this situation. For this, we replace the Hamiltonian (3.6) with $\mathcal{P} h_x \mathcal{P}$. 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.

The general discussions in Section 2 implies that one has low-lying states in the sectors with different particle numbers, and the (candidate of) pure infinite volume ground state $\omega_\theta(\cdots)$ is constructed as in (2.42). The corresponding low-lying state (2.29), in this situation, becomes

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

A remarkable feature of the (presumably pure) ground state $\omega_\theta(\cdots)$ is that it is constructed by summing up the states with different particle numbers as in (3.8). We further find from (2.43) that the state has nonvanishing expectation values of the creation and annihilation operators, for example, as

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

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 certain mean-field theory. We have seen that such states arise naturally if one tries to consider pure 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 discussions.

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. It is clear that the definition of infinite volume ground states employed in Section 2.5 is sensitive to the value of the "chemical potential" ν, once we relax the constraint of the particle number conservation. Better definitions in the present situation are those of $\mathcal{G}_1$ or $\mathcal{G}_2$ in Appendix A, with allowed perturbations (local operators A in the former, and maps T in the latter) restricted only to those preserve the particle number. This definition is clearly independent of the value of ν. To prove that $\omega_\theta(\cdots)$ 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 Section 2.5 or $\mathcal{G}_3$) 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 deal 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 interested readers. We shall 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

$$N_{\mathrm{e}} = \sum_x n_{x\uparrow} + n_{x\downarrow}, \tag{3.10}$$

where $n_{x\sigma} = c_{x\sigma}^* c_{x\sigma}$. A typical example is the so-called Hubbard model. (See, for example, [29, 34].)

A class of Hubbard models with attractive interactions are believed to exhibit superconductivity in their ground states. 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-$T_{\rm c}$ superconductivity, but as a new type of collective phenomena in strongly interacting electron systems.

A standard superconducting phase can be characterized by a condensation of certain electron pairs, which manifests itself as a long range order in electron pairing correlation function. For example the condensation of singlet pairs can be measured as a long range order (2.16) with respect to the order operators defined by

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

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

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 2.2 with $C_\Lambda = (N_{\rm e} - N)/2$, where N denotes the number of sites in Λ. The theorem states that the existence of an electron pair condensation inevitably leads to the appearance of low-lying eigenstates whose number increase faster than any given small order of the system size N. Except for half-filled models with special Hamiltonians, the models do not have a $U(1)\times\mathbf{Z}_2$ symmetry necessary to apply Theorem 2.3.

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 non-overlapping 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".

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

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

We again set $C_\Lambda = (N_{\rm e} - N)/2$, and apply Theorem 2.2 to control low-lying states.

Although there are no nontrivial electron system in which the existence of a superconducting phase is proved, we believe our results have potential usefulness, for example, in future numerical works.

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 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 $\{1, 2, \ldots, N\}$. 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

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

where λ and D are parameters.

Haldane [13] 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 [3].) Haldane's prediction was that the gapful 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 [11], and perturbations to the dimerized VBS model [22]. The ref. [11] contains a general treatment of the VBS-type models, and the $S = 1$ model mentioned here is one of the examples. The $S = 1$ model of [11] and their method of constructing the ground state (but not the proof of the existence of a gap) were rediscovered by other authors [24].

The ground state in the Haldane phase is disordered in the sense that the spin-spin correlation functions decay exponentially. Den Nijs and Rommelse [35] 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

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

If we denote the unique normalized ground state for finite Λ with N sites as Φ_Λ, we expect to have

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

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 [35, 41]. 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

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

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

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

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

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

¿From the difference of parities, we find that the four states $\Phi_\Lambda, \Psi_\Lambda^{(1)}, \Psi_\Lambda^{(2)}$, 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 2.1) 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 have been observed in exact solutions [2], in numerical simulations [19] and in actual experiments in impurity doped samples [12]. The existence of the Kennedy triplet is characteristic in the 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, and there are no low-lying states.

