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Quantum Griffiths inequalities

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Abstract

We present a general framework of Griffiths inequalities for quantum systems. Our approach is based on operator inequalities associated with self-dual cones and provides a consistent viewpoint of the Griffiths inequality. As examples, we discuss the quantum Ising model, quantum rotor model, Bose–Hubbard model, and Hubbard model. We present a model-independent structure that governs the correlation inequalities.

1 Introduction

Ever since its formulation by Lenz [29], the Ising model has been the most fundamental model to illustrate the phenomenon of phase transitions. Let Λ be a finite subset of \mathbb{Z}^d . The system's Hamiltonian is given by the function

$$H_{\Lambda}(\sigma) = -\sum_{x,y\in\Lambda} J_{xy}\sigma_x\sigma_y \tag{1.1}$$

for each $\sigma = \{\sigma_x\}_{x \in \Lambda} \in \{-1, +1\}^{\Lambda}$. J_{xy} is a non-negative coupling constant. The expectation value of the function $f : \{-1, +1\}^{\Lambda} \to \mathbb{R}$ is

$$\langle f \rangle_{\beta} = \sum_{\sigma \in \{-1,+1\}^{\Lambda}} f(\sigma) e^{-\beta H_{\Lambda}(\sigma)} / Z_{\beta},$$
 (1.2)

where Z_{β} is the normalization constant $Z_{\beta} = \sum_{\sigma \in \{-1,+1\}^{\Lambda}} e^{-\beta H_{\Lambda}(\sigma)}$. In [23], Griffiths discovered the following famous inequalities¹:

• First Griffiths inequality:

$$\langle \sigma_A \rangle_\beta \ge 0 \tag{1.3}$$

for each $A \subseteq \Lambda$, where $\sigma_A = \prod_{x \in A} \sigma_x$.

• Second Griffiths inequality:

$$\langle \sigma_A \sigma_B \rangle_\beta \ge \langle \sigma_A \rangle_\beta \langle \sigma_B \rangle_\beta$$
 (1.4)

for each $A, B \subseteq \Lambda$.

¹To be precise, this general formulation was established by Kelly and Sherman [32].

Since Griffiths' discovery, a large number of rigorous studies on the Ising ferromagnets has been successfully undertaken by applying his inequalities. The fact that Griffiths inequalities are so useful indicates that they express the essence of correlations in the Ising system. Therefore, it is natural to ask whether similar inequalities hold true for other models. Studying this problem means trying to seek a model-independent or universal property of the notion of correlations. Griffiths inequalities already hold true for some classical models, e.g., the plane rotor model. This suggests that our problem is certainly meaningful. Ginibre took the first important step toward providing a general framework for Griffiths inequalities [20]. However, we know of only a few concrete examples of quantum (i.e., noncommutative) models that satisfy Griffiths inequalities [8, 10, 19, 36, 52]. Our goals here are as follows:

- (a) To present a general method for constructing Griffiths inequalities for classical and quantum systems.
- (b) According to (a), to highlight a universal property of correlations.

To this end, we advance the technique of operator inequalities associated with self-dual cones.

We already know that the quantum Ising and rotor models satisfy Griffiths inequalities. Thus, these two models can be regarded as role models for our purpose. A standard approach to proving the Griffiths inequality for these systems is to reduce the *d*-dimensional quantum systems to the corresponding d + 1-dimensional classical systems using the Trotter–Kato product formula [4, 9, 10, 36]. However, since known proofs of the quantum Griffiths inequalities rely on the results of classical systems, it is difficult to extend these proofs to quantum models that cannot be reduced to classical ones. Considering this situation, we take the following steps:

- (i) We prove the Griffiths inequality for the quantum Ising and rotor models using a method of operator inequalities and understand common mathematical structures underlying both models.
- (ii) We seek similar structures in other models from our viewpoint of operator inequalities and construct the Griffiths inequality by analogy.

By carrying out these steps, we construct quantum Griffiths inequalities for the Bose– Hubbard and Hubbard models. We note that the proposed method can be applied to many other models, e.g., the Su–Schrieffer–Heeger (SSH) model, Holstein–Hubbard model, and Fröhlich model². Although we present a few concrete applications of our results here, we expect these inequalities to play important roles in statistical physics just as the original Griffiths inequalities did for the Ising system. We also remark that some of results in this paper can be proved by probabilisitc approaches, e.g., random walk representations. However, we believe that the proposed method can be applicable to a wider class of quantum models and clarify new aspects of the quantum Griffiths inequality. Finally, we emphasize the following: from the viewpoint of operator inequalities, we can find a common mathematical structure from among the several models mentioned above. This universal structure enables us to construct the Griffiths inequality for each model. From this fact, we expect to obtain a model-independent

 $^{^{2}}$ The problem of the quantum Heisenberg model is still open.

or general expression of the notion of correlation from our viewpoint, see Section 8 for details.

This paper is organized as follows. In Section 2, we introduce a useful operator inequality induced by self-dual cones. Using this, we develop a general theory of the Griffiths inequality for quantum systems. In the following sections, we will demonstrate how our operator inequalities are effective for the study of correlation functions for quantum models.

In Section 3, we reformulate reflection positivity from the viewpoint of our operator inequalities. We then describe how we construct the Griffiths inequality using reflection positivity. This construction and the one in Section 2 are complementary to each other.

In Sections 4 and 5, we discuss the quantum Ising and rotor models, respectively. These sections provide not only something of a warm-up but also important clues for finding a common structure underlying the Griffiths inequality. Readers can learn how to use the operator inequalities through these sections as well.

Sections 6 and 7 are devoted to advanced applications of the abstract theory established in Sections 2 and 3. We construct the Griffiths inequality for the Bose–Hubbard model (Section 6), and Hubbard model (Section 7). We emphasize that our constructions are natural modifications and extensions of the methods discussed in Sections 4 and 5.

In Section 8, we present concluding remarks. In Appendix A, we collect useful propositions concerning our operator inequalities. These propositions will be used repeatedly in this study.

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2 General theory

2.1 First inequality

Let $(\mathfrak{H}, \langle \cdot | \cdot \rangle)$ be a complex Hilbert space and \mathfrak{P} be a convex cone in \mathfrak{H} . The dual cone \mathfrak{P}^{\dagger} of \mathfrak{P} is defined as

$$\mathfrak{P}^{\dagger} = \left\{ x \in \mathfrak{H} \, \big| \, \langle x | y \rangle \ge 0 \, \forall y \in \mathfrak{P} \right\}.$$

$$(2.1)$$

We say that \mathfrak{P} is *self-dual* if

$$\mathfrak{P} = \mathfrak{P}^{\dagger}.\tag{2.2}$$

Henceforth, we always assume that \mathfrak{P} is self-dual. Each element x in \mathfrak{P} is called positive w.r.t. \mathfrak{P} and written as $x \ge 0$ w.r.t. \mathfrak{P} .

Definition 2.1 Let $\mathscr{B}(\mathfrak{H})$ be the set of all bounded linear operators on \mathfrak{H} . Let $A \in \mathscr{B}(\mathfrak{H})$. If $Ax \geq 0$ w.r.t. \mathfrak{P} for all $x \in \mathfrak{P}$, then we say that A preserves the positivity w.r.t. \mathfrak{P} and write³

$$A \trianglerighteq 0$$
 w.r.t. \mathfrak{P} .

³This symbol was introduced by Miura [42]. Bratteli, Kishimoto and Robinson studied the commutative cases in [7, 35].

Note that

$$A \ge 0 \quad \text{w.r.t.} \quad \mathfrak{P} \Longrightarrow \langle x | Ay \rangle \ge 0 \quad \forall x, y \in \mathfrak{P}. \quad \diamondsuit$$

$$(2.3)$$

The following proposition is often useful.

Proposition 2.2 [42] We have the following:

- (i) If $A \ge 0, B \ge 0$ w.r.t. \mathfrak{P} and $\alpha \ge 0, \beta \ge 0$, then $\alpha A + \beta B \ge 0$ w.r.t. \mathfrak{P} .
- (ii) If $A \ge 0$ and $B \ge 0$ w.r.t. \mathfrak{P} , then $AB \ge 0$ w.r.t. \mathfrak{P} .

Our first setting is as follows.

(A) There exists a complete orthonormal system (CONS) $\{e_n\}_{n\in\mathbb{N}}$ of \mathfrak{H} such that $e_n\in\mathfrak{P}$ for all $n\in\mathbb{N}$.

The system's Hamiltonian is denoted by H. H is self-adjoint and bounded from below. To state the first quantum (i.e., noncommutative) Griffiths inequality, we need the following conditions:

(**H.** 1) $e^{-\beta H} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$.

For each $A \in \mathscr{B}(\mathfrak{H})$, the thermal expectation value of A is defined as

$$\langle A \rangle_{\beta} = \operatorname{Tr} \left[A \, \mathrm{e}^{-\beta H} \right] / Z_{\beta}, \quad Z_{\beta} = \operatorname{Tr} \left[\mathrm{e}^{-\beta H} \right].$$
 (2.4)

Remark 2.3 In this section, we always assume that $e^{-\beta H}$ is in the trace class for all $\beta > 0$. \diamondsuit

Theorem 2.4 is a prototype of the Griffiths inequality.

Theorem 2.4 Assume (A) and (H. 1). If $A \succeq 0$ w.r.t. \mathfrak{P} , then $\langle A \rangle_{\beta} \geq 0$ for all $\beta \geq 0$.

Proof. By our assumptions and Proposition 2.2, we have $A e^{-\beta H} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$. Thus, applying Proposition A.1, we conclude Theorem 2.4. \Box

To discuss the case where $\beta = \infty$, we assume that

(A') H has a unique ground state, i.e., dim ker(H - E) = 1, where $E = \inf \operatorname{spec}(H)$.

Under this condition, we can define the ground state expectation value as

$$\langle A \rangle_{\infty} = \langle \psi | A \psi \rangle, \quad A \in \mathscr{B}(\mathfrak{H}),$$

$$(2.5)$$

where ψ is the unique ground state of H such that $\|\psi\| = 1$.

Theorem 2.5 Assume (A') and (H. 1). If $A \ge 0$ w.r.t. \mathfrak{P} , then $\langle A \rangle_{\infty} \ge 0$.

Proof. By Proposition A.6, we can choose ψ as $\psi \ge 0$ w.r.t. \mathfrak{P} . Thus, this theorem immediately follows from (2.3). \Box

Remark 2.6 If we assume that $e^{-\beta H}$ improves the positivity w.r.t. \mathfrak{P} for all $\beta > 0$, then the ground state of H is automatically unique, see 8.4 for details. \diamond

Theorem 2.7 is a generalization of Theorem 2.4.

Theorem 2.7 Assume (A) and (H. 1). Let $A(s) = e^{-sH}Ae^{sH}$. If $A_j \ge 0$ w.r.t. \mathfrak{P} for all $j = 1, \ldots, n$, we then have

$$\left\langle \prod_{j=1}^{n} A_j(s_j) \right\rangle_{\beta} \ge 0 \tag{2.6}$$

for all $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n < \beta$, where $\prod_{j=1}^n O_j = O_1 O_2 \cdots O_n$, the ordered product.

Proof. Let $S = \left[\prod_{j=1}^{n} A_j(s_j)\right] e^{-\beta H}$. By our assumptions, we see that $S = \underbrace{e^{-s_1 H}}_{\rhd 0} \underbrace{A_1}_{\rhd 0} \underbrace{e^{-(s_2 - s_1)H}}_{\rhd 0} \cdots \underbrace{A_n}_{\rhd 0} \underbrace{e^{-(\beta - s_n)H}}_{\rhd 0} \ge 0 \quad \text{w.r.t.} \mathfrak{P}.$ (2.7)

Thus, by Proposition A.1, we obtain (2.6). \Box

Theorem 2.8 Assume (A') and (H. 1). Then (2.6) holds true at $\beta = \infty$.

2.2 Second inequality

We consider the extended Hilbert space $\mathfrak{H}_{ext} = \mathfrak{H} \otimes \mathfrak{H}$. Let \mathfrak{P}_{ext} be a self-dual cone in $\mathfrak{H} \otimes \mathfrak{H}$. Instead of (A), we assume the following:

(B) There exists a CONS $\{E_n\}_{n\in\mathbb{N}}$ of \mathfrak{H}_{ext} such that $E_n \in \mathfrak{P}_{ext}$ for all $n \in \mathbb{N}$.

To state Theorem 2.9, the following condition is assumed:

(H. 2) Let $H_{\text{ext}} = H \otimes \mathbb{1} + \mathbb{1} \otimes H$. Then there exists a unitary operator \mathscr{U} such that $\mathscr{U}^* e^{-\beta H_{\text{ext}}} \mathscr{U} \succeq 0$ w.r.t. $\mathfrak{P}_{\text{ext}}$ for all $\beta \ge 0$.

There are several ways to state the second quantum Griffiths inequality. First, we give the following formulation.

Theorem 2.9 Assume (B) and (H. 2). Let $A, B, C, D \in \mathscr{B}(\mathfrak{H})$ and $A(s) = e^{-sH}Ae^{sH}$. Assume the following:

- (i) $\mathscr{U}^*A \otimes C\mathscr{U} \geq 0$ w.r.t. $\mathfrak{P}_{\text{ext}}$.
- (ii) $\mathscr{U}^*(B \otimes D D \otimes B) \mathscr{U} \geq 0$ w.r.t. $\mathfrak{P}_{\text{ext}}$.

Then we have

$$\langle A(s)B(t)\rangle_{\beta}\langle C(s)D(t)\rangle_{\beta} - \langle A(s)D(t)\rangle_{\beta}\langle C(s)B(t)\rangle_{\beta} \ge 0$$
 (2.8)

for all $0 \le s \le t < \beta$. In addition, assume (A) and (H. 1). If $A \ge 0, B \ge 0, C \ge 0$ and $D \ge 0$ w.r.t. \mathfrak{P} , we obtain

$$\langle A(s)B(t)\rangle_{\beta} \ge 0, \quad \langle C(s)D(t)\rangle_{\beta} \ge 0, \quad \langle A(s)D(t)\rangle_{\beta} \ge 0, \quad \langle C(s)B(t)\rangle_{\beta} \ge 0$$
 (2.9)

for all $0 \leq s \leq t < \beta$.

Proof. Let

$$\langle\!\langle X \rangle\!\rangle_{\beta} = \operatorname{Tr} \left[X \,\mathrm{e}^{-\beta H_{\mathrm{ext}}} \right] \Big/ Z_{\beta}^2.$$
 (2.10)

Then we can derive (2.8) from the following:

$$\left\langle\!\!\left\langle A(s) \otimes C(s) \left(B(t) \otimes D(t) - D(t) \otimes B(t) \right) \right\rangle\!\!\right\rangle_{\beta} \ge 0.$$
(2.11)

But this follows immediately from Proposition A.1 and the fact that

$$\mathscr{U}^* A(s) \otimes C(s) \Big(B(t) \otimes D(t) - D(t) \otimes B(t) \Big) e^{-\beta H_{\text{ext}}} \mathscr{U}$$
$$= \mathscr{U}^* e^{-sH_{\text{ext}}} A \otimes C e^{-(t-s)H_{\text{ext}}} \Big(B \otimes D - D \otimes B \Big) e^{-(\beta-t)H_{\text{ext}}} \mathscr{U} \succeq 0$$
(2.12)

w.r.t. $\mathfrak{P}_{\text{ext}}$ for all $0 \leq s \leq t < \beta$.

By (H. 1), it follows that $e^{-sH}Ae^{-(t-s)H}Be^{-(\beta-t)H} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$. Thus, by Proposition A.1, we obtain that $\langle A(s)B(t)\rangle_{\beta} \ge 0$ for all $\beta \ge 0$. \Box

Theorem 2.10 If we replace (A) and (B) by (A') in Theorem 2.9, then (2.8) and (2.9) hold true at $\beta = \infty$.

Proof. Since H has a unique ground state ψ , H_{ext} has a unique ground state $\psi \otimes \psi$ as well. By **(H. 2)** and Proposition A.6, it follows that $\Phi = \mathscr{U}^* \psi \otimes \psi \ge 0$ w.r.t. $\mathfrak{P}_{\text{ext}}$. Thus, by (2.3),

$$\left\langle \left\langle e^{-sH_{\text{ext}}}A \otimes Ce^{-(t-s)H_{\text{ext}}}(B \otimes D - D \otimes B)e^{tH_{\text{ext}}}\right\rangle \right\rangle_{\infty}$$
$$=e^{2(t-s)E} \left\langle \underbrace{\Phi}_{\geq 0} \middle| \underbrace{\mathscr{U}^*A \otimes Ce^{-(t-s)H_{\text{ext}}}(B \otimes D - D \otimes B)\mathscr{U}}_{\geq 0} \underbrace{\Phi}_{\geq 0} \right\rangle \geq 0, \qquad (2.13)$$

where $\langle\!\langle X \rangle\!\rangle_{\infty} = \langle \psi \otimes \psi | X \psi \otimes \psi \rangle$. This completes the proof. \Box

We introduce the Duhamel two-point function,

$$(A,B)_{\beta} = Z_{\beta}^{-1} \int_{0}^{1} \operatorname{Tr} \left[A \, \mathrm{e}^{-x\beta H} B \, \mathrm{e}^{-(1-x)\beta H} \right] dx, \quad A,B \in \mathscr{B}(\mathfrak{H}).$$
(2.14)

Corollary 2.11 Assume (B) and (H. 2). Let $A, B \in \mathscr{B}(\mathfrak{H})$. Assume the following:

- (i) $\mathscr{U}^*A \otimes \mathbb{1}\mathscr{U} \succeq 0 \ w.r.t. \ \mathfrak{P}_{ext}.$
- (ii) $\mathscr{U}^*(B \otimes \mathbb{1} \mathbb{1} \otimes B) \mathscr{U} \geq 0 \ w.r.t. \ \mathfrak{P}_{ext}.$

Then we have

$$(A,B)_{\beta} - \langle A \rangle_{\beta} \langle B \rangle_{\beta} \ge 0, \tag{2.15}$$

$$\langle AB \rangle_{\beta} - \langle A \rangle_{\beta} \langle B \rangle_{\beta} \ge 0.$$
 (2.16)

In addition, assume (A) and (H. 1). If $A \ge 0$ and $B \ge 0$ w.r.t. \mathfrak{P} , we obtain

$$(A, B)_{\beta} \ge 0, \quad \langle AB \rangle_{\beta} \ge 0, \quad \langle A \rangle_{\beta} \ge 0, \quad \langle B \rangle_{\beta} \ge 0.$$
 (2.17)

Our second formulation of the second quantum Griffiths inequality is as follows.

Theorem 2.12 Assume (**B**) and (**H. 2**). Let $A, B, C, D \in \mathscr{B}(\mathfrak{H})$ and $A(s) = e^{-sH}Ae^{sH}$. Assume the following:

$$\mathscr{U}^*(A \otimes C - C \otimes A) \mathscr{U} \ge 0, \quad \mathscr{U}^*(B \otimes D - D \otimes B) \mathscr{U} \ge 0 \quad w.r.t. \ \mathfrak{P}_{ext}.$$
 (2.18)

Then we have

$$\langle A(s)B(t)\rangle_{\beta}\langle C(s)D(t)\rangle_{\beta} - \langle A(s)D(t)\rangle_{\beta}\langle C(s)B(t)\rangle_{\beta} \ge 0$$
 (2.19)

for all $0 \le s \le t < \beta$. In addition, assume (A) and (H. 1). If $A \ge 0, B \ge 0, C \ge 0$ and $D \ge 0$ w.r.t. \mathfrak{P} , we obtain

$$\left\langle A(s)B(t)\right\rangle_{\beta} \ge 0, \quad \left\langle C(s)D(t)\right\rangle_{\beta} \ge 0, \quad \left\langle A(s)D(t)\right\rangle_{\beta} \ge 0, \quad \left\langle C(s)B(t)\right\rangle_{\beta} \ge 0 \quad (2.20)$$
 for all $0 \le s \le t < \beta$.

Proof. Note that we can conclude (2.19) from the following:

$$\left\langle\!\!\left\langle \left(A(s)\otimes C(s) - C(s)\otimes A(s)\right) \left(B(t)\otimes D(t) - D(t)\otimes B(t)\right)\right\rangle\!\!\right\rangle_{\beta} \ge 0.$$
(2.21)

To show this, we use Proposition A.1 and the fact that

$$\mathscr{U}^* \Big(A(s) \otimes C(s) - C(s) \otimes A(s) \Big) \Big(B(t) \otimes D(t) - D(t) \otimes B(t) \Big) e^{-\beta H_{\text{ext}}} \mathscr{U}$$

= $\mathscr{U}^* e^{-sH_{\text{ext}}} \Big(A \otimes C - C \otimes A \Big) e^{-(t-s)H_{\text{ext}}} \Big(B \otimes D - D \otimes B \Big) e^{-(\beta-t)H_{\text{ext}}} \mathscr{U} \ge 0$ (2.22)

w.r.t. $\mathfrak{P}_{\text{ext}}$ for all $0 \leq s \leq t < \beta$. \Box

Theorem 2.13 If we replace (A) and (B) by (A') in Theorem 2.12, then (2.19) and (2.20) hold true at $\beta = \infty$.

Corollary 2.14 Assume (B) and (H. 2). Let $A, B \in \mathscr{B}(\mathfrak{H})$. Assume the following:

$$\mathscr{U}^* \Big(A \otimes \mathbb{1} - \mathbb{1} \otimes A \Big) \mathscr{U} \succeq 0, \quad \mathscr{U}^* \Big(B \otimes \mathbb{1} - \mathbb{1} \otimes B \Big) \mathscr{U} \succeq 0 \quad w.r.t. \ \mathfrak{P}_{\text{ext}}.$$
(2.23)

Then we have

$$\langle A(s)B(t)\rangle_{\beta} - \langle A\rangle_{\beta}\langle B\rangle_{\beta} \ge 0$$
 (2.24)

for all $0 \leq s \leq t < \beta$. In particular, we have

$$(A,B)_{\beta} - \langle A \rangle_{\beta} \langle B \rangle_{\beta} \ge 0, \qquad (2.25)$$

$$\langle AB \rangle_{\beta} - \langle A \rangle_{\beta} \langle B \rangle_{\beta} \ge 0.$$
 (2.26)

In addition, assume (A) and (H. 1). If $A \ge 0, B \ge 0$ w.r.t. \mathfrak{P} , then we obtain

$$(A, B)_{\beta} \ge 0, \quad \langle AB \rangle_{\beta} \ge 0, \quad \langle A \rangle_{\beta} \ge 0, \quad \langle B \rangle_{\beta} \ge 0.$$
 (2.27)

2.3 Further generalization

Theorem 2.12 can be generalized as follows.

Theorem 2.15 Assume (B) and (H. 2). Let $A_j, B_j \in \mathscr{B}(\mathfrak{H}), j = 1, ..., n$ and $A(s) = e^{-sH}Ae^{sH}$. Assume the following:

$$\mathscr{U}^*\left(A_j \otimes B_j + \varepsilon_j B_j \otimes A_j\right) \mathscr{U} \ge 0 \quad w.r.t. \ \mathfrak{P}_{\text{ext}}, \quad j = 1, \dots, n,$$
 (2.28)

where $\varepsilon_j = 1$ or -1. Then we have, for all $0 \le s_1 \le s_2 \le \cdots \le s_n < \beta$,

$$\sum_{I \subseteq \{1,2,\dots,n\}} \varepsilon_I \langle T_I \rangle_\beta \langle T_{I^c} \rangle_\beta \ge 0, \tag{2.29}$$

where $I^c = \{1, 2, ..., n\} \setminus I$, $\varepsilon_I = \prod_{j \in I} \varepsilon_j$ and

$$T_{I} = \prod_{j=1}^{n} T_{j}(s_{j}), \quad T_{j}(s_{j}) = \begin{cases} A_{j}(s_{j}) & j \in I \\ B_{j}(s_{j}) & j \in I^{c} \end{cases}.$$
 (2.30)

In addition, assume (A) and (H. 1). If $A_j \ge 0$, $B_j \ge 0$ w.r.t. \mathfrak{P} for all $j = 1, \ldots, n$, we obtain

$$\left\langle T_I \right\rangle_\beta \ge 0 \tag{2.31}$$

for all $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n < \beta$ and $I \subseteq \{1, 2, \dots, n\}$.