Fundamental connection between the hidden order (3.17) and the existence of the low-lying triplet was discussed by Kennedy and Tasaki [22] from the view point 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[8].

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 non-local nature of the order operators. See [2, 19, 22] for more details.

4 Proof of first theorem

In the present section, we prove Theorem 2.2 for $M > 0$. Throughout the proof, we drop the subscript Λ from $O_\Lambda^\pm, H_\Lambda, E_\Lambda, \Phi_\Lambda, \Psi_\Lambda^{(M)}$, etc. Our goal is to bound the quantity

$$\begin{aligned} \Delta^{(M)} &:= \frac{1}{N}\left\{(\Psi^{(M)}, H\,\Psi^{(M)}) - E\right\} \\ &= \frac{(\Phi, (O^-)^M H (O^+)^M\,\Phi) - (\Phi, (O^-)^M (O^+)^M H\,\Phi)}{N(\Phi, (O^-)^M (O^+)^M\,\Phi)} \end{aligned}$$

[8] That the existence of a string 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.

$$= \sum_{x\in\Lambda} \frac{(\Phi, (O^-)^M [h_x, (O^+)^M]\,\Phi)}{N(\Phi, (O^-)^M (O^+)^M\,\Phi)}. \tag{4.1}$$

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

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

with

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

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

Roughly speaking, Q_x is the main part of the operator O^+, and is expected to behave almost similarly to O^+. This is the basic idea of the present proof. The following lemma makes the idea into a precise estimate.

Lemma 4.1 *Suppose that the conditions (2.19) and (2.20) for N and M are satisfied. Then for $k = 1, 2, \ldots, M$, we have*

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

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

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

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

$$\begin{aligned} |(\Phi, A^* BC\,\Phi)| &\le \sqrt{(\Phi, A^*A\,\Phi)(\Phi, C^*B^*BC\,\Phi)} \\ &\le \|B\| \sqrt{(\Phi, A^*A\,\Phi)(\Phi, C^*C\,\Phi)}, \end{aligned} \tag{4.7}$$

for general operators A, B, and C.

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

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

where we have used the bounds (4.4) and (2.20).

Again using (4.5), we get

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

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

$$\begin{aligned}
&\left|\frac{(\Phi,(O^-)^M(O^+)^M\,\Phi)}{(\Phi,(Q_x^*)^M(Q_x)^M\,\Phi)}\right| \\
\ge\;& 1-{\sum_{k,\ell}}'\binom{M}{k}\binom{M}{\ell}(2ro)^{k+\ell}\frac{\sqrt{(\Phi,(Q_x^*)^{M-k}(Q_x)^{M-k}\,\Phi)(\Phi,(Q_x^*)^{M-\ell}(Q_x)^{M-\ell}\,\Phi)}}{(\Phi,(Q_x^*)^M(Q_x)^M\,\Phi)} \\
\ge\;& 1-\left\{\left(1+\frac{2r}{\mu N}\right)^{2M}-1\right\} \\
\ge\;& 2-e^{\mu/2}.
\end{aligned} \tag{4.10}$$

Note that, since $0\le\mu\le1$, we have $2-e^{\mu/2}\ge 2-\sqrt{e}>0$.

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

$$\left|\Delta^{(M)}\right| \le 16rh\frac{e^{\mu/2}-e^{\mu/4}}{\mu^2(2-e^{\mu/2})}\frac{M}{N} = c_1\frac{M}{N}. \tag{4.11}$$

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

$$\frac{a_m}{a_{m-1}} \geq (\mu o N)^2. \tag{4.12}$$

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

$$\begin{aligned} a_1 &= (\Phi, (O^- - R_x^*)(O^+ - R_x)\, \Phi) \\ &\geq (\Phi, O^- O^+ \Phi) - 2(2o)^2 r N \\ &= \frac{1}{2}\left\{(\Phi, O^- O^+ \Phi) + (\Phi, O^+ O^- \Phi) + (\Phi, [O^-, O^+]\, \Phi)\right\} - 8o^2 r N \\ &\geq (\Phi, (O^{(1)})^2\, \Phi) + (\Phi, (O^{(2)})^2\, \Phi) - 2o^2(1+4r^2)N, \end{aligned} \tag{4.13}$$

where we have used i), ii), iii) to bound the norm of the commutators.

By substituting the assumption (2.16) on the existence of a long range order, and the bound (2.19) for N, we get

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

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

Next we use the Schwartz inequality to get

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

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

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

The rest of the proof is easy. Assume that, for a fixed m, $a_{m'} \neq 0$ for all $m' < m \leq M$. Then by summing up (4.16) and using the bounds (4.14), (2.20) and $r \leq 2$, we see that

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

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 shall prove Theorem 2.3. 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*

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

Proof: By using the Schwartz inequality we get

$$(\Phi, (O^{(1)})^{2m-2}\,\Phi)^2 = (\Phi, (O^{(1)})^m (O^{(1)})^{m-2}\,\Phi)^2 \leq (\Phi, (O^{(1)})^{2m}\,\Phi)(\Phi, (O^{(1)})^{2m-4}\,\Phi), \tag{5.3}$$

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

$$\frac{(\Phi, (O^{(1)})^{2(m-1)}\,\Phi)}{(\Phi, (O^{(1)})^{2m}\,\Phi)} \leq \frac{(\Phi, (O^{(1)})^{2(m-2)}\,\Phi)}{(\Phi, (O^{(1)})^{2(m-1)}\,\Phi)} \leq \cdots \leq \frac{1}{(\Phi, (O^{(1)})^2\,\Phi)} \leq \frac{1}{(\mu o N)^2}, \tag{5.4}$$

where we used (2.16). We also note that the definition (2.2) implies

$$(\Phi, (O^{(1)})^{2m}\,\Phi) \leq \left\| O^{(1)} \right\|^2 (\Phi, (O^{(1)})^{2(m-1)}\,\Phi) \leq (oN)^2 (\Phi, (O^{(1)})^{2(m-1)}\,\Phi). \tag{5.5}$$

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). ■

One of the main ingredients in the proof is the following Lemma 5.2, which allows us to approximate expectation values including $O^{\pm}$ with those including the self-adjoint operator $O^{(1)}$. 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 $y \notin \mathcal{S}_x$, and $\|a_x\| \leq a$ with a finite constant a for any x. The support set $\mathcal{S}_x$ 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*

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

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 $0\le k\le K+L$, we have

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

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

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

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

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

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

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

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 form (2.22)), we find that $\Delta^{(M)}$ can be written in terms of a double commutator as follows.

$$\begin{aligned}
&2N\left\|\Psi^{(M)}\right\|^2\Delta^{(M)}\\
=\;&2(\Phi,(O^-)^M H(O^+)^M\,\Phi)-2E(\Phi,(O^-)^M(O^+)^M\,\Phi)\\
=\;&(\Phi,(O^-)^M H(O^+)^M\,\Phi)+(\Phi,(O^+)^M H(O^-)^M\,\Phi)\\
&-(\Phi,(O^-)^M(O^+)^M H\,\Phi)-(\Phi,H(O^+)^M(O^-)^M\,\Phi)\\
=\;&(\Phi,[(O^-)^M,[H,(O^+)^M]]\,\Phi)\\
=\;&\sum_{m=0}^{M-1}(\Phi,[(O^-)^M,(O^+)^m[H,O^+](O^+)^{M-m-1}]\,\Phi)
\end{aligned}$$

$$
\begin{aligned}
= & \sum_{m=1}^{M-1}\sum_{\ell=0}^{M-1}\sum_{n=0}^{m-1} \\
& (\Phi,(O^-)^\ell(O^+)^n[O^-,O^+](O^+)^{m-n-1}[H,O^+](O^+)^{M-m-1}(O^-)^{M-\ell-1}\,\Phi) \\
+ & \sum_{m=0}^{M-1}\sum_{\ell=0}^{M-1} \\
& (\Phi,(O^-)^\ell(O^+)^m[O^-,[H,O^+]](O^+)^{M-m-1}(O^-)^{M-\ell-1}\,\Phi) \\
+ & \sum_{m=0}^{M-2}\sum_{\ell=0}^{M-1}\sum_{n=0}^{M-m-2} \\
& (\Phi,(O^-)^\ell(O^+)^m[H,O^+](O^+)^n[O^-,O^+](O^+)^{M-m-n-2}(O^-)^{M-\ell-1}\,\Phi). \qquad (5.13)
\end{aligned}
$$