Remark 2.16 Let $\langle\!\langle \cdot \rangle\!\rangle_{\beta}$ be defined by (2.10). Then we obtain (2.29) from the following:

$$\left\langle \left\langle \prod_{j=1}^{n} \left[A_j(s_j) \otimes B_j(s_j) + \varepsilon_j B_j(s_j) \otimes A_j(s_j) \right] \right\rangle \right\rangle_{\beta} \ge 0.$$
(2.32)

Thus (2.32) can be regarded as a generalization of the second quantum Griffiths inequality as well. This expression will be useful in the later sections. \diamond

Theorem 2.17 If we replace (A) and (B) by (A') in Theorem 2.15, then (2.29) and (2.31) hold true at $\beta = \infty$.

Example 1 When n = 2, by (2.29), we have

$$\varepsilon_{1}\varepsilon_{2}\langle A_{1}A_{2}\rangle\langle B_{1}B_{2}\rangle + \varepsilon_{1}\langle A_{1}B_{2}\rangle\langle B_{1}A_{2}\rangle + \varepsilon_{2}\langle B_{1}A_{2}\rangle\langle A_{1}B_{2}\rangle + \langle B_{1}B_{2}\rangle\langle A_{1}A_{2}\rangle \ge 0.$$
(2.33)

Here $\langle A_1 A_2 \cdots A_n \rangle$ is an abbreviation of $\langle A_1(s_1) A_2(s_2) \cdots A_n(s_n) \rangle_{\beta}$. Thus, if $\varepsilon_1 = \varepsilon_2 = -1$, we obtain Theorem 2.12. \diamond

Example 2 Consider the case where n = 3 and $B_1 = B_2 = B_3 = 1$. In this case, (2.29) is meaningful only if $\varepsilon_1 \varepsilon_2 \varepsilon_3 = 1$:

$$\langle A_1 A_2 A_3 \rangle + \varepsilon_1 \langle A_1 \rangle \langle A_2 A_3 \rangle + \varepsilon_2 \langle A_2 \rangle \langle A_1 A_3 \rangle + \varepsilon_3 \langle A_3 \rangle \langle A_1 A_2 \rangle \ge 0.$$
 (2.34)

Moreover, suppose that assumption (2.28) is satisfied for

$$(\varepsilon_1, \varepsilon_2, \varepsilon_3) = (1, -1, -1), (-1, 1, -1), (-1, -1, 1),$$
 (2.35)

then we obtain

$$\langle A_1 A_2 A_3 \rangle - \langle A_1 \rangle \langle A_2 A_3 \rangle \ge 0, \tag{2.36}$$

$$\langle A_1 A_2 A_3 \rangle - \langle A_2 \rangle \langle A_1 A_3 \rangle \ge 0, \tag{2.37}$$

$$\langle A_1 A_2 A_3 \rangle - \langle A_3 \rangle \langle A_1 A_2 \rangle \ge 0, \tag{2.38}$$

which implies that

$$3\langle A_1A_2A_3\rangle - \langle A_1\rangle\langle A_2A_3\rangle - \langle A_2\rangle\langle A_1A_3\rangle - \langle A_3\rangle\langle A_1A_2\rangle \ge 0. \quad \diamondsuit \qquad (2.39)$$

Example 3 Consider the case where n = 4, $\varepsilon_1 \varepsilon_2 \varepsilon_3 \varepsilon_4 = 1$, and $B_1 = B_2 = B_3 = B_4 = 1$. In this case, (2.29) implies that

Let $S = \{(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4) \in \{\pm 1\}^4 | \varepsilon_1 \varepsilon_2 \varepsilon_3 \varepsilon_4 = 1\}$. If assumption (2.28) holds true for all $(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4) \in S$, we obtain

$$3\langle A_1A_2A_3A_4\rangle - \langle A_1A_2\rangle\langle A_3A_4\rangle - \langle A_1A_3\rangle\langle A_2A_4\rangle - \langle A_1A_4\rangle\langle A_2A_3\rangle \ge 0. \quad \diamondsuit \quad (2.41)$$

The following theorem offers us a connection between Corollary 2.14 and Theorem 2.15 (similar arguments can be found in [20]):

Theorem 2.18 Assume (B) and (H. 2). Let $A_j \in \mathscr{B}(\mathfrak{H})$, j = 1, ..., n. Assume that

$$\mathscr{U}^*\left(A_j \otimes \mathbb{1} + \mathbb{1} \otimes A_j\right) \mathscr{U} \succeq 0, \quad \mathscr{U}^*\left(A_j \otimes \mathbb{1} - \mathbb{1} \otimes A_j\right) \mathscr{U} \succeq 0 \quad w.r.t. \ \mathfrak{P}_{\text{ext}}$$
(2.42)

for all j = 1, ..., n. For each $I = \{i_1, ..., i_k\} \subseteq \{1, ..., n\}$, we set

$$A_I = \prod_{\ell=1}^k A_{i_\ell}.$$
(2.43)

Then we obtain

$$\langle A_I A_K \rangle_\beta - \langle A_I \rangle_\beta \langle A_K \rangle_\beta \ge 0 \tag{2.44}$$

for all $I, K \subseteq \{1, \ldots, n\}$.

Proof. For each $\varepsilon \in \{\pm 1\}$, define $B_j^{(\varepsilon)} = \frac{1}{2}(A_j \otimes \mathbb{1} + \varepsilon \mathbb{1} \otimes A_j)$. By (2.42), we have $B_j^{(\varepsilon)} \ge 0$ w.r.t. $\mathfrak{P}_{\text{ext}}$ for all $j = 1, \ldots, n$. Since $A_j \otimes \mathbb{1} = B_j^{(+)} + B_j^{(-)}$ and $\mathbb{1} \otimes A_j = B_j^{(+)} - B_j^{(-)}$, we see that

$$A_{I} \otimes 1 - 1 \otimes A_{I} = \prod_{\ell=1}^{k} \left[B_{i_{\ell}}^{(+)} + B_{i_{\ell}}^{(-)} \right] - \prod_{\ell=1}^{k} \left[B_{i_{\ell}}^{(+)} - B_{i_{\ell}}^{(-)} \right]$$
$$= \sum_{\varepsilon_{1}, \dots, \varepsilon_{k} \in \{\pm 1\}} C_{\varepsilon_{1}, \dots, \varepsilon_{k}} B_{i_{1}}^{(\varepsilon_{1})} \cdots B_{i_{k}}^{(\varepsilon_{k})}, \qquad (2.45)$$

where $C_{\varepsilon_1,\ldots,\varepsilon_k} \geq 0$ for all $\varepsilon_1,\ldots,\varepsilon_k \in \{\pm 1\}$. Thus, the RHS of $(2.45) \geq 0$ w.r.t. \mathfrak{P}_{ext} . Similarly, $A_K \otimes \mathbb{1} - \mathbb{1} \otimes A_K \geq 0$ w.r.t. \mathfrak{P}_{ext} . By applying Corollary 2.14, we obtain the result. \Box

3 Reflection positivity

In Section 2, we give a general framework of the Griffiths inequality. In our proofs, assumptions (A) and (B) are basic inputs. Unfortunately, these assumptions are not satisfied in several models. To overcome this situation, we employ the concept of reflection positivity. As we indicated in [44], reflection positivity can be considered an operator inequality associated with a special self-dual cone. This viewpoint makes it possible to visualize a common mathematical structure among various quantum models. Reflection positivity originates from axiomatic quantum field theory [51]. Glimm, Jaffe, and Spencer first applied reflection positivity to the rigorous study of the phase transition [21]. This idea was successfully further developed by Dyson, Fröhlich, Israel, Lieb, Simon, [11, 17, 18] and many others. Lieb also discovered a crucial application of reflection positivity to many-electron systems, called the spin reflection positivity [38]. Recently, Jaffe and Pedrocchi studied the topological order by reflection positivity ity [30, 31].

For each $p \in \mathbb{N}$, we denote the trace ideal by $\mathscr{L}^p(\mathfrak{H})$, which is defined as

$$\mathscr{L}^{p}(\mathfrak{H}) = \left\{ \xi \in \mathscr{B}(\mathfrak{H}) \, \middle| \, \mathrm{Tr}[|\xi|^{p}] < \infty \right\}. \tag{3.1}$$

 $\mathscr{L}^{1}(\mathfrak{H})$ is called the trace class, while $\mathscr{L}^{2}(\mathfrak{H})$ is called the Hilbert–Schmidt class. $\mathscr{L}^{2}(\mathfrak{H})$ becomes a Hilbert space if we define the inner product as $\langle \eta | \xi \rangle_{\mathscr{L}^{2}} = \operatorname{Tr}[\eta^{*}\xi]$ for all $\eta, \xi \in \mathscr{L}^{2}(\mathfrak{H})$.

Definition 3.1 (Bounded operators) Let $A \in \mathscr{B}(\mathfrak{H})$.

- (i) The left multiplication operator $\mathcal{L}(A)$ is defined as $\mathcal{L}(A)\xi = A\xi$ for all $\xi \in \mathscr{L}^2(\mathfrak{H})$.
- (ii) The right multiplication operator $\mathcal{R}(A)$ is defined as $\mathcal{R}(A)\xi = \xi A$ for all $\xi \in \mathscr{L}^2(\mathfrak{H})$.

Remark 3.2 (i) $\mathcal{L}(A), \mathcal{R}(A) \in \mathscr{B}(\mathscr{L}^2(\mathfrak{H}))$, the set of all bounded operators on $\mathscr{L}^2(\mathfrak{H})$.

- (ii) $\mathcal{L}(A)\mathcal{L}(B) = \mathcal{L}(AB).$
- (iii) $\mathcal{R}(A)\mathcal{R}(B) = \mathcal{R}(BA).$

Let ϑ be an antilinear involution on \mathfrak{H} . Let Φ_{ϑ} be an isometric isomorphism from $\mathscr{L}^2(\mathfrak{H})$ onto $\mathfrak{H} \otimes \mathfrak{H}$ defined by

$$\Phi_{\vartheta}(|x\rangle\langle y|) = x \otimes \vartheta y \quad \forall x, y \in \mathfrak{H}.$$

$$(3.2)$$

We have the relations

$$\mathcal{L}(A) = \Phi_{\vartheta}^{-1}A \otimes \mathbb{1}\Phi_{\vartheta}, \quad \mathcal{R}(\vartheta A^*\vartheta) = \Phi_{\vartheta}^{-1}\mathbb{1} \otimes A\Phi_{\vartheta}$$
(3.3)

for each $A \in \mathscr{B}(\mathfrak{H})$. We simply write these facts as

$$\mathfrak{H} \otimes \mathfrak{H} = \mathscr{L}^2(\mathfrak{H}), \quad A \otimes \mathbb{1} = \mathcal{L}(A), \quad \mathbb{1} \otimes A = \mathcal{R}(\vartheta A^* \vartheta),$$
(3.4)

if no confusion arises.

Definition 3.1 can be extended to unbounded operators by (3.3) as follows.

Definition 3.3 (Unbounded operators) Let A be a densely defined closed operator on \mathfrak{H} .

- (i) The left multiplication operator $\mathcal{L}(A)$ is defined as $\mathcal{L}(A) = \Phi_{\vartheta}^{-1}A \otimes \mathbb{1}\Phi_{\vartheta}$.
- (ii) The right multiplication operator $\mathcal{R}(A)$ is defined as $\mathcal{R}(A) = \Phi_{\vartheta}^{-1} \mathbb{1} \otimes \vartheta A^* \vartheta \Phi_{\vartheta}$.

Remark 3.4 (i) Both $\mathcal{L}(A)$ and $\mathcal{R}(A)$ are closed operators on $\mathscr{L}^2(\mathfrak{H})$.

- (ii) If A is self-adjoint, so are $\mathcal{L}(A)$ and $\mathcal{R}(A)$.
- (iii) We will also use the conventional identification (3.4). \diamond

Definition 3.5 A canonical cone in $\mathscr{L}^2(\mathfrak{H})$ is defined by

$$\mathscr{L}^{2}(\mathfrak{H})_{+} = \left\{ \xi \in \mathscr{L}^{2}(\mathfrak{H}) \, \big| \, \xi \ge 0 \text{ as a linear operator in } \mathfrak{H} \right\}.$$
(3.5)

 $\mathscr{L}^2(\mathfrak{H})_+$ is self-dual. \diamondsuit

The following proposition is often useful.

Proposition 3.6 For each $A \in \mathscr{B}(\mathfrak{H})$, we have $\mathcal{L}(A)\mathcal{R}(A^*) \geq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$.

Proof. For each $\xi \in \mathscr{L}^2(\mathfrak{H})_+$, we can see that $\mathcal{L}(A)\mathcal{R}(A^*)\xi = A\xi A^* \geq 0$. \Box

Definition 3.7 We define

$$\mathfrak{A} = \operatorname{Coni}\left\{\mathcal{L}(A)\mathcal{R}(A^*) \in \mathscr{B}(\mathscr{L}^2(\mathfrak{H})) \,\middle|\, A \in \mathscr{B}(\mathfrak{H})\right\}^{-\mathrm{w}},\tag{3.6}$$

where $\operatorname{Coni}(X)$ is the conical hull of X and S^{-W} represents the closure of S under a weak topology in $\mathscr{B}(\mathscr{L}^2(\mathfrak{H}))$.

If $A \in \mathfrak{A}$, then we write $A \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$.

Remark 3.8 (i) $A \succeq 0 \Longrightarrow A \trianglerighteq 0.4$

- (ii) $A \succeq 0, B \succeq 0, a, b \ge 0 \Longrightarrow aA + bB \succeq 0.$
- (iii) $A \succeq 0, B \succeq 0 \Longrightarrow AB \succeq 0.$ \diamondsuit

The following proposition is a guiding principle of reflection positivity [11, 17, 44]. The point is that assumptions (A) and (B) are unnecessary.

Proposition 3.9 (Reflection positivity) Assume that A is a trace class operator on $\mathscr{L}^2(\mathfrak{H})$, i.e., $A \in \mathscr{L}^1(\mathscr{L}^2(\mathfrak{H}))$. If $A \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$, then we have $\operatorname{Tr}_{\mathscr{L}^2}[A] \ge 0$. *Proof.* It suffices to consider the case where $A = \sum_{j=1}^N \mathcal{L}(a_j)\mathcal{R}(a_j^*)$, $N \in \mathbb{N}$. In this case, we can easily see that $\operatorname{Tr}_{\mathscr{L}^2}[A] = \sum_{j=1}^N |\operatorname{Tr}_{\mathfrak{H}}[a_j]|^2 \ge 0$. \Box

As before, the system's Hamiltonian H is a self-adjoint operator acting in $\mathscr{L}^2(\mathfrak{H})$ and bounded from below. In this section, we continue to assume that $e^{-\beta H}$ is a trace class operator for all $\beta > 0$. Corresponding to **(H. 1)**, we need the following condition:

(H. 3) $e^{-\beta H} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$ for all $\beta \ge 0$.

Let $\langle \cdot \rangle_{\beta}$ be the thermal average. Theorem 3.10 is another prototype of the Griffiths inequality.

Theorem 3.10 Assume (**H. 3**). If $A \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$, then $\langle A \rangle_{\beta} \geq 0$ for all $\beta \geq 0$.

Proof. From Remark 3.8 (iii), we have $A e^{-\beta H} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$ for all $\beta \ge 0$. Thus by Proposition 3.9, we conclude the theorem. \Box

Theorem 3.10 can be generalized as follows.

Theorem 3.11 Assume (**H. 3**). If $A_j \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$ for all $j = 1, \ldots, n$, then we have

$$\left\langle \prod_{j=1}^{n} A_j(s_j) \right\rangle_{\beta} \ge 0 \tag{3.7}$$

for all $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n < \beta$.

⁴From this fact, we understand that reflection positivity is closely related to the notion of positivity preservation discussed in Section 2.

Proof. Since

$$\left[\prod_{j=1}^{n} A_j(s_j)\right] e^{-\beta H} = \underbrace{e^{-s_1 H}}_{\succeq 0} \underbrace{A_1}_{\succeq 0} \underbrace{e^{-(s_2 - s_1)H}}_{\succeq 0} \cdots \underbrace{A_n}_{\succeq 0} \underbrace{e^{-(\beta - s_n)H}}_{\succeq 0} \succeq 0$$
(3.8)

w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$, we obtain (3.7) by Proposition 3.9. \Box

Theorem 3.12 Assume (A'). Then Theorem 3.11 holds true at $\beta = \infty$.

Proof. Considering Remark 3.8 (i), we know that Theorem 3.12 follows from Theorem 2.8. \Box

4 Quantum Ising model

4.1 Results

Let Λ be a finite subset of \mathbb{R}^d . The Hamiltonian of the quantum Ising model is given by

$$H_{\Lambda} = -\sum_{x,y\in\Lambda} J_{xy}\sigma_x^{(3)}\sigma_y^{(3)} - \sum_{x\in\Lambda} \mu_x\sigma_x^{(3)} - \sum_{x\in\Lambda} \lambda_x\sigma_x^{(1)}.$$
(4.1)

 $\sigma^{(1)},\sigma^{(2)},$ and $\sigma^{(3)}$ are the Pauli matrices:

$$\sigma^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
(4.2)

 H_{Λ} acts in the Hilbert space $\mathfrak{H}_{\Lambda} = \bigotimes_{x \in \Lambda} \mathbb{C}^2$. $(J_{xy})_{x,y \in \mathbb{Z}^d}$ is a family of coupling constants, and $\mu_x, \lambda_x \in \mathbb{R}$ are the magnetic fields. In this section, we always assume the following:

(J)
$$J_{xy} \ge 0, \quad J_{xy} = J_{yx}, \quad J_{xx} = 0.$$

The thermal average is defined by

$$\langle A \rangle_{\beta} = \operatorname{Tr} \left[A \, \mathrm{e}^{-\beta H_{\Lambda}} \right] / Z_{\beta}, \quad Z_{\beta} = \operatorname{Tr} \left[\mathrm{e}^{-\beta H_{\Lambda}} \right].$$
(4.3)

Let

$$\tau_x = \frac{1}{2} (1 + \sigma_x^{(1)}). \tag{4.4}$$

Set

$$S_x^{(\varepsilon)} = \begin{cases} \tau_x & \text{if } \varepsilon = 1\\ \sigma_x^{(3)} & \text{if } \varepsilon = 3 \end{cases}.$$
(4.5)

We define

$$\mathfrak{A} = \operatorname{Coni}\left\{S_{x_1}^{(\varepsilon_1)} \cdots S_{x_n}^{(\varepsilon_n)} \middle| x_1, \dots, x_n \in \Lambda, \ \varepsilon_1, \dots, \varepsilon_n \in \{1, 3\}, n \in \mathbb{N}\right\},\tag{4.6}$$

where $\operatorname{Coni}(S)$ is the conical hull of S.

Theorem 4.1 (First Griffiths inequality) Assume (**J**). Assume that $\mu_x \ge 0$ for all $x \in \Lambda$. For all $A_1, \ldots, A_n \in \mathfrak{A}, \lambda_x \in \mathbb{R}$ and $0 \le s_1 \le \cdots \le s_n \le \beta$, we have

$$\left\langle \prod_{j=1}^{n} A_j(s_j) \right\rangle_{\beta} \ge 0.$$
(4.7)

For each $A \subseteq \Lambda$, set

$$\sigma_A^{(3)} = \prod_{x \in A} \sigma_x^{(3)}, \quad \tau_A = \prod_{x \in A} \tau_x.$$

$$(4.8)$$

To state the second Griffiths inequality, we introduce the following notations:

$$\langle\!\langle X \rangle\!\rangle_{\beta} = \operatorname{Tr}_{\mathfrak{H}\otimes\mathfrak{H}\otimes\mathfrak{H}}\left[X \,\mathrm{e}^{-\beta H_{\mathrm{ext}}}\right] \Big/ Z_{\beta}^{2},$$
(4.9)

$$H_{\text{ext}} = H_{\Lambda} \otimes 1 \!\!\!1 + 1 \!\!\!1 \otimes H_{\Lambda}. \tag{4.10}$$

Theorem 4.2 (Second Griffiths inequality) Assume (**J**). Assume that $\mu_x \ge 0, \lambda_x \ge 0$ for all $x \in \Lambda$. For all $A, B, C, D \subseteq \Lambda$ and $\beta \ge 0$, we have

$$\left\langle\!\!\left\langle\!\left(\sigma_A^{(3)}(s)\otimes\tau_C(s)-\tau_C(s)\otimes\sigma_A^{(3)}(s)\right)\!\left(\sigma_B^{(3)}(t)\otimes\tau_D(t)-\tau_D(t)\otimes\sigma_B^{(3)}(t)\right)\right\rangle\!\!\right\rangle_{\beta} \ge 0$$

$$(4.11)$$

for all $0 \le s \le t \le \beta$, where $\sigma_A^{(3)}(t) = e^{-tH_\Lambda} \sigma_A^{(3)} e^{tH_\Lambda}$ and $\tau_B(t) = e^{-tH_\Lambda} \tau_B e^{tH_\Lambda}$.

Remark 4.3 (4.11) can be expressed as follows:

$$\left\langle \sigma_A^{(3)}(s)\sigma_B^{(3)}(t)\right\rangle_{\beta} \left\langle \tau_C(s)\tau_D(t)\right\rangle_{\beta} - \left\langle \sigma_A^{(3)}(s)\tau_D(t)\right\rangle_{\beta} \left\langle \tau_C(s)\sigma_B^{(3)}(t)\right\rangle_{\beta} \ge 0. \quad \diamondsuit \quad (4.12)$$

From this theorem (or (4.12)), we can derive the well-known formula.

Corollary 4.4 Under the same assumptions as Theorem 4.2, we have

$$\left\langle \sigma_A^{(3)} \sigma_B^{(3)} \right\rangle_{\beta} - \left\langle \sigma_A^{(3)} \right\rangle_{\beta} \left\langle \sigma_B^{(3)} \right\rangle_{\beta} \ge 0, \quad \left\langle \tau_A \tau_B \right\rangle_{\beta} - \left\langle \tau_A \right\rangle_{\beta} \left\langle \tau_B \right\rangle_{\beta} \ge 0.$$
 (4.13)

The following theorem is an extension of Theorem 4.2.

Theorem 4.5 Assume (**J**). Assume that $\mu_x \ge 0$, $\lambda_x \ge 0$ for all $x \in \Lambda$. Let $A_1, \ldots, A_n, B_1, \ldots, B_n \subseteq \Lambda$. Then, for all $0 \le t_1 \le t_2 \le \cdots \le t_n \le \beta$, we have

$$\left\langle \left\langle \prod_{j=1}^{n} \left(\sigma_{A_j}^{(3)}(t_j) \otimes \tau_{B_j}(t_j) - \tau_{B_j}(t_j) \otimes \sigma_{A_j}^{(3)}(t_j) \right) \right\rangle \right\rangle_{\beta} \ge 0.$$

$$(4.14)$$

By Theorem 2.15, we obtain the following corollary.

Corollary 4.6 Assume (**J**). Assume that $\mu_x \ge 0$, $\lambda_x \ge 0$ for all $x \in \Lambda$. Let $A_1, \ldots, A_n, B_1, \ldots, B_n \subseteq \Lambda$. For each $I = \{i_1, \ldots, i_k\} \subseteq \{1, \ldots, n\}$ with $i_1 < i_2 < \cdots < i_k$, we define

$$S_{I}(\mathbf{t}) = \prod_{j=1}^{k} S_{j}(t_{j}), \quad S_{j}(t_{j}) = \begin{cases} \sigma_{A_{j}}^{(3)}(t_{j}) & \text{if } j \in I \\ \tau_{B_{j}}(t_{j}) & \text{if } j \in I^{c} \end{cases}.$$
(4.15)

Then we have, for all $0 \le t_1 \le t_2 \le \cdots \le t_n \le \beta$,

$$\sum_{I \subseteq \{1,2,\dots,n\}} (-1)^{|I|} \left\langle S_I(\mathbf{t}) \right\rangle_\beta \left\langle S_{I^c}(\mathbf{t}) \right\rangle_\beta \ge 0.$$
(4.16)

In addition, we have

$$\left\langle S_I(\mathbf{t}) \right\rangle_{\beta} \ge 0$$
 (4.17)

for all $0 \le t_1 \le t_2 \le \cdots \le t_n \le \beta$ and $I \subseteq \Lambda$.