Note that the symmetry vi), along with the relation $UCU^{-1}=-C$ (which follows from (2.13) and (2.22)), 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

$$
\begin{aligned}
& \left|2N\left\|\Psi^{(M)}\right\|^2\Delta^{(M)}\right| \\
\le & \sum_{m=1}^{M-1}\sum_{\ell=0}^{M-1}\sum_{n=0}^{m-1} \\
& 2\gamma M\left|(\Phi,(O^-)^\ell(O^+)^{m-1}[H,O^+](O^+)^{M-m-1}(O^-)^{M-\ell-1}\,\Phi)\right| \\
+ & \sum_{m=0}^{M-1}\sum_{\ell=0}^{M-1} \\
& \left|(\Phi,(O^-)^\ell(O^+)^m[O^-,[H,O^+]](O^+)^{M-m-1}(O^-)^{M-\ell-1}\,\Phi)\right| \\
+ & \sum_{m=0}^{M-2}\sum_{\ell=0}^{M-1}\sum_{n=0}^{M-m-2} \\
& 2\gamma M\left|(\Phi,(O^-)^\ell(O^+)^m[H,O^+](O^-)^{M-m-2}(O^-)^{M-\ell-1}\,\Phi)\right| \\
\le & 6\gamma M^4\delta([H,O^+];M-2,M-1)+3M^2\delta([O^-,[H,O^+]];M-1,M-1), \qquad (5.14)
\end{aligned}
$$

where we have used (5.10). The use of Lemma 5.2 is justified since M satisfies (2.23) which (with $K+L\le 2M$) guarantees the condition (5.7).

By using (5.11) and then the bound (5.2), we get

$$
\begin{aligned}
& \left|2N\left\|\Psi^{(M)}\right\|^2\Delta^{(M)}\right| \\
\le\ & 3\gamma M^4(4rohN)(2oN)b_{M-2}+\frac{3}{2}M^2(16r^2o^2hN)b_{M-1} \\
\le\ & \left\{\frac{24\gamma rh}{o^2\mu^4}\frac{M^4}{N^2}+\frac{24r^2h}{\mu^2}\frac{M^2}{N}\right\}b_M. \qquad (5.15)
\end{aligned}
$$

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

$$
\left\|\Psi^{(M)}\right\|^2=(\Phi,(O^-)^M(O^+)^M\,\Phi)\ge\frac{1}{2}b_M. \qquad (5.16)
$$

By combining (5.15) and (5.16), and substituting the assumed bound (2.23), we finally get

$$\begin{aligned}\left|\Delta^{(M)}\right| &\leq \frac{24r^2h}{\mu^2}\left\{1+\frac{\gamma}{o^2\mu^2 r}\frac{M^2}{N}\right\}\left(\frac{M}{N}\right)^2 \\ &\leq c_3\left(\frac{M}{N}\right)^2, \qquad (5.17)\end{aligned}$$

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

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 $\{\sigma_i\}_{i=1,\ldots,K+L}$, $\{\tau\}_{i=1,\ldots,K+L}$ 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 $0 \leq k, \ell \leq K+L$, we have*

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

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

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

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

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

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

$$\left|(\Phi, \left(\prod_{i=1}^{k} O^{\sigma_i}\right) A \left(\prod_{i=k+1}^{K+L} O^{\sigma_i}\right)\Phi) - \frac{2^{2J}(J!)^2}{(2J)!}(\Phi, (O^{(1)})^J A (O^+)^{K-L}(O^{(1)})^J\,\Phi)\right|$$

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

where we have used (5.18).

To prove (5.10), we simply substitute the estimate

$$
\begin{aligned}
&\left|\frac{2^{2J}(J!)^2}{(2J)!}(\Phi, (O^{(1)})^J A (O^+)^{K-L} (O^{(1)})^J \Phi)\right| \\
&\le \left\|A(O^+)^{K-L}\right\| \frac{2^{2J}(J!)^2}{(2J)!}(\Phi, (O^{(1)})^{2J} \Phi) \le 2\delta(A;K,L),
\end{aligned} \tag{5.22}
$$

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 $K \ge L$ (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 $A \ne 1$. We denote by D the left-hand side of (5.18), and bound it as

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

The quantity D_1 in (5.23) can be bounded as

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

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 $[O^{\pm},A]=\sum_{x\in\Lambda}[\sum_{y\in\mathcal{S}_x} o^{\pm}_y, a_x]$, and note that $\left\|[\sum_{y\in\mathcal{S}_x} o^{\pm}_y, a_x]\right\|\le 4rao$. When $\sigma_j=+1$, we get

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

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

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

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

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

$$D_1\le (K+L)\frac{3}{2}(4raoN)(2oN)^{K-L+1}b_{L-1}. \qquad (5.27)$$

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

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

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 (2.22), and $C\Phi=0$, we can further bound D_2 as

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

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

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

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

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

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 readers to have them included in the present paper.

We start by briefly reviewing basic setups in operator algebraic approach to quantum systems with infinitely many degrees of freedom [9, 40]. For simplicity we shall 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 $\mathcal{H}_x$ which is assumed to be identical to $\mathcal{H}_o$ 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

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

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

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

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 $\mathcal{A}$ into a Banach space.

A state $\rho(\cdots)$ is a linear map from $\mathcal{A}$ to $\mathbf{C}$ which satisfies $\rho(1) = 1$, and $\rho(A^*A) \ge 0$ for any $A \in \mathcal{A}$. It can be shown [9] that it automatically holds that $|\rho(A)| \le \|A\|$, and $\rho(A^*) = \rho(A)^*$. We denote by $\mathcal{E}$ the set of all states on $\mathcal{A}$. Since $\mathcal{E}$ is the unit sphere of the dual space $\mathcal{A}^*$, the Banach-Alaoglu theorem [39] implies that $\mathcal{E}$ is compact in the weak-$*$ topology.

The compactness provides us with a useful way of constructing states on $\mathcal{A}$. 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 [42, 40] as $i \uparrow \infty$. For each i we take a state (density matrix) $\rho_i(\cdots)$ on the algebra $\mathcal{A}_{\Omega_i}$. Since $\rho_i(\cdots)$ can be naturally regarded as an element of $\mathcal{E}$ (by defining, for example, $\rho(A) = 0$ for $A \in \mathcal{A}\backslash\mathcal{A}_{\Omega_i}$), 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 $A \in \mathcal{A}$.

As in Section 2, we let h_o be the local Hamiltonian at the origin $o \in \mathbf{Z}^d$, which acts on the finite dimensional Hilbert space $\bigotimes_{x\in\mathcal{S}_o} \mathcal{H}_x$ with the support set $\mathcal{S}_o$ 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

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

Here we introduced

$$\overline{\Omega} := \{x \;\big|\; \mathcal{S}_x \cap \Omega \neq \emptyset\}, \tag{A.7}$$

where $\mathcal{S}_x = \tau_x(\mathcal{S}_o)$ 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 [4].) The definition is useful because of its similarity to "classical" definitions of ground states. It is

$$\mathcal{G}_2 := \{\omega \in \mathcal{E} \;\big|\; \omega(H_{\overline{\Omega}}) \le \omega(T(H_{\overline{\Omega}})) \quad \text{for any } T \in \mathcal{P}_\Omega, \text{ and for any finite } \Omega \subset \mathbf{Z}^d\}, \tag{A.8}$$