Example 4 We have the following:

- (i) $\langle \sigma_A^{(3)} \rangle_{\beta}$ is monotonically increasing in J_{xy} and μ_x .
- (ii) $\langle \tau_A \rangle_{\beta}$ is monotonically decreasing in J_{xy} and μ_x .
- (iii) $\langle \sigma_A^{(3)} \rangle_{\beta}$ is monotonically decreasing in λ_x .
- (iv) $\langle \tau_A \rangle_{\beta}$ is monotonically increasing in λ_x .

We will prove this example in Section 4.4. \Diamond

Remark 4.7 (i) Our results can be extended to a more general Hamiltonian of the form

$$H_{\Lambda} = -\sum_{A \subseteq \Lambda} J_A \sigma_A^{(3)} - \sum_{A \subseteq \Lambda} K_A \tau_A \tag{4.18}$$

with $J_A \ge 0$ and $K_A \ge 0$.

(ii) Assume that $\mu_x > 0$ or $\lambda_x > 0$ for all $x \in \Lambda$. Then since the ground state of H_{Λ} is unique for all Λ^5 , our results are valid at $\beta = \infty$. The results at $\beta = \infty$ are used in the study of quantum phase transitions [9, 10]. \diamond

⁵This fact can be proven by the Perron–Frobenius–Faris theorem [12].

4.2 Proof of Theorem 4.1

Let $\Omega = \{-1, +1\}$ be the set of possible values of a spin. Given Λ , Ω^{Λ} is the set of spin configurations in Λ . Set

$$|+1\rangle = \begin{pmatrix} 1\\0 \end{pmatrix}, \quad |-1\rangle = \begin{pmatrix} 0\\1 \end{pmatrix}.$$
 (4.19)

For each $\boldsymbol{\omega} = \{\omega_x\}_{x \in \Lambda} \in \Omega^{\Lambda}$, we define

$$|\boldsymbol{\omega}\rangle = \bigotimes_{x \in \Lambda} |\omega_x\rangle. \tag{4.20}$$

Then $\{|\boldsymbol{\omega}\rangle | \boldsymbol{\omega} \in \Omega^{\Lambda}\}$ is a CONS of \mathfrak{H}_{Λ} .

Definition 4.8 A standard self-dual cone in \mathfrak{H}_{Λ} is defined by

$$\mathfrak{H}_{\Lambda,+} = \left\{ \Psi \in \mathfrak{H}_{\Lambda} \, \middle| \, \Psi = \sum_{\boldsymbol{\omega} \in \Omega^{\Lambda}} C_{\boldsymbol{\omega}} | \boldsymbol{\omega} \rangle, \quad C_{\boldsymbol{\omega}} \ge 0 \, \forall \boldsymbol{\omega} \in \Omega^{\Lambda} \right\}. \quad \diamondsuit \quad (4.21)$$

Remark 4.9 $|\boldsymbol{\omega}\rangle \in \mathfrak{H}_{\Lambda,+}$ for all $\boldsymbol{\omega} \in \Omega^{\Lambda}$.

Let U be a unitary operator⁶ on \mathfrak{H}_{Λ} given by

$$U = \bigotimes_{x \in \Lambda} u, \quad u = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ -1 & 1 \end{pmatrix}.$$
(4.22)

Since $u^* \sigma^{(3)} u = \sigma^{(1)}$ and $u^* \sigma^{(1)} u = -\sigma^{(3)}$, we have

$$U^* \sigma_x^{(3)} U = \sigma_x^{(1)}, \quad U^* \sigma_x^{(1)} U = -\sigma_x^{(3)}$$
(4.23)

for all $x \in \Lambda$. Thus,

$$\hat{H}_{\Lambda} = U^* H_{\Lambda} U = -\sum_{x,y \in \Lambda} J_{xy} \sigma_x^{(1)} \sigma_y^{(1)} - \sum_{x \in \Lambda} \mu_x \sigma_x^{(1)} + \sum_{x \in \Lambda} \lambda_x \sigma_x^{(3)}.$$
(4.24)

Proposition 4.10 We have the following:

- (i) $\sigma_x^{(1)} \succeq 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$ for all $x \in \Lambda$.
- (ii) $\frac{1}{2}(\mathbb{1} \sigma_x^{(3)}) \ge 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$ for all $x \in \Lambda$.
- (iii) $e^{-\beta \hat{H}_{\Lambda}} \succeq 0 \ w.r.t. \ \mathfrak{H}_{\Lambda,+} \ for \ all \ \beta \geq 0.$

Proof. (i), (ii) Let r be a map on Ω defined by r(-1) = +1 and r(+1) = -1. Clearly, $\sigma^{(1)}|\omega\rangle = |r(\omega)\rangle$ holds. Then $\sigma_x^{(1)}|\omega\rangle = |r_x(\omega)\rangle$, where $(r_x(\omega))_y = r(\omega_x)$ if y = x, $(r_x(\omega))_y = \omega_y$ if $y \neq x$. Thus, for all $\omega \in \Omega^{\Lambda}$, it holds that $\sigma_x^{(1)}|\omega\rangle \in \mathfrak{H}_{\Lambda,+}$. Thus, we conclude (i). (ii) is obvious.

⁶This unitary operator is well-known [34, 43].

(iii) Let

$$\hat{T} = \sum_{x,y\in\Lambda} J_{xy}\sigma_x^{(1)}\sigma_y^{(1)}, \quad \hat{V}_\mu = -\sum_{x\in\Lambda} \mu_x \sigma_x^{(1)}, \quad \hat{V}_\lambda = \sum_{x\in\Lambda} \lambda_x \sigma_x^{(3)}.$$
(4.25)

Set $\hat{V} = \hat{V}_{\mu} + \hat{V}_{\lambda}$. Then we have $\hat{H}_{\Lambda} = -\hat{T} + \hat{V}$. By (i), we have $\hat{T} \geq 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$. On the other hand, since $-\hat{V}_{\mu} \geq 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}^{7}$, we have $e^{-\beta \hat{V}_{\mu}} \geq 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$ for all $\beta \geq 0$ by Proposition A.3. In addition, we have

$$e^{-\beta\hat{V}_{\lambda}}|\boldsymbol{\omega}\rangle = \underbrace{\exp\left\{-\beta\sum_{x\in\Lambda}\lambda_{x}\omega_{x}\right\}}_{\geq 0}|\boldsymbol{\omega}\rangle \in \mathfrak{H}_{\Lambda,+},\tag{4.26}$$

which implies $e^{-\beta \hat{V}_{\lambda}} \geq 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$. By Proposition A.4, we have $e^{-\beta \hat{V}} \geq 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$ for all $\beta \geq 0$. Now we can apply Proposition A.5 with $A = -\hat{V}, B = \hat{T}$. \Box

Proof of Theorem 4.1

For each $x \in \Lambda$, by Proposition 4.10 (i) and (ii), we have

$$\hat{\sigma}_x^{(3)} = U^* \sigma_x^{(3)} U = \sigma_x^{(1)} \ge 0, \quad \hat{\tau}_x = U^* \tau_x U = \frac{1}{2} (1 - \sigma_x^{(3)}) \ge 0 \tag{4.27}$$

w.r.t. $\mathfrak{H}_{\Lambda,+}$. Thus, $U^* S_{x_1}^{(\varepsilon_1)} \cdots S_{x_n}^{(\varepsilon_n)} U \succeq 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$, implying that $\hat{A} = U^* A U \succeq 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$ for all $A \in \mathfrak{A}$. By applying Theorem 2.7, we conclude Theorem 4.1. \Box

4.3 Proof of Theorems 4.2 and 4.5

4.3.1 Preliminaries

Let $\mathfrak{K} = \mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^4$. Then $\{|\omega, \omega'\rangle | \omega, \omega' \in \Omega\}$ is a CONS of \mathfrak{K} , where $|\omega, \omega'\rangle = |\omega\rangle \otimes |\omega'\rangle$. We label $\{|\omega, \omega'\rangle | \omega, \omega' \in \Omega\}$ as

$$|e^{1}\rangle = |+1,+1\rangle, \ |e^{2}\rangle = |-1,-1\rangle, \ |e^{3}\rangle = |+1,-1\rangle, \ |e^{4}\rangle = |-1,+1\rangle.$$
 (4.28)

Thus, each $|\varphi\rangle = \sum_{j=1}^{4} c_j |e_j\rangle \in \mathfrak{K}$ can be identified with $(c_1, c_2, c_3, c_4)^T \in \mathbb{C}^4$. We introduce linear operators on \mathfrak{K} as

$$\psi = \frac{1}{\sqrt{2}} \left(\sigma^{(3)} \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^{(3)} \right), \tag{4.29}$$

$$\phi = \frac{1}{\sqrt{2}} \left(\sigma^{(3)} \otimes \mathbb{1} - \mathbb{1} \otimes \sigma^{(3)} \right), \tag{4.30}$$

$$\eta = \frac{1}{\sqrt{2}} \left(\sigma^{(1)} \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^{(1)} \right), \tag{4.31}$$

$$\xi = \frac{1}{\sqrt{2}} \left(\sigma^{(1)} \otimes \mathbb{1} - \mathbb{1} \otimes \sigma^{(1)} \right).$$
(4.32)

⁷We used the assumption $\mu_x \ge 0$ here.

In general, each operator X in \mathfrak{K} can be expressed as a 4×4 matrix: $X = (X_{ij})_{i,j=1,2,3,4}$ with $X_{ij} = \langle e_i | X e_j \rangle$. In particular, we have

$$\psi = \sqrt{2} \begin{pmatrix} \sigma^{(3)} & 0\\ 0 & 0 \end{pmatrix}, \quad \phi = \sqrt{2} \begin{pmatrix} 0 & 0\\ 0 & \sigma^{(3)} \end{pmatrix},$$
$$\eta = \sqrt{2} \begin{pmatrix} \sigma^{(1)} & \alpha\\ \alpha & \sigma^{(1)} \end{pmatrix}, \quad \xi = \sqrt{2} \begin{pmatrix} 0 & \gamma\\ \gamma & 0 \end{pmatrix}, \quad (4.33)$$

where

$$\alpha = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ 1 & 1 \end{pmatrix}, \quad \gamma = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1\\ 1 & -1 \end{pmatrix}.$$
(4.34)

Let u be the unitary operator given by (4.22) and let

$$\vartheta = \left(\begin{array}{cc} u & 0\\ 0 & u \end{array}\right). \tag{4.35}$$

For each operator X on \mathfrak{K} , we write $\tilde{X} = \vartheta^* X \vartheta$. By (4.33), we obtain

$$\tilde{\psi} = \sqrt{2} \begin{pmatrix} \sigma^{(1)} & 0 \\ 0 & 0 \end{pmatrix}, \quad \tilde{\phi} = \sqrt{2} \begin{pmatrix} 0 & 0 \\ 0 & \sigma^{(1)} \end{pmatrix},
\tilde{\eta} = \sqrt{2} \begin{pmatrix} -\sigma^{(3)} & \hat{\alpha} \\ \hat{\alpha} & -\sigma^{(3)} \end{pmatrix}, \quad \tilde{\xi} = \sqrt{2} \begin{pmatrix} 0 & \hat{\gamma} \\ \hat{\gamma} & 0 \end{pmatrix}$$
(4.36)

where $\hat{\alpha} = u^* \alpha u = (\mathbb{1}_2 - \sigma^{(3)}) / \sqrt{2}$ and $\hat{\gamma} = -(\mathbb{1}_2 + \sigma^{(3)}) / \sqrt{2}$.

Definition 4.11 Let

$$\mathfrak{K}_{+} = \left\{ |\varphi\rangle \in \mathfrak{K} \, \middle| \, |\varphi\rangle = \sum_{j=1}^{4} c_{j} |e_{j}\rangle, \quad c_{j} \ge 0, j = 1, 2, 3, 4 \right\}.$$

$$(4.37)$$

Clearly, \mathfrak{K}_+ is a self-dual cone in \mathfrak{K} .

Proposition 4.12 We have the following:

- (i) $\tilde{\psi} \ge 0$ w.r.t. \Re_+ .
- (ii) $\tilde{\phi} \ge 0$ w.r.t. \Re_+ .
- (iii) $-\tilde{\xi} \ge 0$ w.r.t. \Re_+ .
- (iv) $1_4 + \frac{1}{\sqrt{2}}\tilde{\eta} \ge 0$ w.r.t. \mathfrak{K}_+ .
- (v) $\exp(\beta \tilde{\psi}) \ge 0$ w.r.t. \mathfrak{K}_+ for all $\beta \ge 0$.
- (vi) $\exp(\beta \tilde{\eta}) \ge 0$ w.r.t. \Re_+ for all $\beta \ge 0$.

Proof. Note that by Proposition A.2, a linear operator X on \mathfrak{K} satisfies $X \geq 0$ w.r.t. \mathfrak{K}_+ if and only if $X_{ij} = \langle e_i | X e_j \rangle \geq 0$ for all i, j = 1, 2, 3, 4. Thus, (i), (ii), (iii), and (iv) immediately follow from (4.36).

(v) By (i) and Proposition A.3, we can see that $\exp(\beta \tilde{\psi}) \ge 0$ w.r.t. \mathfrak{K}_+ for all $\beta \ge 0$. To show (vi), we write $\tilde{\eta} = \tilde{\eta}_d + \tilde{\eta}_o$, where

$$\tilde{\eta}_d = \sqrt{2} \begin{pmatrix} -\sigma^{(3)} & 0\\ 0 & -\sigma^{(3)} \end{pmatrix}, \quad \tilde{\eta}_o = \sqrt{2} \begin{pmatrix} 0 & \hat{\alpha}\\ \hat{\alpha} & 0 \end{pmatrix}.$$
(4.38)

Suppose that

- (a) $\exp(\beta \tilde{\eta}_d) \ge 0$ w.r.t. \mathfrak{K}_+ for all $\beta \ge 0$,
- (b) $\exp(\beta \tilde{\eta}_o) \ge 0$ w.r.t. \mathfrak{K}_+ for all $\beta \ge 0$.

Then we can immediately conclude (vi) by Proposition A.4. Hence, it suffices to prove (a) and (b).

To show (a), observe that

$$\exp(\beta \tilde{\eta}_d) = \begin{pmatrix} e^{-\sqrt{2}\beta\sigma^{(3)}} & 0\\ 0 & e^{-\sqrt{2}\beta\sigma^{(3)}} \end{pmatrix}.$$
(4.39)

Since all matrix elements of $\exp(-\sqrt{2}\beta\sigma^{(3)})$ are positive, we conclude that (a) is true by Proposition A.2.

Since $\tilde{\eta}_o \succeq 0$ w.r.t. \mathfrak{K}_+ , we find that $\exp(\beta \tilde{\eta}_o) \succeq 0$ w.r.t. \mathfrak{K}_+ for all $\beta \geq 0$ by Proposition A.3. Thus, we conclude (b). \Box

4.3.2 Completion of proof of Theorems 4.2 and 4.5

Let H_{ext} be given by (4.10). H_{ext} acts in the extended Hilbert space $\mathfrak{K}_{\Lambda} = \mathfrak{H}_{\Lambda} \otimes \mathfrak{H}_{\Lambda}$. For each $x \in \Lambda$, let

$$\psi_x = \frac{1}{\sqrt{2}} \left(\sigma_x^{(3)} \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_x^{(3)} \right), \tag{4.40}$$

$$\phi_x = \frac{1}{\sqrt{2}} \left(\sigma_x^{(3)} \otimes \mathbb{1} - \mathbb{1} \otimes \sigma_x^{(3)} \right), \tag{4.41}$$

$$\eta_x = \frac{1}{\sqrt{2}} \left(\sigma_x^{(1)} \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_x^{(1)} \right), \tag{4.42}$$

$$\xi_x = \frac{1}{\sqrt{2}} \left(\sigma_x^{(1)} \otimes \mathbb{1} - \mathbb{1} \otimes \sigma_x^{(1)} \right).$$

$$(4.43)$$

 $H_{\rm ext}$ can be expressed as

$$H_{\text{ext}} = -\sum_{x,y\in\Lambda} J_{xy}(\psi_x\psi_y + \phi_x\phi_y) - \sqrt{2}\sum_{x\in\Lambda} \mu_x\psi_x - \sqrt{2}\sum_{x\in\Lambda} \lambda_x\eta_x.$$
 (4.44)

We employ the following identification⁸ of \mathfrak{K}_{Λ} :

$$\mathfrak{K}_{\Lambda} = \bigotimes_{x \in \Lambda} \mathfrak{K},\tag{4.45}$$

⁸Indeed, we have $\mathfrak{K}_{\Lambda} = \left(\bigotimes_{x \in \Lambda} \mathbb{C}^2\right) \otimes \left(\bigotimes_{x \in \Lambda} \mathbb{C}^2\right) \cong \bigotimes_{x \in \Lambda} (\mathbb{C}^2 \otimes \mathbb{C}^2) \cong \bigotimes_{x \in \Lambda} \mathfrak{K}.$

where $\mathfrak{K} = \mathbb{C}^4$. Thus, ψ_x, ϕ_x , and η_x can be expressed as

$$\psi_x = \otimes_{y \in \Lambda} (\psi)^{\delta_{xy}}, \quad \phi_x = \otimes_{y \in \Lambda} (\phi)^{\delta_{xy}}, \quad \eta_x = \otimes_{y \in \Lambda} (\eta)^{\delta_{xy}}. \tag{4.46}$$

Here $(X)^{\delta_{xy}} = 1$ if $x \neq y$, $(X)^{\delta_{xy}} = X$ if x = y. Let ϑ be given by (4.35). Set $\Theta = \bigotimes_{x \in \Lambda} \vartheta$. For each linear operator X on \mathfrak{K}_{Λ} , set $\tilde{X} = \Theta^* X \Theta$. Then we obtain

$$\tilde{H}_{\text{ext}} = -\sum_{x,y\in\Lambda} J_{xy}(\tilde{\psi}_x\tilde{\psi}_y + \tilde{\phi}_x\tilde{\phi}_y) - \sqrt{2}\sum_{x\in\Lambda} \mu_x\tilde{\psi}_x - \sqrt{2}\sum_{x\in\Lambda} \lambda_x\tilde{\eta}_x, \qquad (4.47)$$

where $\tilde{\psi}_x, \tilde{\phi}_x, \tilde{\eta}_x, \tilde{\xi}_x$ are defined through (4.36) and (4.46).

Definition 4.13 We define a self-dual cone in \mathfrak{K}_{Λ} by

$$\mathfrak{K}_{\Lambda,+} := \left\{ |\Psi\rangle \in \mathfrak{K}_{\Lambda} \ \middle| \ |\Psi\rangle = \sum_{\mathbf{n} \in \{1,2,3,4\}^{\Lambda}} C_{\mathbf{n}} |e_{\mathbf{n}}\rangle, \ C_{\mathbf{n}} \ge 0 \ \forall \mathbf{n} \in \{1,2,3,4\}^{\Lambda} \right\}, \quad (4.48)$$

where $|e_{\mathbf{n}}\rangle = \bigotimes_{x \in \Lambda} |e_{n_x}\rangle$ for each $\mathbf{n} = \{n_x\}_{x \in \Lambda} \in \{1, 2, 3, 4\}^{\Lambda}$.

Remark 4.14 $|e_{\mathbf{n}}\rangle \in \mathfrak{K}_{\Lambda,+}$ for all $\mathbf{n} \in \{1,2,3,4\}^{\Lambda}$.

Proposition 4.15 We have the following:

- (i) $\tilde{\psi}_x \geq 0$ w.r.t. $\Re_{\Lambda,+}$ for all $x \in \Lambda$.
- (ii) $\tilde{\phi}_x \ge 0$ w.r.t. $\Re_{\Lambda,+}$ for all $x \in \Lambda$.
- (iii) $-\tilde{\xi}_x \ge 0$ w.r.t. $\Re_{\Lambda,+}$ for all $x \in \Lambda$.
- (iv) $1 + \frac{1}{\sqrt{2}} \tilde{\eta}_x \ge 0 \ \mathfrak{K}_{\Lambda,+}$ for all $x \in \Lambda$.
- (v) $\exp(\beta \tilde{\psi}_x) \ge 0$ w.r.t. $\Re_{\Lambda,+}$ for all $x \in \Lambda$ and $\beta \ge 0$.
- (vi) $\exp(\beta \tilde{\eta}_x) \ge 0$ w.r.t. $\Re_{\Lambda,+}$ for all $x \in \Lambda$ and $\beta \ge 0$.

Proof. By Proposition A.2, a linear operator X in \mathfrak{K}_{Λ} satisfies $X \geq 0$ w.r.t. $\mathfrak{K}_{\Lambda,+}$ if and only if $\langle e_{\mathbf{n}} | X e_{\mathbf{m}} \rangle \geq 0$ for all $\mathbf{m}, \mathbf{n} \in \{1, 2, 3, 4\}^{\Lambda}$. Thus, the assertions immediately follow from Proposition 4.12. \Box

Corollary 4.16 $\exp(-\beta H_{\text{ext}}) \geq 0$ w.r.t. $\Re_{\Lambda,+}$ for all $\beta \geq 0$.

Proof. Set $\tilde{H}_{\text{ext}} = -\tilde{T} + \tilde{V}$, where

$$\tilde{T} = \sum_{x,y \in \Lambda} J_{xy} (\tilde{\psi}_x \tilde{\psi}_y + \tilde{\phi}_x \tilde{\phi}_y), \quad \tilde{V} = \tilde{V}_\mu + \tilde{V}_\lambda$$
(4.49)

with $\tilde{V}_{\mu} = -\sqrt{2} \sum_{x \in \Lambda} \mu_x \tilde{\psi}_x$ and $\tilde{V}_{\lambda} = -\sqrt{2} \sum_{x \in \Lambda} \lambda_x \tilde{\eta}_x$. By Proposition 4.15 (i) and (ii), it holds that $\tilde{T} \ge 0$ w.r.t. $\mathfrak{K}_{\Lambda,+}$. On the other hand, we can see that by Proposition 4.15 (v) and (vi),

$$e^{-\beta V_{\mu}} = \prod_{x \in \Lambda} \underbrace{e^{\sqrt{2}\beta\mu_{x}\tilde{\psi}_{x}}}_{\succeq 0} \succeq 0, \quad e^{-\beta V_{\lambda}} = \prod_{x \in \Lambda} \underbrace{e^{\sqrt{2}\beta\lambda_{x}\tilde{\eta}_{x}}}_{\succeq 0} \succeq 0 \tag{4.50}$$

w.r.t. $\mathfrak{K}_{\Lambda,+}$ for all $\beta \geq 0.9$ Thus, by Proposition A.4, we obtain $e^{-\beta \tilde{V}} \geq 0$ w.r.t. $\mathfrak{K}_{\Lambda,+}$ for all $\beta \geq 0$. By applying Proposition A.5, we conclude the desired assertion. \Box

⁹Here we have used the assumptions $\mu_x \ge 0$ and $\lambda_x \ge 0$.

Corollary 4.17 For all $A, B, C, D \subseteq \Lambda$, we have the following:

- (i) $\Theta^* \sigma_A^{(3)} \otimes \tau_C \Theta \succeq 0$ w.r.t. $\Re_{\Lambda,+}$.
- (ii) $\Theta^* (\sigma_B^{(3)} \otimes \tau_D \tau_D \otimes \sigma_B^{(3)}) \Theta \succeq 0 \quad w.r.t. \ \Re_{\Lambda,+}.$

Proof. (i) Let $\tilde{\ell}_x = \frac{1}{2}(\mathbb{1} + \frac{1}{\sqrt{2}}\tilde{\eta}_x)$ and $\tilde{m}_x = -\frac{1}{2\sqrt{2}}\tilde{\xi}_x$. By Proposition 4.15 (iii) and (iv), it holds that $\tilde{\ell}_x \ge 0$ and $\tilde{m}_x \ge 0$ w.r.t. $\mathfrak{K}_{\Lambda,+}$. Thus, we have

$$\Theta^* \sigma_A^{(3)} \otimes \tau_C \Theta = 2^{-|A|/2} \prod_{x \in A} (\tilde{\psi}_x + \tilde{\phi}_x) \prod_{x \in C} (\tilde{\ell}_x + \tilde{m}_x) \ge 0$$

$$(4.51)$$

w.r.t. $\mathfrak{K}_{\Lambda,+}$ by Proposition 4.15.