where $\mathcal{P}_\Omega$ is the set of all local perturbations on Ω. A local perturbation T on Ω is a linear mapping $T : \mathcal{A} \to \mathcal{A}$ which satisfies $T(A) \ge 0$ for any $A \ge 0$, and $T(A) = A$ for any $A \in \mathcal{A}_{\Omega^c}$, where $\mathcal{A}_{\Omega^c} := \overline{\bigcup_{\Omega'} \mathcal{A}_{\Omega'\backslash\Omega}}$ is the operator algebra 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 [2].) It is

$$\mathcal{G}_3 := \{\omega \in \mathcal{E} \;\big|\; \omega(h_x) = \epsilon_0 \quad \text{for any } x \in \mathbf{Z}^d\}, \tag{A.9}$$

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 $\mathcal{A}_\Lambda$ by imposing periodic boundary conditions. Note that a Hamiltonian with periodic boundary conditions is simply denoted as H_Λ except in the present Appendix. Then we define ϵ_0 by

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

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 $\widehat{\mathcal{G}}_i$ the set of $\omega \in \mathcal{G}_i$ which is translation invariant, *i.e.*, $\omega(\tau_x(A)) = \omega(A)$ for any $A \in \mathcal{A}$ 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 $\mathcal{G}_1 = \mathcal{G}_2$.*

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

To prove $\mathcal{G}_1 \subset \mathcal{G}_2$, we note that the above mentioned theorem in [9] says that $\omega \in \mathcal{G}_1$ if and only if

$$\omega(H_{\overline{\Omega}}) \le \omega'(H_{\overline{\Omega}}), \tag{A.12}$$

for any $\omega' \in \mathcal{E}$ such that $\omega(B) = \omega'(B)$ for all $B \in \mathcal{A}_{\Omega^c}$, 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 $\mathcal{G}_2$, we see that $\omega \in \mathcal{G}_2$.

To prove $\mathcal{G}_2 \subset \mathcal{G}_1$, we can follow the part (1) $\Rightarrow$ (2) of the proof of the above mentioned theorem in [9] without any modifications. ■

Next we note that

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

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

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

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

Let ℓ be an integer such that $\overline{\Omega}$ is contained in a suitable d-dimensional $\ell\times\cdots\times\ell$ hypercubic lattice Λ_0. For an integer n, let Λ be the d-dimensional $(n\ell)\times\cdots\times(n\ell)$ 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 $\mathcal{A}_\Lambda$. We further define

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

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

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

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

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

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

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

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

$$(n\ell)^{-d} \omega'_\Lambda(H_\Lambda^{\text{p.b.c.}}) - \epsilon_0 \leq -\ell^{-d}\varepsilon + \beta (n\ell)^{-1}, \tag{A.19}$$

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

It should be noted that we do not have $\mathcal{G}_1 = \mathcal{G}_2 = \mathcal{G}_3$. For example, a state with a single domain wall in the Ising model belongs to $\mathcal{G}_1 = \mathcal{G}_2$ but not to $\mathcal{G}_3$. 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* $\widehat{\mathcal{G}}_1 = \widehat{\mathcal{G}}_2 = \widehat{\mathcal{G}}_3$.

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

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

where $\mathcal{E}_{\text{inv}}$ is the set of translation invariant states in $\mathcal{E}$. We only have to show that $\epsilon_0 = \widetilde{\epsilon}_0$, and this may be done in several ways. Here we offer a simple constructive proof. For each Λ, we can take a ground state $\Phi_\Lambda \in \mathcal{H}_\Lambda$ of the Hamiltonian $H_\Lambda^{\text{p.b.c.}}$, which state is invariant under translations that take into account the periodic boundary conditions imposed on Λ. Define a state $\omega \in \mathcal{E}$ by the (weak-$*$) limiting procedure (2.37). By construction, we see that $\omega \in \widehat{\mathcal{G}}_1$. The above mentioned theorem of [9] then implies that $\omega(h_x) = \widetilde{\epsilon}_0$. 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 $\mathcal{H}_o$, and its lowest eigenvalue is simple. The perturbation p_o is an arbitrary self-adjoint operator on $\bigotimes_{x\in\mathcal{S}_o}\mathcal{H}_x$, and δ is a constant. By using a rigorous perturbation technique, the following was proved in [22].