(ii) We have

$$\Theta^* \left(\sigma_B^{(3)} \otimes \tau_D - \tau_D \otimes \sigma_B^{(3)} \right) \Theta$$

=2^{-|B|/2} $\prod_{x \in B} \prod_{y \in D} (\tilde{\psi}_x + \tilde{\phi}_x) (\tilde{\ell}_y + \tilde{m}_y) - 2^{-|B|/2} \prod_{x \in B} \prod_{y \in D} (\tilde{\psi}_x - \tilde{\phi}_x) (\tilde{\ell}_y - \tilde{m}_y)$ (4.52)

$$= \sum_{X_1, X_2 \subset B} \sum_{Y_1, Y_2 \subset D} K_{X_1 X_2 Y_1 Y_2} \tilde{\psi}_{X_1} \tilde{\phi}_{X_2} \tilde{\ell}_{Y_1} \tilde{m}_{Y_2}$$
(4.53)

with $K_{X_1X_2Y_1Y_2} \geq 0, \tilde{\psi}_{X_1} = \prod_{x \in X_1} \tilde{\psi}_x, \ \tilde{\phi}_{X_2} = \prod_{x \in X_2} \tilde{\phi}_x, \tilde{\ell}_{Y_1} = \prod_{x \in Y_1} \tilde{\ell}_x, \ \tilde{m}_{Y_2} = \prod_{x \in Y_2} \tilde{m}_x$. Thus, $\Theta^*(\sigma_B^{(3)} \otimes \tau_D - \tau_D \otimes \sigma_B^{(3)}) \Theta \geq 0$ w.r.t. $\mathfrak{K}_{\Lambda,+}$. \Box

Proof of Theorems 4.2 and 4.5

By Corollaries 4.16, 4.17 and Theorem A.1, we have

$$\left\langle \left(\left(\sigma_{A}^{(3)}(s) \otimes \tau_{C}(s) - \tau_{C}(s) \otimes \sigma_{A}^{(3)}(s) \right) \left(\sigma_{B}^{(3)}(t) \otimes \tau_{D}(t) - \tau_{D}(t) \otimes \sigma_{B}^{(3)}(t) \right) \right\rangle \right\rangle_{\beta} = Z_{\beta}^{-2} \operatorname{Tr} \left[\underbrace{\operatorname{e}^{-s\tilde{H}_{ext}}}_{\geq 0} \underbrace{\Theta^{*} \left(\sigma_{A}^{(3)} \otimes \tau_{C} - \tau_{C} \otimes \sigma_{A}^{(3)} \right) \Theta}_{\geq 0} \underbrace{\operatorname{e}^{-(t-s)\tilde{H}_{ext}}}_{\geq 0} \right] \\ \times \underbrace{\Theta^{*} \left(\sigma_{B}^{(3)} \otimes \tau_{D} - \tau_{D} \otimes \sigma_{B}^{(3)} \right) \Theta}_{\geq 0} \underbrace{\operatorname{e}^{-(\beta-t)\tilde{H}_{ext}}}_{\geq 0} \right] \geq 0. \tag{4.54}$$

This concludes Theorem 4.2.

Similarly, we can show Theorem 4.5 by Corollary 4.17 and Theorem A.1. \square

4.4 Proof of Example 4

We only prove (i) and (ii), since (iii) and (iv) can be proved in a similar manner. Recall the Duhamel formula

$$e^{-t(A+B)} = \sum_{n\geq 0} \int_{0\leq t_1\leq t_2\leq \cdots\leq t_n\leq \beta} (-B(t_1))\cdots (-B(t_n)) e^{-tA} dt_1\cdots dt_n$$
(4.55)

for any bounded self-adjoint operators A and B with $B(t) = e^{-tA}Be^{tA}$. Using this, we have

$$\frac{\partial}{\partial J_{xy}} e^{-\beta H} = \sum_{n \ge 1} D_n, \tag{4.56}$$

$$D_n = n(J_{xy})^{n-1} \int_{0 \le t_1 \le \dots \le t_n \le \beta} T_{xy}[t_1] \cdots T_{xy}[t_n] e^{-\beta H'} dt_1 \cdots dt_n, \qquad (4.57)$$

where $T_{xy} = \sigma_x^{(3)} \sigma_y^{(3)}$, $H' = H_{\Lambda} + J_{xy} \sigma_x^{(3)} \sigma_y^{(3)}$ and $T_{xy}[t] = e^{-tH'} T_{xy} e^{tH'}$. Note that in a similar manner to Sections 4.2 and 4.3, we have the following:

- (a) $e^{-\beta \hat{H}'} \ge 0$ w.r.t. $\mathfrak{H}_{\Lambda,+}$ for all $\beta \ge 0$, where $\hat{H}' = U^* H' U$.
- (b) $e^{-\beta \tilde{H}'_{ext}} \ge 0$ w.r.t. $\Re_{\Lambda,+}$ for all $\beta \ge 0$, where $H'_{ext} = H' \otimes 1 \!\!1 + 1 \!\!1 \otimes H'$.

Hence, by setting $M_n = T_{xy}[t_1] \cdots T_{xy}[t_n]$, we obtain

$$\frac{\partial}{\partial J_{xy}} \langle \sigma_A^{(3)} \rangle_{\beta}$$

$$= \sum_{n \ge 1} n (J_{xy})^{n-1} \int_{0 \le t_1 \le \dots \le \beta} \left\{ \langle \sigma_A^{(3)} \mathsf{M}_n \rangle_{H',\beta} - \langle \sigma_A^{(3)} \rangle_{H',\beta} \langle \mathsf{M}_n \rangle_{H',\beta} \right\} dt_1 \cdots dt_n$$

$$= \sum_{n \ge 1} \frac{n (J_{xy})^{n-1}}{2} \int_{0 \le t_1 \le \dots \le \beta} \left\langle \left\langle \left(\sigma_A^{(3)} \otimes 1\!\!1 - 1\!\!1 \otimes \sigma_A^{(3)} \right) \left(\mathsf{M}_n \otimes 1\!\!1 - 1\!\!1 \otimes \mathsf{M}_n \right) \right\rangle \right\rangle_{H',\beta} dt_1 \cdots dt_n$$

$$\ge 0, \qquad (4.58)$$

where $\langle \cdot \rangle_{H',\beta}$ and $\langle \! \langle \cdot \rangle \! \rangle_{H',\beta}$ are the thermal averages associated with H' and H'_{ext} . (Here we used the facts that $\Theta^*(\sigma_A^{(3)} \otimes 1\!\!1 - 1\!\!1 \otimes \sigma_A^{(3)}) \Theta \succeq 0$ and $\Theta^*(\mathsf{M}_n \otimes 1\!\!1 - 1\!\!1 \otimes \mathsf{M}_n) e^{-\beta H'_{\text{ext}}} \Theta \succeq 0$ w.r.t. $\mathfrak{K}_{\Lambda,+}$, which follow from Corollary 4.17.) Thus, we have proved (i). Similarly, by applying the fact that $\Theta^*(\tau_A \otimes 1\!\!1 - 1\!\!1 \otimes \tau_A) \Theta \leq 0$ w.r.t. $\mathfrak{K}_{\Lambda,+}$, which follows from Corollary 4.17, we have

$$\frac{\partial}{\partial J_{xy}} \langle \tau_A \rangle_{\beta} = \sum_{n \ge 1} \frac{n (J_{xy})^{n-1}}{2} \int_{0 \le t_1 \le \dots \le \beta} \left\langle \! \left\langle \left(\tau_A \otimes 1\!\!\!1 - 1\!\!\!1 \otimes \tau_A \right) \left(\mathsf{M}_n \otimes 1\!\!\!1 - 1\!\!\!1 \otimes \mathsf{M}_n \right) \right\rangle \!\! \right\rangle_{H',\beta} dt_1 \cdots dt_n \\ \le 0. \tag{4.59}$$

Thus, we have proved (ii). \Box

5 Quantum rotor model

5.1 Results

Let Λ be a finite subset of \mathbb{R}^2 . The quantum rotor model on Λ is defined by

$$H = \sum_{x \in \Lambda} \frac{U_x}{2} \left(-i \frac{\partial}{\partial \theta_x} \right)^2 - \sum_{x,y \in \Lambda} t_{xy} \cos(\theta_x - \theta_y).$$
(5.1)

The Hilbert space is $\mathfrak{H} = \bigotimes_{x \in \Lambda} L^2(\mathbb{T})$ with $\mathbb{T} = [-\pi, \pi]$. $U_x > 0$ being the strength of the on site repulsion and $t_{xy} \ge 0$ being the hopping strength. H is a self-adjoint operator acting in the Hilbert space \mathfrak{H} .¹⁰ We refer readers who want to learn the physical background to [6, 54].

Remark 5.1 In this study, we simply write M_f , the multiplication operator by the function f, as $f(\theta)$ if no confusion occurs. \diamond

Let $T_x = e^{i\theta_x}$. For each $A = \{m_x\}_{x \in \Lambda} \in \mathbb{Z}^{\Lambda}$, we set

$$T^A = \prod_{x \in \Lambda} (T_x)^{m_x}.$$
(5.2)

Let

$$\mathfrak{A} = \operatorname{Coni}\left\{T^A \,|\, A \in \mathbb{Z}^\Lambda\right\}^{-\mathrm{w}}.$$
(5.3)

The thermal expectation value $\langle \cdot \rangle_{\beta}$ is defined by

$$\langle A \rangle_{\beta} = \operatorname{Tr} \left[A e^{-\beta H} \right] / Z_{\beta}, \quad Z_{\beta} = \operatorname{Tr} \left[e^{-\beta H} \right]$$
 (5.4)

for all $A \in \mathscr{B}(\mathfrak{H})$.

Theorem 5.2 (First Griffiths inequality) Let $A_1, \ldots, A_n \in \mathfrak{A}$. For all $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n < \beta$, we have

$$\left\langle \prod_{j=1}^{n} A_j(s_j) \right\rangle_{\beta} \ge 0.$$
(5.5)

To state second Griffiths inequality, some conditions are required. We introduce an extended Hilbert space \mathfrak{H}_{ext} by $\mathfrak{H}_{ext} = \mathfrak{H} \otimes \mathfrak{H}$. For each $X \in \mathscr{B}(\mathfrak{H}_{ext})$, we set

$$\langle\!\langle X \rangle\!\rangle_{\beta} = \operatorname{Tr}_{\mathfrak{H}_{ext}} \left[X \,\mathrm{e}^{-\beta H_{ext}} \right] \Big/ Z_{\beta}^2,$$
(5.6)

$$H_{\text{ext}} = H \otimes \mathbb{1} + \mathbb{1} \otimes H.$$
(5.7)

Let $C_x = \cos \theta_x$ and

$$C_x(s) = \mathrm{e}^{-sH} C_x \mathrm{e}^{sH}.$$
(5.8)

Theorem 5.3 (Second Griffiths inequality) For all $x_1, \ldots, x_n \in \Lambda$, $0 \le s_1 \le s_2 \le \cdots \le s_n < \beta$ and $\varepsilon_1, \ldots, \varepsilon_n \in \{\pm 1\}$, we have

$$\left\langle \left\langle \prod_{j=1}^{n} \left[C_{x_j}(s_j) \otimes 1 + \varepsilon_j 1 \otimes C_{x_j}(s_j) \right] \right\rangle \right\rangle_{\beta} \ge 0.$$
(5.9)

¹⁰The precise definition of $-i\frac{\partial}{\partial\theta}$ is given by

$$\operatorname{dom}\left(-i\frac{\partial}{\partial\theta}\right) = \{f \in C^{1}(\mathbb{T}) \mid f(-\pi) = f(\pi)\},\$$
$$-i\frac{\partial}{\partial\theta}f = -if' \quad \forall f \in \operatorname{dom}\left(-i\frac{\partial}{\partial\theta}\right).$$

Then $-i\frac{\partial}{\partial\theta}$ is essentially self-adjoint. We still denote its closure by the same symbol.

From Theorem 5.3, we immediately obtain Corollary 5.4, which has a form similar to (1.4). (This is why we call Theorem 5.3 the second Griffiths inequality, see Remark 2.16 and Theorem 2.18 for general arguments.)

Corollary 5.4 For each $A = \{m_x\}_{x \in \Lambda} \in \mathbb{N}^{\Lambda}$, set

$$C^A = \prod_{x \in \Lambda} (C_x)^{m_x}.$$
(5.10)

For all $A, B \in \mathbb{N}^{\Lambda}$, we obtain

$$\langle C^A C^B \rangle_\beta \ge \langle C^A \rangle_\beta \langle C^B \rangle_\beta.$$
 (5.11)

Let

$$n_x = -i\frac{\partial}{\partial\theta_x}.\tag{5.12}$$

Set $n_x(s) = e^{-sH} n_x e^{sH}$. We have the following.

Theorem 5.5 For all $x_1, \ldots, x_n \in \Lambda$, $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n < \beta$ and $\varepsilon_1, \ldots, \varepsilon_n \in \{\pm 1\}$, we have

$$\left\langle\!\!\left\langle\prod_{j=1}^{n}\left[n_{x_{j}}(s_{j})\otimes\mathbb{1}+\varepsilon_{j}\mathbb{1}\otimes n_{x_{j}}(s_{j})\right]\left[n_{x_{j}}(s_{j})\otimes\mathbb{1}+\overline{\varepsilon}_{j}\mathbb{1}\otimes n_{x_{j}}(s_{j})\right]\right\rangle\!\!\right\rangle_{\beta}\geq0,\qquad(5.13)$$

where $\overline{\varepsilon}_j = -\varepsilon_j$.

We can construct several extensions of Theorems 5.3 and 5.5. Theorem 5.6 illustrates this fact. Let

$$\alpha_x^{(1)}(s) = C_x(s) \otimes \mathbb{1} + \mathbb{1} \otimes C_x(s), \tag{5.14}$$

$$\alpha_x^{(2)}(s) = C_x(s) \otimes \mathbb{1} - \mathbb{1} \otimes C_x(s), \tag{5.15}$$

$$\alpha_x^{(3)}(s) = \left[n_x(s) \otimes \mathbb{1} + \mathbb{1} \otimes n_x(s) \right] \left[n_x(s) \otimes \mathbb{1} - \mathbb{1} \otimes n_x(s) \right].$$
(5.16)

Theorem 5.6 For all $x_1, \ldots, x_n \in \Lambda$, $\mu_1, \ldots, \mu_n \in \{1, 2, 3\}$ and $0 \le s_1 \le s_2 \le \cdots \le s_n \le \beta$, we have

$$\left\langle\!\!\left\langle \prod_{j=1}^{n} \alpha_{x_{j}}^{(\mu_{j})}(s_{j}) \right\rangle\!\!\right\rangle_{\beta} \ge 0.$$
(5.17)

Example 5 For all $A \subseteq \Lambda$ and $x, y, z \in \Lambda$, we have the following:

- (i) $\langle C^A \rangle_\beta$ is monotonically increasing in t_{xy} .
- (ii) $\langle n_z^2 \rangle_\beta$ is monotonically increasing in t_{xy} .
- (iii) $\left. \frac{\partial}{\partial U_x} \langle C^A \rangle_\beta \right|_{U_x=0} \le 0.$

We will provide a proof of this example in Section 5.4. \Diamond

Remark 5.7 (i) Our results can be extended to a more general Hamiltonian of the form

$$H = \sum_{x \in \Lambda} \frac{U_x}{2} \left(-i \frac{\partial}{\partial \theta_x} \right)^2 - \sum_{A \in \mathbb{N}^\Lambda} J_A C^A$$
(5.18)

with $J_A \ge 0$, where the sum converges under a uniform topology.

(ii) Since the ground state of H is unique, our results are valid at $\beta = \infty$. The results at $\beta = \infty$ are essential for the study of quantum phase transitions [36]. \diamond

5.2 Proof of Theorem 5.2

Let \mathcal{F} be the Fourier transformation ¹¹ on \mathfrak{H} and let $\hat{H} = \mathcal{F}H\mathcal{F}^{-1}$. We have

$$\hat{H} = \sum_{x \in \Lambda} \frac{U_x}{2} \hat{n}_x^2 + \frac{1}{2} \sum_{x,y \in \Lambda} (-t_{xy}) (\hat{T}_x \hat{T}_y^* + \hat{T}_x^* \hat{T}_y).$$
(5.20)

 \hat{H} acts in the Hilbert space $\hat{\mathfrak{H}} = \mathcal{F}\mathfrak{H} = \otimes_{x \in \Lambda} \ell^2(\mathbb{Z})$. \hat{n}_x and \hat{T}_x are defined by $\hat{n}_x = \mathcal{F}n_x \mathcal{F}^{-1}$ and $\hat{T}_x = \mathcal{F}T_x \mathcal{F}^{-1}$.

For each $n \in \mathbb{Z}$, set $e_n(m) = \delta_{mn} \in \ell^2(\mathbb{Z})$. $\{e_n \mid n \in \mathbb{Z}\}$ is a CONS in $\ell^2(\mathbb{Z})$. For each $\mathbf{n} = \{n_x\}_{x \in \Lambda} \in \mathbb{Z}^{\Lambda}$, let $e_{\mathbf{n}} = \bigotimes_{x \in \Lambda} e_{n_x}$. Clearly, $\{e_{\mathbf{n}} \mid \mathbf{n} \in \mathbb{Z}^{\Lambda}\}$ is a CONS of $\hat{\mathfrak{H}}$ as well. Remarkably, for each $\mathbf{n} = \{n_x\}_{x \in \Lambda} \in \mathbb{Z}^{\Lambda}$,

$$\hat{n}_x e_{\mathbf{n}} = n_x e_{\mathbf{n}}, \quad T_x e_{\mathbf{n}} = e_{\mathbf{n} + \boldsymbol{\delta}_x}, \tag{5.21}$$

where $\delta_x = {\delta_{xy}}_{y \in \Lambda} \in \mathbb{Z}^{\Lambda}$. In other words, \hat{n}_x is the number operator and \hat{T}_x is the creation operator at site x.

Definition 5.8 Let

$$\hat{\mathfrak{H}}_{+} = \left\{ F = \sum_{\mathbf{n}\in\mathbb{Z}^{\Lambda}} F(\mathbf{n})e_{\mathbf{n}} \in \hat{\mathfrak{H}} \, \middle| \, F(\mathbf{n}) \ge 0 \; \forall \mathbf{n}\in\mathbb{Z}^{\Lambda} \right\}.$$
(5.22)

Note that $\hat{\mathfrak{H}}_+$ is a self-dual cone in $\hat{\mathfrak{H}}$. Clearly, $e_{\mathbf{n}} \in \hat{\mathfrak{H}}_+$ for all $\mathbf{n} \in \mathbb{Z}^{\Lambda}$.

Proposition 5.9 We have the following:

- (i) $\hat{T}_x \ge 0$ w.r.t. $\hat{\mathfrak{H}}_+$ for all $x \in \Lambda$.
- (ii) $e^{-\beta \hat{H}} \ge 0$ w.r.t. $\hat{\mathfrak{H}}_+$ for all $\beta \ge 0$.

$$(\mathcal{F}f)(\mathbf{n}) = (2\pi)^{-|\Lambda|/2} \int_{\mathbb{T}^{\Lambda}} f(\boldsymbol{\theta}) e^{-i\boldsymbol{\theta}\cdot\mathbf{n}} d\boldsymbol{\theta} \quad \forall f \in \mathfrak{H}.$$
(5.19)

¹¹To be precise, \mathcal{F} is a unitary operator given by

Proof. (i) Note that $\hat{\mathfrak{H}}_+ = \operatorname{Coni}\{e_{\mathbf{n}} | \mathbf{n} \in \mathbb{Z}^{\Lambda}\}^-$, where $\operatorname{Coni}(S)^-$ is the closure of $\operatorname{Coni}(S)$. Thus, it suffices to show that $\hat{T}_x e_{\mathbf{n}} \geq 0$ w.r.t. $\hat{\mathfrak{H}}_+$ for all $\mathbf{n} \in \mathbb{Z}^{\Lambda}$. This is trivial according to (5.21).

(ii) Let

$$-\hat{\mathbf{K}} = \frac{1}{2} \sum_{x,y \in \Lambda} t_{xy} (\hat{T}_x \hat{T}_y^* + \hat{T}_x^* \hat{T}_y), \quad \hat{\mathbf{U}} = \sum_{x \in \Lambda} \frac{U_x}{2} \hat{n}_x^2.$$
(5.23)

By (i), we can see that $-\hat{\mathbf{K}} \ge 0$ w.r.t. $\hat{\mathfrak{H}}_+$. On the other hand, since

$$e^{-\beta \hat{\mathbf{U}}} e_{\mathbf{n}} = \underbrace{\exp\left\{-\beta \sum_{x \in \Lambda} \frac{U_x}{2} n_x^2\right\}}_{\geq 0} e_{\mathbf{n}} \text{ for all } \mathbf{n} = \{n_x\} \in \mathbb{Z}^{\Lambda},$$
(5.24)

we have $e^{-\beta \hat{\mathbf{U}}} \geq 0$ w.r.t. $\hat{\mathfrak{H}}_+$. Thus, by Proposition A.5, we conclude (ii). \Box

5.2.1 Completion of proof of Theorem 5.2

By Proposition 5.9 (i), we have $A \ge 0$ w.r.t. $\hat{\mathfrak{H}}_+$ for all \mathfrak{A} . Applying Theorem 2.7, we prove Theorem 5.2. \Box

5.3 Proof of Theorems 5.3, 5.5, and 5.6 and Corollary 5.4

First, note the following identification:

$$\mathfrak{H}_{\text{ext}} = L^2 \big(\mathbb{T}^{\Lambda} \times \mathbb{T}^{\Lambda}, d\boldsymbol{\theta} d\boldsymbol{\theta}' \big).$$
(5.25)

Under the identification (5.25), we see that

$$H_{\text{ext}} = H \otimes \mathbb{1} + \mathbb{1} \otimes H$$
$$= \sum_{x \in \Lambda} \frac{U_x}{2} \left\{ \left(-i \frac{\partial}{\partial \theta_x} \right)^2 + \left(-i \frac{\partial}{\partial \theta'_x} \right)^2 \right\}$$
$$- \sum_{x,y \in \Lambda} t_{xy} \left\{ \cos(\theta_x - \theta_y) + \cos(\theta'_x - \theta'_y) \right\}.$$
(5.26)

Next, we introduce a new coordinate system $\{\phi_x, \phi'_x\}$ with

$$\phi_x = \frac{1}{2}(\theta'_x - \theta_x), \quad \phi'_x = \frac{1}{2}(\theta'_x + \theta_x).$$
(5.27)

Then we easily see that

$$\mathfrak{H}_{\text{ext}} = L^2 \big(\mathbb{T}^{\Lambda} \times \mathbb{T}^{\Lambda}, d\phi d\phi' \big).$$
(5.28)

Using the identity

$$\cos\theta + \cos\theta' = 2\cos\frac{\theta' + \theta}{2}\cos\frac{\theta' - \theta}{2}, \qquad (5.29)$$

we obtain

$$H_{\text{ext}} = \sum_{x \in \Lambda} \frac{U_x}{4} (\nu_x^2 + \nu_x'^2) - 2 \sum_{x,y \in \Lambda} t_{xy} \cos(\phi_x - \phi_y) \cos(\phi_x' - \phi_y'), \qquad (5.30)$$

where

$$\nu_x = -i\frac{\partial}{\partial\phi_x}, \quad \nu'_x = -i\frac{\partial}{\partial\phi'_x}.$$
(5.31)

Let $\mathfrak{X} = L^2(\mathbb{T}^{\Lambda}, d\phi)$. Then by (5.28), we obtain the following identification:

$$\mathfrak{H}_{\text{ext}} = L^2(\mathbb{T}^\Lambda, d\phi) \otimes L^2(\mathbb{T}^\Lambda, d\phi) = \mathfrak{X} \otimes \mathfrak{X}.$$
(5.32)

Moreover, we obtain the following proposition.

Proposition 5.10 We have $H_{\text{ext}} = T - V$, where

$$\mathsf{T} = \sum_{x \in \Lambda} \frac{U_x}{4} \left(\nu_x^2 \otimes \mathbb{1} + \mathbb{1} \otimes \nu_x^2 \right), \tag{5.33}$$

$$\mathsf{V} = 2\sum_{x,y\in\Lambda} t_{xy}\cos(\phi_x - \phi_y) \otimes \cos(\phi_x - \phi_y). \tag{5.34}$$

Let ϑ be the antilinear isomorphism defined by

$$(\vartheta f)(\phi) = \overline{f}(\phi) \quad \text{a.e.}, \quad f \in L^2(\mathbb{T}^\Lambda, d\phi).$$
 (5.35)

By (3.4) and (5.32), we have the identification $\mathfrak{H}_{ext} = \mathscr{L}^2(\mathfrak{X})$ by ϑ . Moreover, by (3.4), we have the following proposition:

Proposition 5.11 We have $H_{ext} = T - V$, where

$$\mathsf{T} = \sum_{x \in \Lambda} \frac{U_x}{4} \big\{ \mathcal{L}(\nu_x^2) + \mathcal{R}(\nu_x^2) \big\},\tag{5.36}$$

$$\mathsf{V} = 2 \sum_{x,y \in \Lambda} t_{xy} \mathcal{L} \Big[\cos(\phi_x - \phi_y) \Big] \mathcal{R} \Big[\cos(\phi_x - \phi_y) \Big].$$
(5.37)

By Corollary A.9, we immediately obtain the following:

Corollary 5.12 We have $\exp(-\beta H_{\text{ext}}) \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$ for all $\beta \ge 0$.

5.3.1 Completion of proof of Theorem 5.3 and Corollary 5.4

Proposition 5.13 We have the following:

- (i) $\cos \theta_x \otimes \mathbb{1} + \mathbb{1} \otimes \cos \theta_x = 2\mathcal{L}(\cos \phi_x)\mathcal{R}(\cos \phi_x) \succeq 0 \ w.r.t. \ \mathscr{L}^2(\mathfrak{X})_+.$
- (ii) $\cos \theta_x \otimes \mathbb{1} \mathbb{1} \otimes \cos \theta_x = 2\mathcal{L}(\sin \phi_x)\mathcal{R}(\sin \phi_x) \succeq 0 \ w.r.t. \ \mathscr{L}^2(\mathfrak{X})_+.$

Proof. (i), (ii) We apply Ginibre's idea [20]:

$$\cos a + \cos b = 2\cos\frac{b+a}{2}\cos\frac{b-a}{2},$$
 (5.38)

$$\cos a - \cos b = 2\sin\frac{b+a}{2}\sin\frac{b-a}{2}. \quad \Box$$
(5.39)

Put

$$2V_x^{(\varepsilon)} = C_x \otimes 1 + \varepsilon 1 \otimes C_x, \quad \varepsilon = \pm 1.$$
(5.40)

Then by Proposition 5.13, we have $V_x^{(\varepsilon)} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$ for all $x \in \Lambda$ and $\varepsilon \in \{\pm 1\}$. Since $\exp(-\beta H_{\text{ext}}) \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$ for all $\beta \ge 0$ by Corollary 5.12, we can apply Theorem 3.11. Thus, we conclude Theorem 5.3.

For each $\mathcal{A} \subseteq \Lambda$, define $[\mathcal{A}] = \{m_x\}_{x \in \Lambda} \in \{0, 1\}^{\Lambda}$ by $m_x = 1$ if $x \in \mathcal{A}$ and $m_x = 0$ otherwise. For simplicity, we will consider the case where $\mathcal{A} = [\mathcal{A}]$ and $\mathcal{B} = [\mathcal{B}]$. To prove Corollary 5.4, we note

$$C_x \otimes \mathbb{1} = V_x^{(+1)} + V_x^{(-1)}, \quad \mathbb{1} \otimes C_x = V_x^{(+1)} - V_x^{(-1)}.$$
 (5.41)

Observe that

$$2\langle C^{A}C^{B}\rangle_{\beta} - 2\langle C^{A}\rangle_{\beta}\langle C^{B}\rangle_{\beta}$$

$$= \left\langle \left\langle \left(C^{A} \otimes \mathbb{1} - \mathbb{1} \otimes C^{A}\right) \left(C^{B} \otimes \mathbb{1} - \mathbb{1} \otimes C^{B}\right) \right\rangle \right\rangle_{\beta}$$

$$= \sum_{\mathcal{X} \subseteq \mathcal{A}} \sum_{\mathcal{Y} \subseteq \mathcal{B}} \underbrace{\left[1 - (-1)^{|\mathcal{X}|}\right] \left[1 - (-1)^{|\mathcal{Y}|}\right]}_{\geq 0} \underbrace{\left\langle \left\langle V_{\mathcal{A} \setminus \mathcal{X}}^{(+1)} V_{\mathcal{X}}^{(-1)} V_{\mathcal{B} \setminus \mathcal{Y}}^{(+1)} V_{\mathcal{Y}}^{(-1)} \right\rangle \right\rangle_{\beta}}_{\geq 0 \text{ by Theorem 5.3}} \geq 0, \quad (5.42)$$

where $V_{\mathcal{A}}^{(\pm 1)} = \prod_{x \in \mathcal{A}} V_x^{(\pm 1)}$. Hence, we conclude Corollary 5.4. \Box

5.3.2 Completion of proof of Theorem 5.5

Proposition 5.14 For all $x \in \Lambda, \beta \ge 0$ and $\varepsilon \in \{\pm 1\}$, we have

$$(n_x \otimes \mathbb{1} + \mathbb{1} \otimes n_x)(n_x \otimes \mathbb{1} - \mathbb{1} \otimes n_x) \succeq 0 \quad w.r.t. \ \mathscr{L}^2(\mathfrak{X})_+.$$
(5.43)

Proof. Note that since $\vartheta \nu_x^* \vartheta = -\nu_x$, we have

$$n_x \otimes 1 + 1 \otimes n_x = 1 \otimes \nu_x = -\mathcal{R}(\nu_x), \tag{5.44}$$

and

$$n_x \otimes \mathbb{1} - \mathbb{1} \otimes n_x = -\nu_x \otimes \mathbb{1} = -\mathcal{L}(\nu_x).$$
(5.45)

Thus, we have $(n_x \otimes 1 + 1 \otimes n_x)(n_x \otimes 1 - 1 \otimes n_x) = \mathcal{L}(\nu_x)\mathcal{R}(\nu_x) \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$. \Box

By Proposition 5.14, we see that

$$\prod_{j=1}^{n} \left[n_{x_{j}}(s_{j}) \otimes \mathbb{1} + \mathbb{1} \otimes n_{x_{j}}(s_{j}) \right] \left[n_{x_{j}}(s_{j}) \otimes \mathbb{1} - \mathbb{1} \otimes n_{x_{j}}(s_{j}) \right] e^{-\beta H_{\text{ext}}}$$

$$= \underbrace{e^{-sH_{\text{ext}}}}_{\geq 0} \underbrace{\left[n_{x_{1}} \otimes \mathbb{1} + \mathbb{1} \otimes n_{x_{1}} \right] \left[n_{x_{1}} \otimes \mathbb{1} - \mathbb{1} \otimes n_{x_{1}} \right]}_{\geq 0} \underbrace{e^{-(s_{2}-s_{1})H_{\text{ext}}}}_{\geq 0} \times \cdots}_{\geq 0} \times \cdots$$

$$\cdots \times \underbrace{\left[n_{x_{n}} \otimes \mathbb{1} + \mathbb{1} \otimes n_{x_{n}} \right] \left[n_{x_{n}} \otimes \mathbb{1} - \mathbb{1} \otimes n_{x_{n}} \right]}_{\geq 0} \underbrace{e^{-(\beta-s_{n})H_{\text{ext}}}}_{\geq 0} \geq 0 \quad \text{w.r.t. } \mathscr{L}^{2}(\mathfrak{X})_{+}.$$

$$(5.46)$$

Therefore, Theorem 5.5 follows from Proposition 3.9. \Box

5.3.3 Completion of proof of Theorem 5.6

By Propositions 5.13 and 5.14, we know $\left[\prod_{j=1}^{n} \alpha_{x_j}^{(\mu_j)}(s_j)\right] e^{-\beta H_{\text{ext}}} \succeq 0 \text{ w.r.t. } \mathscr{L}^2(\mathfrak{X})_+.$ Thus, Theorem 5.6 immediately follows from Proposition 3.9. \Box

5.4 Proof of Example 5

The proof of Example 5 is similar to that of Example 4, so we only provide a sketch. By the Duhamel formula (4.55), we obtain

$$\frac{\partial}{\partial t_{xy}} \langle C^A \rangle_{\beta} = \sum_{n \ge 1} \frac{n(t_{xy})^{n-1}}{2} \int_{0 \le t_1 \le \dots \le t_n \le \beta} \left\langle \! \left\langle \left(C^A \otimes 1\!\!\!1 - 1\!\!1 \otimes C^A \right) \left(\mathsf{K}_n \otimes 1\!\!1 - 1\!\!1 \otimes \mathsf{K}_n \right) \right\rangle \! \right\rangle_{H'_{\text{ext}},\beta} dt_1 \cdots dt_n \right\rangle \right\rangle$$
(5.47)

where $\mathsf{K}_n = \mathrm{e}^{-t_1 H'} \cos(\theta_x - \theta_y) \mathrm{e}^{t_1 H'} \cdots \mathrm{e}^{-t_n H'} \cos(\theta_x - \theta_y) \mathrm{e}^{t_n H'}$ with $H' = H + t_{xy} \cos(\theta_x - \theta_y)$ and $H'_{\text{ext}} = H' \otimes \mathbb{1} + \mathbb{1} \otimes H'$. Since $\mathrm{e}^{-t H'_{\text{ext}}} \succeq 0$, $C^A \otimes \mathbb{1} - \mathbb{1} \otimes C^A \succeq 0$ and $\mathsf{K}_n \otimes \mathbb{1} - \mathbb{1} \otimes \mathsf{K}_n \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$, we know that the RHS of (5.47) is positive. Thus, we obtain (i). Similarly, we have

Hence, we arrive at (ii).

(iii) Let $H'' = H - \frac{U_x}{2}n_x^2$. By Proposition 5.14, Corollary 5.12, and the Duhamel formula (4.55), we obtain

$$\frac{\partial}{\partial U_x} \langle C^A \rangle_\beta \Big|_{U_x=0} = -\frac{\beta}{2} \int_0^\beta \left\langle \!\! \left\langle \underbrace{\left(C^A \otimes 1\!\!\!1 - 1\!\!\!1 \otimes C^A \right)}_{\succeq 0} \underbrace{\mathrm{e}^{-tH_{\mathrm{ext}}''}}_{\succeq 0} \underbrace{\left(n_x^2 \otimes 1\!\!\!1 - 1\!\!\!1 \otimes n_x^2 \right)}_{\succeq 0} \operatorname{e}^{tH_{\mathrm{ext}}''} \right\rangle \!\! \right\rangle_{H_{\mathrm{ext}}'',\beta} dt \le 0,$$
(5.49)

where $H''_{\text{ext}} = H'' \otimes \mathbb{1} + \mathbb{1} \otimes H''$. This completes the proof. \Box

6 Bose–Hubbard model

6.1 Results

Let Λ be a finite subset of \mathbb{R}^d . The Bose–Hubbard model on Λ is defined by

$$H = \sum_{x,y \in \Lambda} (-t_{xy}) a_x^* a_y + \sum_{x \in \Lambda} U_x n_x (n_x - 1) - \sum_{x \in \Lambda} \lambda_x (a_x^* + a_x) - \mu N_{\rm b}.$$
(6.1)

H acts in the bosonic Fock space $\mathfrak{B} = \bigoplus_{n=0}^{\infty} \otimes_{\mathrm{s}}^{n} \ell^{2}(\Lambda)$, where $\otimes_{\mathrm{s}}^{n} \ell^{2}(\Lambda)$ is the *n*-fold symmetric tensor product of $\ell^{2}(\Lambda)$ with $\otimes_{\mathrm{s}}^{0} \ell^{2}(\Lambda) = \mathbb{C}$. a_{x} is the bosonic annihilation operator satisfying the canonical commutation relations (CCRs):

$$[a_x, a_y^*] = \delta_{xy}, \quad [a_x, a_y] = 0.$$
(6.2)

 $n_x = a_x^* a_x$ is the number operator at site $x \in \Lambda$ and $N_b = \sum_{x \in \Lambda} n_x$ is the total number operator.

We assume the following:

- (A. 1) $t_{xy} \ge 0$, $U_x > 0$, $\lambda_x \ge 0$ for all $x, y \in \Lambda$.
- (A. 2) $t_{xy} = t_{yx}$ for all $x, y \in \Lambda$ and $t_{xx} = 0$ for all $x \in \Lambda$.
- (A. 3) $\mu \in \mathbb{R}$.

Under these conditions, we see that $e^{-\beta H}$ is in the trace class for all $\beta > 0$. The thermal expectation value is defined as

$$\langle X \rangle_{\beta} = \operatorname{Tr} \left[X e^{-\beta H} \right] / Z_{\beta}, \quad Z_{\beta} = \operatorname{Tr} \left[e^{-\beta H} \right].$$
 (6.3)

For each densely defined linear operator X, $X^{\#}$ (# = + or -) means

$$X^{\#} = \begin{cases} X & \text{if } \# = -\\ X^* & \text{if } \# = +. \end{cases}$$
(6.4)

Set $\mathbb{N}_0 = \{0\} \cup \mathbb{N}$. For each $\mathbf{m} = \{m_x\}_{x \in \Lambda} \in \mathbb{N}_0^{\Lambda}$ and $\# = \{\#_x\}_{x \in \Lambda} \in \{\pm\}^{\Lambda}$, define

$$I(\mathbf{m}; \#) = \prod_{x \in \Lambda} \left(a_x^{\#_x} \right)^{m_x} \tag{6.5}$$

with $(a_x^{\#_x})^0 = 1$. Now we define

$$\mathfrak{A} = \operatorname{Coni}\Big\{ I(\mathbf{m}; \#) \ \Big| \ \mathbf{m} \in \mathbb{N}_0^{\Lambda}, \ \# \in \{\pm\}^{\Lambda} \Big\}.$$
(6.6)

Note that for all $A \in \mathfrak{A}$, $A e^{-\beta H}$ is in the trace class for all $\beta > 0$. Thus, $\langle A \rangle_{\beta}$ is finite.

Theorem 6.1 (First Griffiths inequality) Let $A_1, \ldots, A_n \in \mathfrak{A}$. For all $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n < \beta$, we have

$$\left\langle \prod_{j=1}^{n} A_j(s_j) \right\rangle_{\beta} \ge 0, \tag{6.7}$$

where $A(s) = e^{-sH}Ae^{sH}$.

To state the second quantum Griffiths inequality, we introduce the following notation:

$$\langle\!\langle Y \rangle\!\rangle_{\beta} := \operatorname{Tr}_{\mathfrak{B}\otimes\mathfrak{B}} \left[Y \,\mathrm{e}^{-\beta H_{\mathrm{ext}}} \right] / Z_{\beta}^2, \quad H_{\mathrm{ext}} = H \otimes \mathbb{1} + \mathbb{1} \otimes H.$$
 (6.8)

Theorem 6.2 Let $x_1, \ldots, x_n, y_1, \ldots, y_n \in \Lambda$. For each $0 \le s_1 \le t_1 \le s_2 \le t_2 \le \cdots \le s_n \le t_n < \beta$, $\#_1, \ldots, \#_n \in \{\pm\}$ and $\varepsilon_1, \ldots, \varepsilon_n \in \{\pm 1\}$, we have

$$\left\langle\!\!\left\langle\prod_{j=1}^{n}\left[a_{x_{j}}^{\#_{j}}(s_{j})\otimes\mathbb{1}+\varepsilon_{j}\mathbb{1}\otimes a_{x_{j}}^{\#_{j}}(s_{j})\right]\left[a_{y_{j}}^{\overline{\#}_{j}}(t_{j})\otimes\mathbb{1}+\varepsilon_{j}\mathbb{1}\otimes a_{y_{j}}^{\overline{\#}_{j}}(t_{j})\right]\right\rangle\!\!\right\rangle_{\beta}\geq0,\qquad(6.9)$$

where $\overline{\#} = -\# {}^{12}$ and $a_x^{\#}(s) = e^{-sH} a_x^{\#} e^{sH}$.

Example 6 Consider the case where n = 1, $\varepsilon_1 = -1$, and $\#_1 = +$. Then we have

$$\langle a_x^*(s)a_y(t)\rangle_\beta - \langle a_x^*\rangle_\beta \langle a_y\rangle_\beta \ge 0 \tag{6.10}$$

for all $x, y \in \Lambda$ and $0 \le s \le t < \beta$. From this, we have

$$(a_x^*, a_y)_\beta - \langle a_x^* \rangle_\beta \langle a_y \rangle_\beta \ge 0.$$
(6.11)

In addition, by Theorem 6.1, it follows that

$$(a_x^*, a_y)_{\beta} \ge 0, \quad \langle a_x^* \rangle_{\beta} \ge 0, \quad \langle a_y \rangle_{\beta} \ge 0. \qquad \diamondsuit$$
 (6.12)

We can generalize Theorem 6.2. To state our result, we need to introduce the following:

$$\alpha_{\pm 1,x} = a_x \otimes 1 \!\!\!1 + 1 \!\!1 \otimes a_x, \tag{6.13}$$

$$\alpha_{-1,x} = -i \big(a_x \otimes \mathbb{1} - \mathbb{1} \otimes a_x \big), \tag{6.14}$$

where $i = \sqrt{-1}$.

¹²To be precise, $\overline{+} = -$ and $\overline{-} = +$.

Theorem 6.3 (Second Griffiths inequality) Let $x_1, \ldots, x_n \in \Lambda$. For all $\#_1, \ldots, \#_n \in \{\pm\}$, $\varepsilon_1, \ldots, \varepsilon_n \in \{\pm1\}$ and $0 \le s_1 \le s_2 \le \cdots \le s_n < \beta$, we have

$$\left\langle\!\!\left\langle\prod_{j=1}^{n} \alpha_{\varepsilon_{j}, x_{j}}^{\#_{j}}(s_{j})\right\rangle\!\!\right\rangle_{\beta} \ge 0, \tag{6.15}$$

where $\alpha_{\varepsilon,x}^{\#}(s) = e^{-sH_{\text{ext}}} \alpha_{\varepsilon,x}^{\#} e^{sH_{\text{ext}}}$.

Remark 6.4 If $\lambda_x > 0$ for all $x \in \Lambda$, then we can prove that the ground state of H is unique¹³. In this case, our results are valid at $\beta = \infty$.

Example 7 Consider the case where n = 3, $\#_1 = +, \#_2 = \#_3 = -$, and $\varepsilon_1 \varepsilon_2 \varepsilon_3 = 1$. We have

$$\langle a_1^* a_2 a_3 \rangle - \langle a_1^* \rangle \langle a_2 a_3 \rangle - \langle a_2 \rangle \langle a_1^* a_3 \rangle + \langle a_3 \rangle \langle a_1^* a_2 \rangle \ge 0$$
(6.16)

for $(\varepsilon_1, \varepsilon_2, \varepsilon_3) = (-1, -1, +1)$, and

$$\langle a_1^* a_2 a_3 \rangle - \langle a_1^* \rangle \langle a_2 a_3 \rangle + \langle a_2 \rangle \langle a_1^* a_3 \rangle - \langle a_3 \rangle \langle a_1^* a_2 \rangle \ge 0$$
(6.17)

for $(\varepsilon_1, \varepsilon_2, \varepsilon_3) = (-1, +1, -1)$, where we use the abbreviation $a_j^{\#} = a_{x_j}^{\#}(s_j)$. On the other hand, we have

$$\langle a_1^* a_2 a_3 \rangle + \langle a_1^* \rangle \langle a_2 a_3 \rangle - \langle a_2 \rangle \langle a_1^* a_3 \rangle - \langle a_3 \rangle \langle a_1^* a_2 \rangle \le 0$$
(6.18)

for $(\varepsilon_1, \varepsilon_2, \varepsilon_3) = (+1, -1, -1)$. Combining (6.16) and (6.17), we get

$$\langle a_1^* a_2 a_3 \rangle - \langle a_1^* \rangle \langle a_2 a_3 \rangle \ge 0.$$
 \diamond (6.19)

If $U_x \equiv 0$, then we obtain a stronger result as follows.

Theorem 6.5 Assume that $U_x = 0$ for all $x \in \Lambda$. Assume that the matrix $(-t_{xy} - \mu \delta_{xy})_{x,y}$ is positive-definite.¹⁴ Let $x_1, \ldots, x_n \in \Lambda$. For all $\#_1, \ldots, \#_n \in \{\pm\}, \varepsilon_1, \ldots, \varepsilon_n \in \{\pm1\}$ and $0 \leq s_1 \leq \cdots \leq s_n < \beta$, we have

$$\left\langle \left\langle \prod_{j=1}^{n} \left[a_{x_j}^{\#_j}(s_j) \otimes 1 + \varepsilon_j 1 \otimes a_{x_j}^{\#_j}(s_j) \right] \right\rangle \right\rangle_{\beta} \ge 0.$$
(6.20)

Corollary 6.6 Under the same assumptions as Theorem 6.5, we have

$$\langle A_1 A_2 \rangle_\beta - \langle A_1 \rangle_\beta \langle A_2 \rangle_\beta \ge 0 \tag{6.21}$$

for all $A_1, A_2 \in \mathfrak{A}$.

Example 8 Let $A \in \mathfrak{A}$. Under the same assumptions as in Theorem 6.5, we have the following:

- (i) $\langle A \rangle_{\beta}$ is monotonically increasing in t_{xy} .
- (ii) $\langle A \rangle_{\beta}$ is monotonically increasing in λ_x .

The proofs of these properties are similar to those of Examples 4 and 5. \Diamond

¹³This fact follows from an application of the Perron–Frobenius–Faris theorem[12].

¹⁴This assumption is needed in order to guarantee that $e^{-\beta H}$ is a trace class operator.

6.2 Proof of Theorem 6.1

In this section, we will often discuss unbounded operators. Thus, we have to extend definitions of our operator inequalities as follows:

Definition 6.7 Let A be a densely defined linear operator in \mathfrak{H} . If $Ax \ge 0$ w.r.t. \mathfrak{P} for all $x \in \mathfrak{P} \cap \operatorname{dom}(A)$, then we also write $A \ge 0$ w.r.t. \mathfrak{P} . Note that

$$\langle x|Ay \rangle \ge 0 \quad \text{for all } x \in \mathfrak{P} \text{ and } y \in \mathfrak{P} \cap \operatorname{dom}(A). \quad \diamondsuit$$
 (6.22)

For each $\mathbf{N} = \{N_x\}_{x \in \Lambda} \in \mathbb{N}_0^{\Lambda}$, we set

$$|\mathbf{N}\rangle = \left(\prod_{x\in\Lambda} N_x!\right)^{-1/2} \prod_{x\in\Lambda} (a_x^*)^{N_x} \Omega, \qquad (6.23)$$

where Ω is the Fock vacuum. Then $\{|\mathbf{N}\rangle | \mathbf{N} \in \mathbb{N}_0^{\Lambda}\}$ is a CONS of \mathfrak{B} .

Definition 6.8 A standard self-dual cone in \mathfrak{B} is defined by

$$\mathfrak{B}_{+} = \left\{ \psi \in \mathfrak{B} \ \middle| \ \psi = \sum_{\mathbf{N} \in \mathbb{N}_{0}^{\Lambda}} \psi_{\mathbf{N}} | \mathbf{N} \rangle, \ \psi_{\mathbf{N}} \ge 0 \ \forall \mathbf{N} \in \mathbb{N}_{0}^{\Lambda} \right\}.$$
(6.24)

 \mathfrak{B}_+ was introduced by Fröhlich [16], see also [46]. \diamond

Remark 6.9 $|\mathbf{N}\rangle \in \mathfrak{B}_+$ for all $\mathbf{N} \in \mathbb{N}_0^{\Lambda}$.

The following lemma is useful in this section.