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 $|\delta| \le \delta_0$, the set of ground states $\widehat{\mathcal{G}}_1 = \widehat{\mathcal{G}}_2 = \widehat{\mathcal{G}}_3$ 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 $h_o = S_o^{(1)}$.

B Pure 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 a *pure* infinite volume ground state.

As far as we know this is the first rigorous and general result which explicitly tells one how to construct a pure 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[9]. 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 2.1, but with additional assumption on the translation invariance. The translation invariance is by no means essential in proving the main theorem, but the 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 Section 2.1. The Hilbert space is constructed as in (2.1), the Hamiltonian as (2.3), and the order operator as (2.4). 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

[9] Even in the 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.

$\mathcal{H}_x$. 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

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

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

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

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

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 [14]

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

and its linear combination with the ground state

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

which was first considered by Kaplan, Horsch, and von der Linden [17]. ¿From a straightforward calculation using the definitions (B.5), (B.6), and the assumed (B.2), (B.3), and (B.4), we find [17] that the above state (B.6) exhibits a symmetry breaking as

$$\begin{aligned}
(\Xi_\Lambda, O_\Lambda\, \Xi_\Lambda) &= \frac{1}{2} \left\{ (\Phi_\Lambda^{(0)}, O_\Lambda\, \Phi_\Lambda^{(0)}) + \frac{2(\Phi_\Lambda^{(0)}, (O_\Lambda)^2\, \Phi_\Lambda^{(0)})}{\left\| O_\Lambda \Phi_\Lambda^{(0)} \right\|} + \frac{(\Phi_\Lambda^{(0)}, (O_\Lambda)^3\, \Phi_\Lambda^{(0)})}{\left\| O_\Lambda \Phi_\Lambda^{(0)} \right\|^2} \right\} \\
&= \sqrt{(\Phi_\Lambda^{(0)}, (O_\Lambda)^2\, \Phi_\Lambda^{(0)})} \geq \mu o N.
\end{aligned} \tag{B.7}$$

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*

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

for any local operator A.

¿From the Definition 2.9 of pure 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 a pure 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*

$$\begin{aligned}
&\left|(\Phi^{(i)}, BC\,\Phi^{(j)}) - \sum_{k=0,1} (\Phi^{(i)}, B\,\Phi^{(k)})(\Phi^{(k)}, C\,\Phi^{(j)})\right| \\
= &\left|(\Phi^{(i)}, B\mathcal{P}C\,\Phi^{(j)})\right| \\
\le &\frac{\sqrt{\|[B,[H,B]]\|\,\|[C,[H,C]]\|}}{2E_{\mathrm{G}}},
\end{aligned} \tag{B.11}$$

where $\mathcal{P}$ 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 $\mathcal{P} \le (H - E_i)/E_{\mathrm{G}}$ for $i = 0, 1$. By using the Schwartz inequality, we have

$$\begin{aligned}
&\left|(\Phi^{(i)}, B\mathcal{P}C\,\Phi^{(j)})\right|^2 \\
\le &(\Phi^{(i)}, B\mathcal{P}B\,\Phi^{(i)})(\Phi^{(j)}, C\mathcal{P}C\,\Phi^{(j)}) \\
\le &(\Phi^{(i)}, B\frac{H-E_i}{E_{\mathrm{G}}}B\,\Phi^{(i)})(\Phi^{(j)}, C\frac{H-E_i}{E_{\mathrm{G}}}C\,\Phi^{(j)}) \\
= &(2E_{\mathrm{G}})^{-2}(\Phi^{(i)}, [B,[H,B]]\,\Phi^{(i)})(\Phi^{(j)}, [C,[H,C]]\,\Phi^{(j)}) \\
\le &(2E_{\mathrm{G}})^{-2}\,\|[B,[H,B]]\|\,\|[C,[H,C]]\|,
\end{aligned} \tag{B.12}$$

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*

$$\left\|\Phi^{(1)} - \Psi\right\|^2 \le \frac{4hr^2}{E_{\mathrm{G}}\mu^2}\frac{1}{N} \tag{B.13}$$

holds.

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

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

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

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

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

$$\left|\left\{(\Xi,(A_\Omega)^2\,\Xi)-(\Xi,A_\Omega\,\Xi)^2\right\}-\left\{(\Xi',(A_\Omega)^2\,\Xi')-(\Xi',A_\Omega\,\Xi')^2\right\}\right|\le\frac{a_1\,\|A\|^2}{\sqrt{N}}|\Omega|^2.\tag{B.18}$$

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

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

The remaining term R can be further rewritten as

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

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

$$
\begin{aligned}
&\left|(\Xi',(A_\Omega)^2\,\Xi')-(\Xi',A_\Omega\,\Xi')^2\right|\\
\le\ & \frac{1}{2}\left|(\Phi^{(1)},A_\Omega\,\Phi^{(0)})(\Phi^{(0)},A_\Omega\,\Phi^{(1)})-(\Phi^{(1)},A_\Omega\,\Phi^{(0)})^2\right|\\
+\ & \frac{1}{4}(\Phi^{(1)},A_\Omega\,\Phi^{(1)})^2\\
+\ & \frac{1}{E_{\mathrm{G}}}\left\|[A_\Omega,[H,A_\Omega]]\right\|. \qquad\qquad \text{(B.21)}
\end{aligned}
$$

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

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

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

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

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

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

$$
\begin{aligned}
&\left|(\Phi^{(0)}, OA_\Omega O\,\Phi^{(0)})\right| \le \left|(\Phi^{(0)}, O^2 A_\Omega\,\Phi^{(0)})\right| + \left|(\Phi^{(0)}, O[A_\Omega, O]\,\Phi^{(0)})\right| \\
&\le \left|(\Phi^{(0)}, O^2\,\Phi^{(1)})(\Phi^{(1)}, A_\Omega\,\Phi^{(0)})\right| + \frac{\sqrt{\|[O^2,[H,O^2]]\|\,\|[A_\Omega,[H,A_\Omega]]\|}}{2E_{\mathrm{G}}} + \|O[A_\Omega, O]\| \\
&\le \left|(\Phi^{(0)}, O^2\,\Phi^{(1)})\,\|A_\Omega\|\right| + \frac{\sqrt{16o^4h^2rN^3 \times 4\,\|A\|^2\,hrr'^2|\Omega|}}{2E_{\mathrm{G}}} + \|A\|\,o^2r'|\Omega|N. \qquad \text{(B.24)}
\end{aligned}
$$

We further use (B.13) to see

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

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

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

where c is an N-independent constant.

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

$$
\frac{1}{|\Omega|^2}\left|(\Xi, (A_\Omega)^2\,\Xi) - (\Xi, A_\Omega\,\Xi)^2\right| \le \frac{4\,\|A\|^2\,hrr'^2}{E_{\mathrm{G}}}\frac{1}{|\Omega|} + O(N^{-1/2}). \qquad \text{(B.27)}
$$

C Lower bound for fluctuation of bulk quantities

In the present Appendix, we prove simple lemmas which characterize the behavior of 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 pure.

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

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

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*

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

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) assumed in our previous publication [25], when we mentioned that the naive infinite volume limit of the Gibbs states without symmetry breaking is not pure.

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

$$\frac{1}{|\Omega|^2} Z(\beta)^{-1} \mathrm{Tr}\left[B_\Omega^* B_\Omega e^{-\beta H_\Lambda}\right] \geq \frac{1}{N^2} Z(\beta)^{-1} \mathrm{Tr}\left[B_\Lambda^* B_\Lambda e^{-\beta H_\Lambda}\right], \tag{C.3}$$

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

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

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

where we used the translation invariance and the periodic boundary conditions to get the final line. If $\mathcal{P}_B = 0$, 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

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

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