Lemma 6.10 Let A be a densely defined linear operator on \mathfrak{B} . Let P_{ℓ} be the orthogonal projection onto $\bigoplus_{n=0}^{\ell} \bigotimes_{s}^{n} \ell^{2}(\Lambda)$. Assume the following:

- (i) $|\mathbf{N}\rangle \in \operatorname{dom}(A)$ for all $\mathbf{N} \in \mathbb{N}_0^{\Lambda}$.
- (ii) $AP_{\ell}\varphi \to A\varphi \text{ as } \ell \to \infty \text{ for all } \varphi \in \operatorname{dom}(A).$

Then the following are equivalent.

- (a) $A \succeq 0$ w.r.t. \mathfrak{B}_+ .
- (b) $\langle \mathbf{M} | A | \mathbf{N} \rangle \geq 0$ for all $\mathbf{M}, \mathbf{N} \in \mathbb{N}_0^{\Lambda 15}$.

Proof. (a) \Longrightarrow (b): This is immediate.

(b) \Longrightarrow (a): Let $A_{\ell} = P_{\ell}AP_{\ell}$. Then, for all $\varphi \in \mathfrak{B}_+$ and $\psi \in \operatorname{dom}(A) \cap \mathfrak{B}_+$, we see that

$$\langle \varphi | A_{\ell} \psi \rangle = \sum_{|\mathbf{M}| \le \ell, |\mathbf{N}| \le \ell} \underbrace{\varphi_{\mathbf{M}}}_{\ge 0} \underbrace{\psi_{\mathbf{N}}}_{\ge 0} \underbrace{\langle \mathbf{M} | A | \mathbf{N} \rangle}_{\ge 0} \ge 0, \tag{6.25}$$

where $|\mathbf{N}| = \sum_{x \in \Lambda} N_x$. Taking $\ell \to \infty$, we obtain $\langle \varphi | A \psi \rangle \ge 0$, which implies $A \psi \ge 0$ w.r.t. \mathfrak{B}_+ . \Box

 $^{^{15}\}langle\psi|X|\phi\rangle := \langle\psi|X\phi\rangle.$

Proposition 6.11 We have $a_x \ge 0$, $a_x^* \ge 0$ w.r.t. \mathfrak{B}_+ for all $x \in \Lambda$.

Proof. It is not difficult to verify that a_x and a_x^* satisfy the assumptions of Lemma 6.10. Moreover, we see that $\langle \mathbf{M} | a_x | \mathbf{N} \rangle \geq 0$ and $\langle \mathbf{M} | a_x^* | \mathbf{N} \rangle \geq 0$ for all $\mathbf{M}, \mathbf{N} \in \mathbb{N}_0^{\Lambda}$. Thus, we obtain the desired assertion by Lemma 6.10. \Box

Corollary 6.12 For all $A \in \mathfrak{A}$, it holds that $A \succeq 0$ w.r.t. \mathfrak{B}_+ .

Proposition 6.13 We have $e^{-\beta H} \ge 0$ w.r.t. \mathfrak{B}_+ for all $\beta \ge 0$.

Proof. Let P_{ℓ} be the orthogonal projection defined in Lemma 6.10. Let $H_{\ell} = P_{\ell}HP_{\ell}$. Since H_{ℓ} converges to H in the strong resolvent sense as $\ell \to \infty$, it suffices to show that

$$e^{-\beta H_{\ell}} \ge 0$$
 w.r.t. \mathfrak{B}_+ for all $\beta \ge 0$ and $\ell \in \mathbb{N}$. (6.26)

To this end, we set

$$T = \sum_{x,y \in \Lambda} t_{xy} a_x^* a_y + \sum_{x \in \Lambda} \lambda_x (a_x + a_x^*) + \mu N_{\rm b}, \quad U = \sum_{x \in \Lambda} U_x n_x (n_x - 1).$$
(6.27)

Let $T_{\ell} = P_{\ell}TP_{\ell}$, $U_{\ell} = P_{\ell}UP_{\ell}$. Then T_{ℓ} and U_{ℓ} are bounded for each $\ell \in \mathbb{N}$. We observe that $\langle \mathbf{M} | T_{\ell} | \mathbf{N} \rangle \geq 0$. Thus, by Proposition A.2, $T_{\ell} \geq 0$ w.r.t. \mathfrak{B}_{+} holds for all $\ell \in \mathbb{N}$. On the other hand,

$$\langle \mathbf{M} | \mathrm{e}^{-\beta U_{\ell}} | \mathbf{N} \rangle = \begin{cases} \exp\left\{ -\beta \sum_{x \in \Lambda} N_x (N_x - 1) \right\} \delta_{\mathbf{MN}} & \text{if } |\mathbf{M}| \le \ell \text{ and } |\mathbf{N}| \le \ell \\ \delta_{\mathbf{MN}} & \text{if } |\mathbf{M}| > \ell \text{ or } |\mathbf{N}| > \ell \end{cases}.$$
(6.28)

This means $\langle \mathbf{M} | e^{-\beta U_{\ell}} | \mathbf{N} \rangle \geq 0$. Thus, applying Proposition A.2, we conclude $e^{-\beta U_{\ell}} \geq 0$ w.r.t. \mathfrak{B}_+ for all $\beta \geq 0$ and $\ell \in \mathbb{N}$. Hence, by Proposition A.5, we conclude $e^{-\beta H_{\ell}} \geq 0$ w.r.t. \mathfrak{B}_+ for all $\beta \geq 0$ and $\ell \in \mathbb{N}$. \Box

Corollary 6.14 Let $x_1, \ldots, x_n \in \Lambda$. For all $\#_1, \ldots, \#_n \in \{\pm\}$ and $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n < \beta$, we have

$$e^{-s_1 H} a_{x_1}^{\#_1} e^{-(s_2 - s_1)H} a_{x_2}^{\#_2} e^{-(s_3 - s_2)H} \cdots e^{-(s_n - s_{n-1})H} a_{x_n}^{\#_n} e^{-(\beta - s_n)H} \ge 0$$
(6.29)

w.r.t. \mathfrak{B}_+ .

6.2.1 Completion of proof of Theorem 6.1

By Corollary 6.12 and Proposition 6.13, we have

$$\begin{bmatrix} \prod_{j=1}^{n} A_{j}(s_{j}) \end{bmatrix} e^{-\beta H}$$

= $\underbrace{e^{-sH}}_{\geq 0} \underbrace{A_{1}}_{\geq 0} \underbrace{e^{-(s_{2}-s_{1})H}}_{\geq 0} \cdots \underbrace{A_{n}}_{\geq 0} \underbrace{e^{-(\beta-s_{n})H}}_{\geq 0} \geq 0 \quad \text{w.r.t.} \ \mathfrak{B}_{+}.$ (6.30)

Thus, by Proposition A.1, we conclude Theorem 6.1. \Box

6.3 Proof of Theorems 6.2 and 6.3

Let $\mathfrak{B}_{ext} = \mathfrak{B} \otimes \mathfrak{B}$. We introduce a new representation of the CCRs as follows. Let

$$\xi_x = \frac{1}{\sqrt{2}} \left(a_x \otimes \mathbb{1} + \mathbb{1} \otimes a_x \right), \quad \eta_x = -\frac{1}{\sqrt{2}} \left(a_x \otimes \mathbb{1} - \mathbb{1} \otimes a_x \right). \tag{6.31}$$

 ξ_x and η_x act in \mathfrak{B}_{ext} and are closable. We denote their closures by the same symbols. Then $\{\xi_x, \eta_x\}$ satisfies the following CCRs:

$$[\xi_x, \xi_y] = 0, \quad [\eta_x, \eta_y] = 0, \quad [\xi_x, \eta_y] = 0, \tag{6.32}$$

$$[\xi_x, \xi_y^*] = \delta_{xy}, \ [\eta_x, \eta_y^*] = \delta_{xy}, \ [\xi_x, \eta_y^*] = 0.$$
(6.33)

Using ξ_x and η_x , we can rewrite H as

$$H_{\text{ext}} = -\mathbb{T} + \mathbb{U},\tag{6.34}$$

where

$$\mathbb{T} = \sum_{x,y\in\Lambda} t_{xy}(\xi_x^*\xi_y + \eta_x^*\eta_y) + \sqrt{2}\sum_{x\in\Lambda}\lambda_x(\xi_x + \xi_x^*)$$
(6.35)

and

$$\mathbb{U} = \mathbb{U}_{d} + \mathbb{U}_{o},$$
(6.36)
$$\mathbb{U}_{d} = \sum_{x \in \Lambda} \frac{U_{x}}{2} \left(\xi_{x}^{*} \xi_{x} \xi_{x}^{*} \xi_{x} + 4 \xi_{x}^{*} \xi_{x} \eta_{x}^{*} \eta_{x} + \eta_{x}^{*} \eta_{x} \eta_{x}^{*} \eta_{x} \right)$$

$$- \sum_{x \in \Lambda} \left(\frac{1}{2} U_{x} + \mu \right) (\xi_{x}^{*} \xi_{x} + \eta_{x}^{*} \eta_{x}),$$

$$\mathbb{U}_{o} = \sum_{x \in \Lambda} \frac{U_{x}}{2} \left(\xi_{x}^{*} \xi_{x}^{*} \eta_{x} \eta_{x} + \xi_{x} \xi_{x} \eta_{x}^{*} \eta_{x}^{*} \right).$$
(6.37)

Let $\Omega_{\text{ext}} = \Omega \otimes \Omega \in \mathfrak{B}_{\text{ext}}$. For each $\mathbf{M}, \mathbf{N} \in \mathbb{N}_0^{\Lambda}$, we define

$$|\mathbf{M}, \mathbf{N}\rangle\rangle = \left(\prod_{x \in \Lambda} M_x! N_x!\right)^{-1/2} \prod_{x \in \Lambda} (\xi_x^*)^{M_x} (\eta_x^*)^{N_x} \Omega_{\text{ext}}.$$
 (6.38)

Clearly, $\{ |\mathbf{M}, \mathbf{N}\rangle | \mathbf{M}, \mathbf{N} \in \mathbb{N}_0^{\Lambda} \}$ is a CONS of \mathfrak{B}_{ext} .

Definition 6.15 We define a self-dual cone in \mathfrak{B}_{ext} by

$$\mathfrak{B}_{\text{ext},+} = \left\{ \Psi \in \mathfrak{B}_{\text{ext}} \mid \Psi = \sum_{\mathbf{M},\mathbf{N} \in \mathbb{N}_{0}^{\Lambda}} \Psi_{\mathbf{M},\mathbf{N}} | \mathbf{M}, \mathbf{N} \rangle \rangle, \ \Psi_{\mathbf{M},\mathbf{N}} \ge 0 \ \forall \mathbf{M}, \mathbf{N} \in \mathbb{N}_{0}^{\Lambda} \right\}. \quad \diamondsuit$$

$$(6.39)$$

We can prove the following in a manner similar to that used for Proposition 6.11. **Proposition 6.16** We have $\xi_x^{\#} \ge 0$, $\eta_x^{\#} \ge 0$ w.r.t. $\mathfrak{B}_{\text{ext},+}$ for all $x \in \Lambda$ and $\# \in \{\pm\}$. Proposition 6.17 Let

$$\mathscr{U} = \exp\left\{-i\frac{\pi}{2}\sum_{x\in\Lambda}\eta_x^*\eta_x\right\}.$$
(6.40)

Then we have $\mathscr{U}^* e^{-\beta H_{ext}} \mathscr{U} \geq 0$ w.r.t. $\mathfrak{B}_{ext,+}$ for all $\beta \geq 0$.

Proof. Let $\hat{H}_{ext} = \mathscr{U}^* H_{ext} \mathscr{U}$. It is important to note that

$$\mathscr{U}^* \mathbb{U}_o \mathscr{U} = -\mathbb{U}_o. \tag{6.41}$$

Thus, we have

$$\hat{H}_{\text{ext}} = -\mathbb{K} + \mathbb{U}_d, \tag{6.42}$$

where $\mathbb{K} = \mathbb{T} + \mathbb{U}_o$. Let \mathcal{P}_{ℓ} be the orthogonal projection onto the closed subspace spanned by $\{|\mathbf{M}, \mathbf{N}\rangle | \mathbf{M}, \mathbf{N} \in \mathbb{N}_0^{\Lambda}, |\mathbf{M}| + |\mathbf{N}| \leq \ell\}$. Let $\hat{H}_{\text{ext},\ell} = \mathcal{P}_{\ell}\hat{H}_{\text{ext}}\mathcal{P}_{\ell}$. Since $\hat{H}_{\text{ext},\ell}$ converges to \hat{H}_{ext} in the strong resolvent sense as $\ell \to \infty$, it suffices to show that

$$\exp\left(-\beta \hat{H}_{\text{ext},\ell}\right) \ge 0 \quad \text{w.r.t.} \ \mathfrak{B}_{\text{ext},+} \text{ for all } \beta \ge 0 \text{ and } \ell \in \mathbb{N}.$$
(6.43)

The proof of this is almost parallel to that of Proposition 6.13. For reader's convenience, we provide a sketch of it. Let $\mathbb{K}_{\ell} = \mathcal{P}_{\ell} \mathbb{K} \mathcal{P}_{\ell}$ and $\mathbb{U}_{d,\ell} = \mathcal{P}_{\ell} \mathbb{U}_d \mathcal{P}_{\ell}$. First, we show that $\mathbb{K}_{\ell} \geq 0$ w.r.t. $\mathfrak{B}_{\text{ext},+}$ for all $\ell \in \mathbb{N}$. Next we show that $\exp(-\beta \mathbb{U}_{d,\ell}) \geq 0$ w.r.t. $\mathfrak{B}_{\text{ext},+}$ for all $\beta \geq 0$ and $\ell \in \mathbb{N}$. Then by Proposition A.5, we conclude (6.43). \Box

Proposition 6.18 Set $\hat{\alpha}_{\varepsilon,x}^{\#} = \mathscr{U}^* \alpha_{\varepsilon,x}^{\#} \mathscr{U}$. Then we have $\hat{\alpha}_{\varepsilon,x}^{\#} \ge 0$ w.r.t. $\mathfrak{B}_{\text{ext},+}$ for all $x \in \Lambda, \varepsilon \in \{\pm 1\}$ and $\# \in \{-,+\}$.

Proof. By Proposition 6.16, we have

$$\hat{\alpha}_{\pm 1.x}^{\#} = \sqrt{2}\xi_x^{\#} \ge 0 \quad \text{w.r.t.} \quad \mathfrak{B}_{\text{ext},\pm}, \tag{6.44}$$

$$\hat{\alpha}_{-1.x}^{\#} = \sqrt{2}\eta_x^{\#} \ge 0 \quad \text{w.r.t.} \ \mathfrak{B}_{\text{ext},+}. \quad \Box \tag{6.45}$$

6.3.1 Completion of proofs of Theorems 6.2 and 6.3

We only prove Theorem 6.3, since Theorem 6.2 is a corollary of it. Let $\hat{H}_{\text{ext}} = \mathscr{U}^* H_{\text{ext}} \mathscr{U}$. Then we have

$$\mathscr{U}^{*} \prod_{j=1}^{n} \alpha_{\varepsilon_{j},x_{j}}^{\#_{j}}(s_{j}) \mathscr{U} e^{\beta \hat{H}_{ext}}$$

$$= \underbrace{e^{-s_{1}\hat{H}_{ext}}}_{\geqq 0} \underbrace{\hat{\alpha}_{\varepsilon_{1},x_{1}}^{\#_{1}}}_{\geqq 0} \underbrace{e^{-(s_{2}-s_{1})\hat{H}_{ext}}}_{\geqq 0} \underbrace{\hat{\alpha}_{\varepsilon_{2},x_{2}}^{\#_{2}}}_{\geqq 0} \cdots \underbrace{\hat{\alpha}_{\varepsilon_{n},x_{n}}^{\#_{n}}}_{\geqq 0} \underbrace{e^{-(\beta-s_{n})\hat{H}_{ext}}}_{\geqq 0} \geqq 0 \quad \text{w.r.t.} \quad \mathfrak{B}_{ext,+} \quad (6.46)$$

by Propositions 6.17 and 6.18. Thus, by Proposition A.1, we obtain Theorem 6.3. \Box

6.4 Proof of Theorem 6.5 and Corollary 6.6

If $U_x = 0$, then we have H = -T, where T is given by (6.27). Thus, instead of Proposition 6.17, we have the following:

Proposition 6.19 We have $e^{-\beta H_{ext}} \geq 0$ w.r.t. $\mathfrak{B}_{ext,+}$ for all $\beta \geq 0$.

Note that the unitary operator \mathscr{U} is unnecessary to prove Proposition 6.19. Hence, instead of (6.46), we obtain

$$\prod_{j=1}^{n} \left[a_{x_{j}}^{\#_{j}}(s_{j}) \otimes 1\!\!1 + \varepsilon_{j} 1\!\!1 \otimes a_{x_{j}}^{\#_{j}}(s_{j}) \right] e^{-\beta H_{\text{ext}}}$$

$$= e^{-s_{1}H_{\text{ext}}} \left[a_{x_{1}}^{\#_{1}} \otimes 1\!\!1 + \varepsilon_{1} 1\!\!1 \otimes a_{x_{1}}^{\#_{1}} \right] e^{-(s_{2}-s_{1})H_{\text{ext}}} \cdots \left[a_{x_{n}}^{\#_{n}} \otimes 1\!\!1 + \varepsilon_{n} 1\!\!1 \otimes a_{x_{n}}^{\#_{n}} \right] e^{-(\beta-s_{n})H_{\text{ext}}}$$

$$\geq 0 \quad \text{w.r.t. } \mathfrak{B}_{\text{ext},+}. \tag{6.47}$$

This completes the proof of Theorem 6.5. By applying Theorem 2.18, we prove Corollary 6.6. \Box

7 Hubbard model

7.1 Results

7.1.1 The finite temperature case

Let $G = (\Lambda, E)$ be a graph with vertex set Λ and edge collection E. An edge with end-points x and y will be denoted by $\{x, y\}$. We assume that $\{x, x\} \notin E$ for all $x \in \Lambda$, i.e., any loops are excluded. In this section, we assume the following:

- (G. 1) $|\Lambda|$ is even.
- (G. 2) G is bipartite, i.e., Λ admits a partition into two classes such that every edge has its ends in different classes.

The Hubbard model on G is given by

$$H = \sum_{\{x,y\}\in E} \sum_{\sigma\in\{\uparrow,\downarrow\}} (-t_{xy}) c_{x\sigma}^* c_{y\sigma} + U \sum_{x\in\Lambda} (n_{x\uparrow} - \frac{1}{2})(n_{x\downarrow} - \frac{1}{2}).$$
(7.1)

H acts in the Hilbert space $\mathfrak{H} = \mathfrak{F} \otimes \mathfrak{F}$. \mathfrak{F} is the fermionic Fock space defined by $\mathfrak{F} = \bigoplus_{n \geq 0} \wedge^n \ell^2(\Lambda)$, where $\wedge^n \ell^2(\Lambda)$ is the *n*-fold antisymmetric tensor product of $\ell^2(\Lambda)$ with $\wedge^0 \ell^2(\Lambda) = \mathbb{C}$. $c_{x\sigma}$ is the electron annihilation operator that satisfies the canonical anticommutation relations (CARs):

$$\{c_{x\sigma}, c_{x'\sigma'}^*\} = \delta_{xx'}\delta_{\sigma\sigma'}, \quad \{c_{x\sigma}, c_{x'\sigma'}\} = 0.$$

$$(7.2)$$

 $n_{x\sigma} = c_{x\sigma}^* c_{x\sigma}$ is the number operator at vertex $x \in \Lambda$. $t_{xy} \in \mathbb{R}$ is the quantum mechanical amplitude of an electron hopping from y to x. We assume that

(T) $t_{xy} = t_{yx} \neq 0$ for all $\{x, y\} \in E$.

U is the strength of the Coulomb repulsion¹⁶ such that

(U) $U \ge 0$.

Since G is bipartite, Λ can be divided into two disjoint sets Λ_e and Λ_o . We set $\mu(x) = 0$ if $x \in \Lambda_e$, $\mu(x) = 1$ if $x \in \Lambda_o$. For each $x \in \Lambda$, define

$$b_x = (-1)^{\mu(x)} c_{x\uparrow}^* \gamma_{\uparrow} c_{x\downarrow}, \tag{7.3}$$

where $\gamma_{\uparrow} = (-1)^{N_{\uparrow}}$ with $N_{\sigma} = \sum_{x \in \Lambda} n_{x\sigma}$. Let

$$\mathfrak{A} = \operatorname{Coni}\left\{ b_{x_1}^{\#_1} b_{x_2}^{\#_2} \cdots b_{x_n}^{\#_n} \mid x_1, \dots, x_n \in \Lambda, \ \#_1, \dots, \#_n \in \{+, -\}, \ n \in \mathbb{N} \right\}.$$
(7.4)

We use the thermal average associated with the grand canonical Gibbs state at inverse temperature β :

$$\langle X \rangle_{\beta} = \operatorname{Tr} \left[X \, \mathrm{e}^{-\beta H} \right] / \Xi_{\beta}, \quad \Xi_{\beta} = \operatorname{Tr} \left[\mathrm{e}^{-\beta H} \right].$$
 (7.5)

For each $\beta > 0$, we can verify that $\langle n_x \rangle_{\beta} = 1$, where $n_x = n_{x\uparrow} + n_{x\downarrow}$. This means that the system at half-filling will be considered.

Theorem 7.1 (First Griffiths inequality) Let $A_1, \ldots, A_n \in \mathfrak{A}$. For all $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n \leq \beta$, we have

$$\left\langle \prod_{j=1}^{n} A_j(s_j) \right\rangle_{\beta} \ge 0, \tag{7.6}$$

where $A(s) = e^{-sH}Ae^{sH}$.

Example 9 For each $x_1, \ldots, x_n \in \Lambda$, $\#_1, \ldots, \#_n \in \{+, -\}$ and $0 \le s_1 \le s_2 \le \cdots \le s_n \le \beta$, we have

$$\left\langle b_{x_1}^{\#_1}(s_1)b_{x_2}^{\#_2}(s_n)\cdots b_{x_n}^{\#_n}(s_n)\right\rangle_{\beta} \ge 0,$$
(7.7)

where $b_x^{\#}(s) = e^{-sH} b_x^{\#} e^{sH}$.

To state the second quantum Griffiths inequality, we introduce the following notation:

$$\langle\!\langle Y \rangle\!\rangle_{\beta} = \operatorname{Tr}_{\mathfrak{H} \otimes \mathfrak{H}} \left[Y \,\mathrm{e}^{-\beta H_{\mathrm{ext}}} \right] \Big/ \Xi_{\beta}^2, \quad H_{\mathrm{ext}} = H \otimes 1\!\!1 + 1\!\!1 \otimes H.$$
 (7.8)

Theorem 7.2 (Second Griffiths inequality) For each $x \in \Lambda, \varepsilon \in \{\pm 1\}, \# \in \{\pm\}, \sigma \in \{\uparrow, \downarrow\}$ and $s \ge 0$, we introduce

$$\alpha_{x\sigma;\varepsilon}^{\#}(s) = c_{x\sigma}^{\#}(s) \otimes 1 + \varepsilon \gamma \otimes c_{x\sigma}^{\#}(s),$$
(7.9)

¹⁶All results in this section can be extended to a more general Coulomb interaction of the form $\sum_{x,y\in\Lambda} U_{xy}(n_{x\uparrow}-\frac{1}{2})(n_{y\downarrow}-\frac{1}{2})$, where U_{xy} is real and positive semidefinite.

where $\gamma = (-1)^{N_e}$ with $N_e = N_{\uparrow} + N_{\downarrow}$ and $c_{x\sigma}^{\#}(s) = e^{-sH}c_{x\sigma}^{\#}e^{sH}$. Let $x_1, \ldots, x_n \in \Lambda$. For each $0 \le s_1 \le s_2 \le \cdots \le s_n \le \beta$, $\#_1, \ldots, \#_n \in \{+, -\}$ and $\varepsilon_1, \ldots, \varepsilon_n \in \{\pm 1\}$, we have

$$\left\langle\!\!\left\langle\prod_{j=1}^{n}\left[(-1)^{\mu(x_{j})}\alpha_{x_{j}\uparrow;\varepsilon_{j}}^{\#_{j}}(s_{j})\gamma_{\uparrow}\otimes\gamma_{\uparrow}\alpha_{x_{j}\downarrow;\varepsilon_{j}}^{\overline{\#}_{j}}(s_{j})\right]\right\rangle\!\!\right\rangle_{\beta} \ge 0$$
(7.10)

and

$$\left\langle \left\langle \prod_{j=1}^{n} \left[(-1)^{\mu(x_j)} \alpha_{x_j\uparrow;\varepsilon_j}^{\#_j}(s_j) \gamma_{\uparrow} \otimes \gamma_{\uparrow} \alpha_{x_j\downarrow;-\varepsilon_j}^{\overline{\#}_j}(s_j) \right] \right\rangle \right\rangle_{\beta} \ge 0.$$
(7.11)

Corollary 7.3 Let $x_1, \ldots, x_n \in \Lambda$. For each $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n \leq \beta$ and $\#_1, \ldots, \#_n \in \{+, -\}$, we have

$$\left\langle\!\!\left\langle\prod_{j=1}^{n}\left[b_{x_{j}}^{\#_{j}}(s_{j})\otimes\gamma_{\uparrow}-\gamma_{\uparrow}\otimes b_{x_{j}}^{\#_{j}}(s_{j})\right]\right\rangle\!\!\right\rangle_{\beta}\geq0.$$
(7.12)

Corollary 7.4 Let $x_1, ..., x_{2n} \in \Lambda$. For each $0 \le s_1 \le s_2 \le \cdots \le s_{2n} \le \beta$ and $\#_1, ..., \#_{2n} \in \{+, -\}$, we have

$$\left\langle \left\langle \prod_{j=1}^{2n} \left[b_{x_j}^{\#_j}(s_j) \otimes \gamma_{\uparrow} - \gamma_{\uparrow} \otimes b_{x_j}^{\#_j}(s_j) \right] \right\rangle \right\rangle_{\beta} \\
\geq \left\langle \left\langle \prod_{j=1}^{2n} (-1)^{\mu(x_j)} \left[c_{x_j\uparrow}^{\#_j}(s_j) \gamma_{\downarrow} \otimes \gamma_{\uparrow} c_{x_j\downarrow}^{\#_j}(s_j) - \gamma_{\downarrow} c_{x_j\downarrow}^{\#_j}(s_j) \otimes c_{x_j\uparrow}^{\#_j}(s_j) \gamma_{\uparrow} \right] \right\rangle \right\rangle_{\beta} \\
\geq 0.$$
(7.13)

Example 10 Consider the case where n = 2. We then have

$$(-1)^{\mu(x)+\mu(y)} \left(\left\langle c_{x\downarrow}^* c_{x\uparrow} c_{y\uparrow}^* c_{y\downarrow} \right\rangle_{\beta} - \left\langle c_{x\downarrow}^* c_{x\uparrow} \right\rangle_{\beta} \left\langle c_{y\uparrow}^* c_{y\downarrow} \right\rangle_{\beta} \right)$$

$$\geq (-1)^{\mu(x)+\mu(y)} \left(\left\langle c_{x\uparrow} c_{y\uparrow}^* \right\rangle_{\beta} \left\langle c_{x\downarrow}^* c_{y\downarrow} \right\rangle_{\beta} + \left\langle c_{x\uparrow} c_{y\downarrow} \right\rangle_{\beta} \left\langle c_{x\downarrow}^* c_{y\uparrow}^* \right\rangle_{\beta} \right)$$

$$\geq 0.$$
(7.14)

Since $\langle c_{x\downarrow}^* c_{x\uparrow} \rangle_{\beta} = 0 = \langle c_{x\uparrow} c_{y\downarrow} \rangle_{\beta}$ by the symmetries of the system, we arrive at

$$(-1)^{\mu(x)+\mu(y)} \langle c_{x\downarrow}^* c_{x\uparrow} c_{y\uparrow}^* c_{y\downarrow} \rangle_{\beta} \ge (-1)^{\mu(x)+\mu(y)} \langle c_{x\uparrow} c_{y\uparrow}^* \rangle_{\beta} \langle c_{x\downarrow}^* c_{y\downarrow} \rangle_{\beta} \ge 0.$$
(7.15)

If $x, y \in \Lambda_e$ or $x, y \in \Lambda_o$, then $(-1)^{\mu(x)+\mu(y)} = 1$, so that we obtain a standard-type correlation inequality. \diamondsuit

Corollary 7.5 Let $\overline{n}_{x\uparrow} = \mathbb{1} - n_{x\uparrow}$. Let $x_1, \ldots, x_n \in \Lambda$. We have

$$\left\langle \left\langle \prod_{j=1}^{n} \left[\overline{n}_{x_{j}\uparrow} n_{x_{j}\downarrow} \otimes 1 + 1 \otimes \overline{n}_{x_{j}\uparrow} n_{x_{j}\downarrow} \right] \right\rangle \right\rangle_{\beta} \\
\geq \left\langle \left\langle \prod_{j=1}^{n} \left[\overline{n}_{x_{j}\uparrow} \otimes n_{x_{j}\downarrow} + n_{x_{j}\downarrow} \otimes \overline{n}_{x_{j}\uparrow} \right] \right\rangle \right\rangle_{\beta} \\
\geq 0.$$
(7.16)

Example 11 In the case where n = 2, we have

$$\left\langle \overline{n}_{x\uparrow} \overline{n}_{y\uparrow} n_{x\downarrow} n_{y\downarrow} \right\rangle_{\beta} + \left\langle \overline{n}_{x\uparrow} n_{x\downarrow} \right\rangle_{\beta} \left\langle \overline{n}_{y\uparrow} n_{y\downarrow} \right\rangle_{\beta} - \left\langle \overline{n}_{x\uparrow} \overline{n}_{y\uparrow} \right\rangle_{\beta} \left\langle n_{x\downarrow} n_{y\downarrow} \right\rangle_{\beta} - \left\langle \overline{n}_{x\uparrow} n_{y\downarrow} \right\rangle_{\beta} \left\langle \overline{n}_{y\uparrow} n_{x\downarrow} \right\rangle_{\beta} \ge 0. \quad \diamondsuit$$
(7.17)

Remark 7.6 Our results can be extended to a general class of electron–phonon(or photon) Hamiltonians, including the Holstein–Hubbard model and the SSH model. \diamond

7.1.2 The zero-temperature case

Our results can be extended to the case where $\beta = \infty$. Unfortunately, the general theorems in Section 3 cannot be directly applied to this model. To clarify the main points of modification, we state results without proofs.

We assume an additional condition.

(G. 3) G is connected, i.e., any of its vertices are linked by a path in G.

We consider a half-filled system. Thus, our Hilbert space is restricted to

$$\mathfrak{E} = \mathfrak{H} \cap \ker(N_{\mathrm{e}} - |\Lambda|). \tag{7.18}$$

Let $S^{(z)} = \frac{1}{2}(N_{\uparrow} - N_{\downarrow})$. Since $S^{(z)}$ commutes with H, we have the following decomposition:

$$\mathfrak{E} = \bigoplus_{M=-|\Lambda|/2}^{|\Lambda|/2} \mathfrak{E}_M, \quad \mathfrak{E}_M = \mathfrak{E} \cap \ker(S^{(z)} - M).$$
(7.19)

 \mathfrak{E}_M is called the *M*-subspace. For each $M \in \operatorname{spec}(S^{(z)})$, set $H_M = H \upharpoonright \mathfrak{E}_M$. The following theorem is important.

Theorem 7.7 [38, 44] For each $M \in \{-|\Lambda|/2, -(|\Lambda|-2)/2, ..., |\Lambda|/2\}$, H_M has a unique ground state.

We denote the normalized ground state of H_M by ψ_M . We define the ground state expectation value by

$$\langle X \rangle_{\infty,M} = \langle \psi_M | X \psi_M \rangle. \tag{7.20}$$

Theorem 7.8 Let $A_1, \ldots, A_n \in \mathfrak{A}$. For all $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n$, we have

$$\left\langle \prod_{j=1}^{n} A_j(s_j) \right\rangle_{\infty,M} \ge 0.$$
(7.21)

We introduce the following notation:

$$\langle\!\langle Y \rangle\!\rangle_{\infty,M} = \left\langle \psi_M \otimes \psi_M \middle| Y \psi_M \otimes \psi_M \right\rangle.$$
 (7.22)

Theorem 7.9 Let $x_1, \ldots, x_n \in \Lambda$. For each $0 \leq s_1 \leq s_2 \leq \cdots \leq s_n$, $\#_1, \ldots, \#_n \in \{+, -\}$ and $\varepsilon_1, \ldots, \varepsilon_n \in \{\pm 1\}$, we have

$$\left\langle \left\langle \prod_{j=1}^{n} \left[(-1)^{\mu(x_j)} \alpha_{x_j \uparrow; \varepsilon_j}^{\#_j}(s_j) \gamma_{\uparrow} \otimes \gamma_{\uparrow} \alpha_{x_j \downarrow; \varepsilon_j}^{\overline{\#}_j}(s_j) \right] \right\rangle \right\rangle_{\infty, M} \ge 0$$
(7.23)

and

$$\left\langle \left\langle \prod_{j=1}^{n} \left[(-1)^{\mu(x_j)} \alpha_{x_j\uparrow;\varepsilon_j}^{\#_j}(s_j) \gamma_{\uparrow} \otimes \gamma_{\uparrow} \alpha_{x_j\downarrow;-\varepsilon_j}^{\overline{\#}_j}(s_j) \right] \right\rangle \right\rangle_{\infty,M} \ge 0.$$
(7.24)

7.2 Proof of Theorem 7.1

The hole–particle transformation \mathcal{U} is a unitary operator such that

$$\mathcal{U}c_{x\uparrow}\mathcal{U}^* = (-1)^{\mu(x)}c_{x\uparrow}^*, \quad \mathcal{U}c_{x\downarrow}\mathcal{U}^* = c_{x\downarrow}.$$
(7.25)

Let $\hat{H} = \mathcal{U}H\mathcal{U}^*$. Then we obtain the attractive Hubbard model:

$$\hat{H} = \sum_{\{x,y\}\in E} \sum_{\sigma\in\{\uparrow,\downarrow\}} (-t_{xy}) c_{x\sigma}^* c_{y\sigma} - U \sum_{x\in\Lambda} (n_{x\uparrow} - \frac{1}{2})(n_{x\downarrow} - \frac{1}{2}).$$
(7.26)

Let c_x be the annihilation operator on \mathfrak{F} . We note that

$$c_{x\uparrow} = c_x \otimes \mathbb{1}, \quad c_{x\downarrow} = (-\mathbb{1})^{\mathsf{N}} \otimes c_x,$$
(7.27)

where $\mathsf{N} = \sum_{x \in \Lambda} c_x^* c_x$. Then we obtain

$$\hat{H} = \mathsf{T} \otimes \mathbb{1} + \mathbb{1} \otimes \mathsf{T} - U \sum_{x \in \Lambda} (\mathsf{n}_x - \frac{1}{2}) \otimes (\mathsf{n}_x - \frac{1}{2}),$$
(7.28)

where $\mathbf{n}_x = c_x^* c_x$ and

$$\mathsf{T} = \sum_{\{x,y\}\in E} (-t_{xy})c_x^* c_y.$$
(7.29)

Let ϑ_1 be an antilinear involution on \mathfrak{F} defined by

$$\vartheta_1 c_{x_1}^* \cdots c_{x_n}^* \Omega = c_{x_1}^* \cdots c_{x_n}^* \Omega, \quad x_1, \dots, x_n \in \Lambda,$$
(7.30)

where Ω is the Fock vacuum in \mathfrak{F} . By (3.4), we have the following identification:

$$\mathfrak{H} = \mathscr{L}^2(\mathfrak{F}). \tag{7.31}$$

Moreover, by (3.4) and (7.28), we obtain the following:

Proposition 7.10 We have

$$\hat{H} = \mathcal{L}(\mathsf{T}) + \mathcal{R}(\mathsf{T}) - U \sum_{x \in \Lambda} \mathcal{L}(\mathsf{n}_x - \frac{1}{2}) \mathcal{R}(\mathsf{n}_x - \frac{1}{2}),$$
(7.32)

Proposition 7.11 We have the following:

- (i) $\hat{b}_x := \mathcal{U}b_x\mathcal{U}^* \succeq 0 \ w.r.t. \ \mathscr{L}^2(\mathfrak{F})_+ \ for \ all \ x \in \Lambda.$
- (ii) $e^{-\beta \hat{H}} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{F})_+$ for all $\beta \ge 0$.
- Proof. (i) This immediately follows from the identification $\hat{b}_x = \mathcal{L}(c_x)\mathcal{R}(c_x^*)$. (ii) By Proposition 7.10 and Corollary A.9, we obtain (ii) \Box

Corollary 7.12 For all $A \in \mathfrak{A}$, we have $\mathcal{U}A\mathcal{U}^* \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{F})_+$.

7.2.1 Completion of proof of Theorem 7.1

By Theorem 3.11 and Corollary 7.12, we obtain Theorem 7.1. \Box

7.3 Proof of Theorem 7.2

Let $\mathfrak{H}_{ext} = \mathfrak{H} \otimes \mathfrak{H}$. Let

$$\phi_{x\sigma} = \frac{1}{\sqrt{2}} \big(c_{x\sigma} \otimes \mathbb{1} + \gamma \otimes c_{x\sigma} \big), \quad \psi_{x\sigma} = \frac{1}{\sqrt{2}} \big(c_{x\sigma} \otimes \mathbb{1} - \gamma \otimes c_{x\sigma} \big). \tag{7.33}$$

 $\phi_{x\sigma}$ and $\psi_{x\sigma}$ act in \mathfrak{H}_{ext} as well. These operators satisfy the following CARs:

$$\{\phi_{x\sigma}, \phi_{y\sigma'}^*\} = \delta_{xy}\delta_{\sigma\sigma'}, \quad \{\phi_{x\sigma}, \phi_{y\sigma'}\} = 0, \tag{7.34}$$

$$\{\psi_{x\sigma}, \psi_{u\sigma'}^*\} = \delta_{xy}\delta_{\sigma\sigma'}, \quad \{\psi_{x\sigma}, \psi_{y\sigma'}\} = 0, \tag{7.35}$$

$$\{\phi_{x\sigma}, \psi_{y\sigma'}^*\} = 0, \qquad \{\phi_{x\sigma}, \psi_{y\sigma'}\} = 0. \tag{7.36}$$

Let $\{\phi_x, \psi_x \mid x \in \Lambda\}$ be new annihilation operators on $\mathfrak{X} = \mathfrak{F} \otimes \mathfrak{F}$ such that

$$\{\phi_x, \phi_y^*\} = \delta_{xy}, \ \{\phi_x, \phi_y\} = 0, \tag{7.37}$$

$$\{\psi_x, \psi_y^*\} = \delta_{xy}, \ \{\psi_x, \psi_y\} = 0, \tag{7.38}$$

$$\{\phi_x, \psi_y^*\} = 0, \qquad \{\phi_x, \psi_y\} = 0, \tag{7.39}$$

and $\phi_x \Omega_{\mathfrak{X}} = 0 = \psi_x \Omega_{\mathfrak{X}}$, where $\Omega_{\mathfrak{X}}$ is the Fock vacuum in \mathfrak{X} . Then we have the following identifications:

$$\phi_{x\uparrow} = \phi_x \otimes \mathbb{1}, \quad \phi_{x\downarrow} = (-\mathbb{1})^{\mathcal{N}} \otimes \phi_x, \quad \psi_{x\uparrow} = \psi_x \otimes \mathbb{1}, \quad \psi_{x\downarrow} = (-\mathbb{1})^{\mathcal{N}} \otimes \psi_x, \qquad (7.40)$$

where $\mathcal{N} = \sum_{x \in \Lambda} (\phi_x^* \phi_x + \psi_x^* \psi_x)$. Let

$$\mathscr{U} = \mathcal{U} \otimes \mathcal{U}. \tag{7.41}$$

Set

$$\hat{H}_{\text{ext}} = \mathscr{U}H_{\text{ext}}\mathscr{U}^* + \frac{1}{2}U|\Lambda|.$$
(7.42)

Then \hat{H}_{ext} can be expressed as

$$\hat{H}_{\text{ext}} = \mathbb{T} \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{T} - \mathbb{V}, \qquad (7.43)$$

where

$$\mathbb{T} = \sum_{\{x,y\}\in E} (-t_{xy})(\phi_x^*\phi_y + \psi_x^*\psi_y) + \frac{U}{2}\mathcal{N},$$
(7.44)

$$\mathbb{V} = \frac{U}{2} \sum_{x \in \Lambda} (\mathcal{N}_x \otimes \mathcal{N}_x + \mathcal{M}_x \otimes \mathcal{M}_x), \tag{7.45}$$

$$\mathcal{N}_x = \phi_x^* \phi_x + \psi_x^* \psi_x, \quad \mathcal{M}_x = \phi_x^* \psi_x + \psi_x^* \phi_x. \tag{7.46}$$

Let ϑ_2 be an antilinear involution on \mathfrak{X} defined by

$$\vartheta_2 \phi_x \vartheta_2 = \phi_x, \quad \vartheta_2 \psi_x \vartheta_2 = \psi_x, \quad \vartheta_2 \Omega_{\mathfrak{X}} = \Omega_{\mathfrak{X}}.$$
 (7.47)

By (3.4), we have the identification

$$\mathfrak{H}_{\text{ext}} = \mathscr{L}^2(\mathfrak{X}). \tag{7.48}$$

In addition, we have the following expression:

Proposition 7.13 We have $\hat{H}_{ext} = \mathcal{L}(\mathbb{T}) + \mathcal{R}(\mathbb{T}) - \mathbb{V}$, where

$$\mathbb{V} = \frac{U}{2} \sum_{x \in \Lambda} \Big\{ \mathcal{L}(\mathcal{N}_x) \mathcal{R}(\mathcal{N}_x) + \mathcal{L}(\mathcal{M}_x) \mathcal{R}(\mathcal{M}_x) \Big\}.$$
(7.49)

By Corollary A.9, we obtain the following:

Corollary 7.14 For all $\beta \geq 0$, we have $\exp(-\beta \hat{H}_{ext}) \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$.

The below proposition immediately follows from the definitions (note that $\mathscr{U}\gamma \otimes \mathbb{1}\mathscr{U}^* = \gamma \otimes \mathbb{1}$ by (G. 1)).

Proposition 7.15 We have the following:

- (i) $\mathscr{U}(-1)^{\mu(x)}(c_{x\uparrow}^{\#} \otimes 1 + \gamma \otimes c_{x\uparrow}^{\#}) \mathscr{U}^* = \sqrt{2}\mathcal{L}(\phi_x^{\overline{\#}}).$
- (ii) $\mathscr{U}(-1)^{\mu(x)}(c_{x\uparrow}^{\#}\otimes 1\!\!1 \gamma \otimes c_{x\uparrow}^{\#})\mathscr{U}^* = \sqrt{2}\mathcal{L}(\psi_x^{\overline{\#}}).$
- (iii) $\mathscr{U}\gamma_{\uparrow} \otimes \gamma_{\uparrow}(c_{x\downarrow}^{\#} \otimes 1 + \gamma \otimes c_{x\downarrow}^{\#})\mathscr{U}^{*} = \sqrt{2}\mathcal{R}(\phi_{x}^{\overline{\#}}).$
- (iv) $\mathscr{U}\gamma_{\uparrow}\otimes\gamma_{\uparrow}(c_{x\downarrow}^{\#}\otimes\mathbb{1}-\gamma\otimes c_{x\downarrow}^{\#})\mathscr{U}^{*}=\sqrt{2}\mathcal{R}(\psi_{x}^{\overline{\#}}).$

Corollary 7.16 Let

$$\alpha_{x\sigma;\varepsilon} = c_{x\sigma} \otimes 1 + \varepsilon \gamma \otimes c_{x\sigma}. \tag{7.50}$$

For all $\varepsilon \in \{\pm 1\}$, $\# \in \{\pm\}$ and $x \in \Lambda$, we have

$$\mathscr{U}(-1)^{\mu(x)}\alpha^{\#}_{x\uparrow,\varepsilon}\gamma_{\uparrow}\otimes\gamma_{\uparrow}\alpha^{\overline{\#}}_{x\downarrow,\varepsilon}\mathscr{U}^{*}\succeq0$$
(7.51)

w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$.

Proof. By Proposition 7.15, we have

$$\mathscr{U}(-1)^{\mu(x)}\alpha^{\#}_{x\uparrow,-1}\gamma_{\uparrow} \otimes \gamma_{\uparrow}\alpha^{\overline{\#}}_{x\downarrow,-1}\mathscr{U}^{*} = 2\mathcal{L}\left(\psi^{\overline{\#}}_{x}\right)\mathcal{R}\left(\psi^{\#}_{x}\right) \succeq 0 \quad \text{w.r.t.} \quad \mathscr{L}^{2}(\mathfrak{X})_{+} , \quad (7.52)$$
$$\mathscr{U}(-1)^{\mu(x)}\alpha^{\#}_{x\uparrow,+1}\gamma_{\uparrow} \otimes \gamma_{\uparrow}\alpha^{\overline{\#}}_{x\downarrow,+1}\mathscr{U}^{*} = 2\mathcal{L}\left(\phi^{\overline{\#}}_{x}\right)\mathcal{R}\left(\phi^{\#}_{x}\right) \succeq 0 \quad \text{w.r.t.} \quad \mathscr{L}^{2}(\mathfrak{X})_{+} , \quad \Box$$
$$(7.53)$$

7.3.1 Completion of proof of Theorem 7.2

Proof of (7.10)

Let $D_{\varepsilon,\#,x} = (-1)^{\mu(x)} \alpha_{x\uparrow,\varepsilon}^{\#} \gamma_{\uparrow} \otimes \gamma_{\uparrow} \alpha_{x\downarrow,\varepsilon}^{\overline{\#}}$. Then we see that by Corollaries 7.14 and 7.16,

$$\mathscr{U}\left[\prod_{j=1}^{n} (-1)^{\mu(x_{j})} \alpha_{x_{j}\uparrow;\varepsilon_{j}}^{\#_{j}}(s_{j})\gamma_{\uparrow} \otimes \gamma_{\uparrow} \alpha_{x_{j}\downarrow;\varepsilon_{j}}^{\#_{j}}(s_{j})\right] e^{-\beta H_{\text{ext}}} \mathscr{U}^{*}$$

$$= \underbrace{e^{-s_{1}\hat{H}_{\text{ext}}}}_{\succeq 0} \underbrace{\mathscr{U}D_{\varepsilon_{1},\#_{1},x_{1}}\mathscr{U}^{*}}_{\succeq 0} \underbrace{e^{-(s_{2}-s_{1})\hat{H}_{\text{ext}}}}_{\succeq 0} \cdots \underbrace{\mathscr{U}D_{\varepsilon_{n},\#_{n},x_{n}}}_{\succeq 0} \underbrace{e^{-(\beta-s_{n})\hat{H}_{\text{ext}}}}_{\succeq 0}}_{\succeq 0} \succeq 0 \quad (7.54)$$

w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$. Thus, by Theorem 3.10, we obtain (7.10). \Box

Proof of (7.11)

Let \mathscr{Q} be a unitary operator defined by $\mathscr{Q} = \mathbb{1} \otimes (-\mathbb{1})^{N_{\downarrow}}$. Then we see that

$$\mathscr{Q}H_{\mathrm{ext}}\mathscr{Q}^{-1} = H_{\mathrm{ext}}, \quad \mathscr{Q}\alpha_{x\uparrow,\varepsilon}\mathscr{Q}^{-1} = \alpha_{x\uparrow,\varepsilon}, \quad \mathscr{Q}\alpha_{x\downarrow,\varepsilon}\mathscr{Q}^{-1} = \alpha_{x\downarrow,-\varepsilon}. \tag{7.55}$$

Thus, (7.11) follows from (7.10). \Box

7.4 Proof of Corollary 7.3

Lemma 7.17 Let $C_{x,\varepsilon} = (-1)^{\mu(x)} \alpha_{x\uparrow,\varepsilon}^{\#} \gamma_{\uparrow} \otimes \gamma_{\uparrow} \alpha_{x\downarrow,-\varepsilon}^{\overline{\#}}$. Set $\mathscr{W} = \mathscr{U}\mathscr{Q}$. Then we obtain $\mathscr{W}C_{x,\varepsilon}\mathscr{W}^{-1} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$.

Proof. By Corollary 7.16 and (7.55), we see that

$$\mathscr{W}C_{x,\varepsilon}\mathscr{W}^{-1} = \mathscr{U}D_{\varepsilon,+1,x}\mathscr{U}^{-1} \succeq 0 \quad \text{w.r.t.} \ \mathscr{L}^2(\mathfrak{X})_+. \quad \Box$$
(7.56)

Lemma 7.18 For all $\beta \geq 0$, we have $\mathscr{W} e^{-\beta H_{ext}} \mathscr{W}^{-1} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$.

Proof. Since $\mathscr{Q}H_{\text{ext}}\mathscr{Q}^{-1} = H_{\text{ext}}$, we see that $\mathscr{W}e^{-\beta H_{\text{ext}}}\mathscr{W}^{-1} = e^{-\beta \hat{H}_{\text{ext}}} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$. \Box

7.4.1 Completion of proof of Corollary 7.3

By Lemma 7.17, we obtain

$$\mathscr{W}C_{x,\varepsilon}\mathscr{W}^{-1} = \mathscr{W}A_x\mathscr{W}^{-1} + \varepsilon \mathscr{W}B_x\mathscr{W}^{-1} \succeq 0 \quad \text{w.r.t.} \ \mathscr{L}^2(\mathfrak{X})_+, \tag{7.57}$$

where

$$A_x = \mathscr{Q}^{-1} (b_x \otimes \gamma_{\uparrow} - \gamma_{\uparrow} \otimes b_x) \mathscr{Q}, \qquad (7.58)$$

$$B_x = -(-1)^{\mu(x)} \mathscr{Q}^{-1} (c_{x\uparrow}^* \gamma_{\downarrow} \otimes \gamma_{\uparrow} c_{x\downarrow} - \gamma_{\downarrow} c_{x\downarrow} \otimes c_{x\uparrow}^* \gamma_{\uparrow}) \mathscr{Q}.$$
(7.59)

Thus, we have

$$\mathscr{W}A_{x}\mathscr{W}^{-1} = \frac{1}{2}\underbrace{\mathscr{W}C_{x,+}\mathscr{W}^{-1}}_{\succeq 0} + \frac{1}{2}\underbrace{\mathscr{W}C_{x,-}\mathscr{W}^{-1}}_{\succeq 0} \succeq 0 \quad \text{w.r.t. } \mathscr{L}^{2}(\mathfrak{X})_{+}.$$
(7.60)

Finally, observe that

$$\mathscr{W}\left[\prod_{j=1}^{n} A_{x_{j}}^{\#_{j}}(s_{j})\right] e^{-\beta H_{\text{ext}}} \mathscr{W}^{-1} \\
= \underbrace{\mathscr{W}e^{-s_{1}H_{\text{ext}}} \mathscr{W}^{-1}}_{\succeq 0} \underbrace{\mathscr{W}A_{x_{1}}^{\#_{1}} \mathscr{W}^{-1}}_{\succeq 0} \underbrace{\mathscr{W}e^{-(s_{2}-s_{1})H_{\text{ext}}} \mathscr{W}^{-1}}_{\succeq 0} \cdots \underbrace{\mathscr{W}e^{-(\beta-s_{n})H_{\text{ext}}} \mathscr{W}^{-1}}_{\succeq 0} \succeq 0 \quad (7.61)$$

w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$. By Theorem 3.10, we conclude Corollary 7.3. \Box

7.5 Proof of Corollary 7.4

7.5.1 First part of the proof

Note that $\mathscr{W}B_x\mathscr{W}^{-1} = \frac{1}{2}\mathscr{W}C_{x,+}\mathscr{W}^{-1} - \frac{1}{2}\mathscr{W}C_{x,-}\mathscr{W}^{-1}$. Combining this with (7.60), we have

$$\mathscr{W}\left[\prod_{j=1}^{2n} A_{x_j}^{\#_j}(s_j)\right] e^{-\beta H_{\text{ext}}} \mathscr{W}^{-1} - \mathscr{W}\left[\prod_{j=1}^{2n} B_{x_j}^{\#_j}(s_j)\right] e^{-\beta H_{\text{ext}}} \mathscr{W}^{-1}$$
$$= \sum_{\delta_1, \dots, \delta_n \in \{\pm\}} X_{\delta_1, \dots, \delta_n} \underbrace{\mathscr{W}C_{x_1, \delta_1}(s_1) \cdots C_{x_n, \delta_n}(s_n) e^{\beta H_{\text{ext}}} \mathscr{W}^{-1}}_{\succeq 0}, \tag{7.62}$$

where each $X_{\delta_1,\ldots,\delta_n}$ is a positive constant. Thus, the RHS of $(7.62) \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$. By Theorem 3.10, we obtain the first inequality in (7.13).

7.5.2 Second part of the proof

We will show the second inequality in (7.13). Let Θ be an antilinear involution on \mathfrak{H} such that

$$\Theta c_{x\sigma} \Theta = c_{x\sigma}, \quad \Theta \Omega_{\mathfrak{H}} = \Omega_{\mathfrak{H}}, \tag{7.63}$$

where $\Omega_{\mathfrak{H}} = \Omega \otimes \Omega$. Then by (3.4), we have $\mathfrak{H}_{ext} = \mathscr{L}^2(\mathfrak{H})$ and

$$\hat{H}_{\text{ext}} = \mathcal{L}(\hat{H}) + \mathcal{R}(\hat{H}). \tag{7.64}$$

By Corollary A.9, we have the following:

Proposition 7.19 For all $\beta \geq 0$, we have $\exp(-\beta \hat{H}_{ext}) \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$.

Let S be the unitary operator on \mathfrak{H} given by

$$Sc_{x\uparrow}S^{-1} = c_{x\downarrow}, \quad Sc_{x\downarrow}S^{-1} = c_{x\uparrow}.$$

$$(7.65)$$

Set $\mathscr{R} = \mathbb{1} \otimes S \mathscr{U}$. Remark that since $S \hat{H} S^{-1} = \hat{H}$, we know that

$$\mathscr{R}e^{-\beta H_{\text{ext}}}\mathscr{R}^{-1} = e^{-\beta \hat{H}_{\text{ext}}} \succeq 0 \text{ w.r.t. } \mathscr{L}^2(\mathfrak{H})_+$$
 (7.66)

by Proposition 7.19.

Proposition 7.20 We have the following:

- (i) $\mathscr{R}(-1)^{\mu(x)}c_{x\uparrow}\gamma_{\downarrow}\otimes \mathbb{1}\mathscr{R}^{-1} = \mathcal{L}(c_{x\uparrow}^{*}\gamma_{\downarrow}).$
- (ii) $\mathscr{R}c_{x\downarrow}\gamma_{\downarrow}\otimes \mathbb{1}\mathscr{R}^{-1} = \mathcal{L}(c_{x\downarrow}\gamma_{\downarrow}).$
- (iii) $\mathscr{R}(-1)^{\mu(x)} \mathbb{1} \otimes c_{x\uparrow} \gamma_{\uparrow} \mathscr{R}^{-1} = \mathcal{R}(\gamma_{\downarrow} c_{x\downarrow}).$
- (iv) $\mathscr{R}\mathbb{1} \otimes \gamma_{\uparrow} c_{x\downarrow} \mathscr{R}^{-1} = \mathcal{R}(\gamma_{\downarrow} c_{x\uparrow}^{*}).$

Corollary 7.21 We have the following:

- (i) $\mathscr{R}(-1)^{\mu(x)}c_{x\uparrow}^*\gamma_{\downarrow}\otimes\gamma_{\uparrow}c_{x\downarrow}\mathscr{R}^{-1}\succeq 0 \ w.r.t. \ \mathscr{L}^2(\mathfrak{H})_+.$
- (ii) $-\mathscr{R}(-1)^{\mu(x)}\gamma_{\downarrow}c_{x\downarrow}\otimes c_{x\uparrow}^{*}\gamma_{\uparrow}\mathscr{R}^{-1}\succeq 0 \ w.r.t. \ \mathscr{L}^{2}(\mathfrak{H})_{+}.$

Proof. By Proposition 7.20, we see that

$$\mathscr{R}(-1)^{\mu(x)}c_{x\uparrow}^*\gamma_{\downarrow}\otimes\gamma_{\uparrow}c_{x\downarrow}\mathscr{R}^{-1} = \mathcal{L}(c_{x\uparrow}\gamma_{\downarrow})\mathcal{R}(\gamma_{\downarrow}c_{x\uparrow}^*) \succeq 0 \quad \text{w.r.t.} \quad \mathscr{L}^2(\mathfrak{H})_+,$$
(7.67)

$$-\mathscr{R}(-1)^{\mu(x)}\gamma_{\downarrow}c_{x\downarrow}\otimes c_{x\uparrow}^{*}\gamma_{\uparrow}\mathscr{R}^{-1} = \mathcal{L}(c_{x\downarrow}\gamma_{\downarrow})\mathscr{R}((c_{x\downarrow}\gamma_{\downarrow})^{*}) \succeq 0 \quad \text{w.r.t.} \quad \mathscr{L}^{2}(\mathfrak{H})_{+}.$$
(7.68)

This completes the proof. \Box

Set

$$K_x = (-1)^{\mu(x)} \Big(c_{x\uparrow}^* \gamma_{\downarrow} \otimes \gamma_{\uparrow} c_{x\downarrow} - \gamma_{\downarrow} c_{x\downarrow} \otimes c_{x\uparrow}^* \gamma_{\uparrow} \Big).$$
(7.69)

By Corollary 7.21, we know that $\mathscr{R}K_x\mathscr{R}^{-1} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$. Thus, by (7.66), we obtain

$$\mathscr{R}\prod_{j=1}^{2n} (-1)^{\mu(x_j)} \left[c_{x_j\uparrow}^{\overline{\#}_j}(s_j)\gamma_{\downarrow} \otimes \gamma_{\uparrow} c_{x_j\downarrow}^{\#_j}(s_j) - \gamma_{\downarrow} c_{x_j\downarrow}^{\#_j}(s_j) \otimes c_{x_j\uparrow}^{\overline{\#}_j}(s_j)\gamma_{\uparrow} \right] e^{-\beta H_{\text{ext}}} \mathscr{R}^{-1}$$
$$= \underbrace{\mathscr{R}e^{-s_1 H_{\text{ext}}} \mathscr{R}^{-1}}_{\succeq 0} \underbrace{\mathscr{R}K_{x_1}^{\#_1} \mathscr{R}^{-1}}_{\succeq 0} \underbrace{\mathscr{R}e^{-(s_2-s_1)H_{\text{ext}}} \mathscr{R}^{-1}}_{\succeq 0} \cdots \underbrace{\mathscr{R}e^{-(\beta-s_n)H_{\text{ext}}} \mathscr{R}^{-1}}_{\succeq 0} \succeq 0 \quad (7.70)$$

w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$. Hence, by Theorem 3.10, we obtain the second inequality in (7.13). \Box

7.6 Proof of Corollary 7.5

Let

$$A_{x,+} = \overline{n}_{x\uparrow} n_{x\downarrow} \otimes 1 + 1 \otimes \overline{n}_{x\uparrow} n_{x\downarrow}, \quad A_{x,-} = \overline{n}_{x\uparrow} \otimes n_{x\downarrow} + n_{x\downarrow} \otimes \overline{n}_{x\uparrow}.$$
(7.71)

Observe that

$$\mathscr{U}A_{x,+}\mathscr{U}^* = \frac{1}{2} \Big\{ \mathcal{L}(\mathcal{N}_x)\mathcal{R}(\mathcal{N}_x) + \mathcal{L}(\mathcal{M}_x)\mathcal{R}(\mathcal{M}_x) \Big\}, \\ \mathscr{U}A_{x,-}\mathscr{U}^* = \frac{1}{2} \Big\{ \mathcal{L}(\mathcal{N}_x)\mathcal{R}(\mathcal{N}_x) - \mathcal{L}(\mathcal{M}_x)\mathcal{R}(\mathcal{M}_x) \Big\}.$$
(7.72)

Clearly, $\mathcal{L}(\mathcal{N}_x)\mathcal{R}(\mathcal{N}_x) \succeq 0$, $\mathcal{L}(\mathcal{M}_x)\mathcal{R}(\mathcal{M}_x) \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{X})_+$. Thus, we have

$$\mathscr{U}\left(\prod_{j=1}^{n} A_{x_{j},+} - \prod_{j=1}^{n} A_{x_{j},-}\right) \mathscr{U}^{*} \succeq 0 \quad \text{w.r.t.} \quad \mathscr{L}^{2}(\mathfrak{X})_{+}.$$
(7.73)

By applying Theorem 3.10, we obtain the first inequality in (7.16). Proof of the second inequality in (7.16) is similar to that of Section 7.5.2. \Box

8 Concluding remarks

Let \mathfrak{P} be a self-dual cone in the Hilbert space \mathfrak{H} . Let H_0 and V be self-adjoint operators in \mathfrak{H} . For simplicity, we assume that H_0 and V are bounded.¹⁷ H_0 is the free Hamiltonian and V is the interaction. The system's Hamiltonian is given by $H = H_0 - V$. Through our studies of the quantum Griffiths inequality, we recognize that the following are model-independent properties:¹⁸

(\mathfrak{P} i) $e^{-\beta H_0} \succeq 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$.

(\mathfrak{P} ii) $V \succeq 0$ w.r.t. \mathfrak{P} .

(\mathfrak{P} ii) is equivalent to $-V \leq 0$ w.r.t. \mathfrak{P} . Thus, if (\mathfrak{P} ii) is satisfied, we say that -V is *attractive* w.r.t. \mathfrak{P} . As we have discussed in the previous sections, when we construct the Griffiths inequality, it is most important to find a self-dual cone \mathfrak{P} such that -V becomes attractive w.r.t. \mathfrak{P} . In this step, we are faced with the following difficulty: in general, there are infinitely many self-dual cones in a single Hilbert space. Let us assume that (\mathfrak{P} i) and (\mathfrak{P} ii) are satisfied by choosing some self-dual cone \mathfrak{P} . Now let us choose another self-dual cone \mathfrak{P}' . Even if (\mathfrak{P} i) and (\mathfrak{P} ii) are satisfied, we can never conclude that (\mathfrak{P}' i) and (\mathfrak{P}' ii) are fulfilled. Therefore, to apply our theory, we have to choose a proper self-dual cone \mathfrak{P} such that (\mathfrak{P} i) and (\mathfrak{P} ii) are satisfied. In other words, a suitable choice of a self-dual cone makes the interaction -V attractive. In this sense, our theory is a kind of representation theory of attraction.

We remark upon some additional conclusions from $(\mathfrak{P} i)$ and $(\mathfrak{P} ii)$. First, we obtain the positivity of a ground state.

¹⁷This assumption can be relaxed [44].

¹⁸Even when we show the second Griffiths inequality, the properties (\mathfrak{P} i) and (\mathfrak{P} ii) are essential for our proof. Namely, (\mathfrak{P} i) and (\mathfrak{P} ii) still hold true for the extended Hamiltonian acting in the doubled Hilbert space $\mathfrak{H} \otimes \mathfrak{H}$, see Sections 2–7.

Theorem 8.1 [44] Assume (\mathfrak{P} i) and (\mathfrak{P} ii). Assume that $E = \inf \operatorname{spec}(H)$ is an eigenvalue of H. Then there exists a nonzero vector $\psi \in \ker(H - E)$ such that $\psi \ge 0$ w.r.t. \mathfrak{P} . Namely, among all the ground states of H, there exists at least one ground state that is positive w.r.t. \mathfrak{P} .

Theorem 8.2 claims that the attractive interaction makes the system more stable.

Theorem 8.2 [44] Assume (\mathfrak{P} i) and (\mathfrak{P} ii). Let $E_0 = \inf \operatorname{spec}(H_0)$. Then $E \leq E_0$.

To describe further effects of $(\mathfrak{P} i)$ and $(\mathfrak{P} ii)$, we define the following:

- **Definition 8.3** (i) A vector $y \in \mathfrak{H}$ is called strictly positive w.r.t. \mathfrak{P} , whenever $\langle x|y \rangle > 0$ for all $x \in \mathfrak{P} \setminus \{0\}$. We write this as y > 0 w.r.t. \mathfrak{P} .
 - (ii) We write $A \succ 0$ w.r.t. \mathfrak{P} , if Ax > 0 w.r.t. \mathfrak{P} for all $x \in \mathfrak{P} \setminus \{0\}$. In this case, we say that A improves the positivity w.r.t. \mathfrak{P} .

Theorem 8.4 [12, 43] Assume (\mathfrak{P} i) and (\mathfrak{P} ii). Assume that $e^{-\beta H} \ge 0$ w.r.t. \mathfrak{P} for all $\beta > 0$. If $E = \inf \operatorname{spec}(H)$ is an eigenvalue, then $\dim \ker(H - E) = 1$ (equivalently, if H has a ground state, then it is unique). Moreover, the unique ground state is strictly positive w.r.t. \mathfrak{P} .

Remark 8.5 If we impose additional conditions on V, we can prove $E < E_0$ [44].

As a corollary of Theorem 8.4, we obtain information about structure of the ground state.

Corollary 8.6 Let G be a group and let π be an irreducible representation of G on \mathfrak{H} . Assume that $\pi_g \geq 0$ w.r.t. \mathfrak{P} for all $g \in G$. Under the same assumptions as in Theorem 8.4, let φ be the ground state of H, i.e., $\varphi \in \ker(H - E)$. Then we have $\pi_g \varphi = \varphi$ for all $g \in G$.

In the theory of strongly correlated electron systems, we can investigate the magnetic properties of the ground state by Theorem 8.4 and Corollary 8.6 [14, 15, 37, 38, 39, 40, 43, 45, 46, 48, 49, 50, 55, 56, 57]. Furthermore, we can find the same structures ((\mathfrak{P} i) and (\mathfrak{P} ii)) in several areas, e.g., in the quantum field theory [16, 22, 26, 43, 46, 47, 51], open quantum systems [41], topological orders [30, 31], and the theory of phase transitions [1, 2, 3, 11, 17, 18, 21, 27, 33]. These facts indicate that (\mathfrak{P} i) and (\mathfrak{P} ii) are universal expressions of the notion of correlations. If this hypothesis is correct, then several areas could be described by the same language and a new discovery in some areas would automatically influence other areas. To reinforce this vision of unification, we must continue to collect evidence.

A Fundamental properties of operator inequalities associated with self-dual cones

A.1 Positivity preserving operators

In this appendix, we review useful operator inequalities studied in [43].

Let \mathfrak{H} be a complex Hilbert space and \mathfrak{P} be a self-dual cone in \mathfrak{H} .

Proposition A.1 Let $\{x_n\}_{n\in\mathbb{N}}$ be a CONS of \mathfrak{H} . Assume that $x_n \in \mathfrak{P}$ for all $n \in \mathbb{N}$. Assume that $A \ge 0$ w.r.t. \mathfrak{P} . Then we have $\operatorname{Tr}[A] \ge 0$.

Proof. Since $x_n \in \mathfrak{P}$, we see that $\langle x_n | A x_n \rangle \ge 0$ for all $n \in \mathbb{N}$. Thus, we arrive at $\operatorname{Tr}[A] = \sum_{n=1}^{\infty} \langle x_n | A x_n \rangle \ge 0$. \Box

Proposition A.2 Let $N = \dim \mathfrak{H} \in \mathbb{N} \cup \{\infty\}$. Let $\{x_n\}_{n=1}^N$ be a CONS of \mathfrak{H} . Assume that $x_n \in \mathfrak{P}$ for all $n \in \{1, \ldots, N\}$.¹⁹ Then the following (i) and (ii) are equivalent.

- (i) $A \succeq 0$ w.r.t. \mathfrak{P} .
- (ii) $A_{mn} = \langle x_m | A x_n \rangle \ge 0$ for all $m, n \in \{1, \dots, N\}$.

Proof. (i) \implies (ii): Trivial.

(ii) \implies (i): Let $w, z \in \mathfrak{P}$. Then we can write

$$w = \sum_{n=1}^{N} c_n x_n, \quad c_n = \langle w | x_n \rangle, \tag{A.1}$$

$$z = \sum_{n=1}^{N} d_n x_n, \quad d_n = \langle z | x_n \rangle.$$
(A.2)

Since $w, z \ge 0$ w.r.t. \mathfrak{P} , we see that $c_n \ge 0, d_n \ge 0$ for all $n \in \mathbb{N}$. Thus, we have

$$\langle w|Az \rangle = \sum_{m,n=1}^{N} c_m d_n A_{mn} \ge 0.$$
(A.3)

Since \mathfrak{P} is self-dual, we have $Az \ge 0$ w.r.t. \mathfrak{P} . Thus, we conclude that $A \ge 0$ w.r.t. \mathfrak{P} . \Box

Proposition A.3 Assume that $A \succeq 0$ w.r.t. \mathfrak{P} . Then $e^{\beta A} \succeq 0$ w.r.t. \mathfrak{P} for all $\beta \geq 0$.

Proof. Since $A \ge 0$ w.r.t. \mathfrak{P} , it holds that $A^n \ge 0$ w.r.t. \mathfrak{P} for all $n \in \mathbb{N}$. Thus,

$$e^{\beta A} = \sum_{n \ge 0} \underbrace{\frac{\beta^n}{n!}}_{\ge 0} \underbrace{A^n}_{\ge 0} \ge 0 \quad \text{w.r.t. } \mathfrak{P} \text{ for all } \beta \ge 0. \qquad \Box \qquad (A.4)$$

Proposition A.4 Assume that $e^{\beta A} \ge 0$ and $e^{\beta B} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$. Then $e^{\beta(A+B)} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$.

Proof. Note that $e^{\beta A}e^{\beta B} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$. Thus, $(e^{\beta A/n}e^{\beta B/n})^n \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$ and $n \in \mathbb{N}$. By the Trotter–Kato product formula, we obtain the desired assertion. \Box

The following proposition is repeatedly used in this study.

Proposition A.5 Assume the following:

¹⁹In the case where $N = \infty$, the symbol $\{1, \ldots, N\}$ denotes \mathbb{N} .

- (i) $e^{\beta A} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$.
- (ii) $B \ge 0$ w.r.t. \mathfrak{P} .

Then we have $e^{\beta(A+B)} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$.

Proof. By (ii) and Proposition A.3, it holds that $e^{\beta B} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$. Thus, applying Proposition A.4, we conclude the assertion. \Box

Proposition A.6 Let A be a positive self-adjoint operator. Assume that $e^{-\beta A} \ge 0$ w.r.t. \mathfrak{P} for all $\beta \ge 0$. Assume that $E = \inf \operatorname{spec}(A)$ is an eigenvalue of A. Then there exists a nonzero vector $x \in \operatorname{ker}(A - E)$ such that $x \ge 0$ w.r.t. \mathfrak{P} .

Proof. **STEP 1.** Let J be an antilinear involution given by Proposition A.7 below. Set $\mathfrak{H}_J = \{x \in \mathfrak{H} \mid Jx = x\}$. We will show that $\ker(A - E) \cap \mathfrak{H}_J \neq \{0\}$.

To see this, let $x \in \ker(A - E)$. Then we have the decomposition $x = \Re x + i\Im x$ with $\Re x = \frac{1}{2}(\mathbb{1} + J)x$ and $\Im x = \frac{1}{2i}(\mathbb{1} - J)x$. Clearly, $\Re x, \Im x \in \mathfrak{H}_J$. Since $x \neq 0$, it holds that $\Re x \neq 0$ or $\Im x \neq 0$. Since $e^{-\beta A} \geq 0$ w.r.t. \mathfrak{P} for all $\beta \geq 0$, A commutes with J. Thus, $\Re x, \Im x \in \ker(A - E) \cap \mathfrak{H}_J$.

STEP 2. Take $x \in \ker(A - E) \cap \mathfrak{H}_J$. By Proposition A.7 (iii), we have a unique decomposition $x = x_+ - x_-$, where $x_{\pm} \in \mathfrak{P}$ and $\langle x_+ | x_- \rangle = 0$. Let $|x| = x_+ + x_-$. Then we have

$$e^{-\beta E} \|x\| = \langle x|e^{-\beta A}x\rangle \le \langle |x||e^{-\beta A}|x|\rangle \le e^{-\beta E} \underbrace{\||x|\|}_{=\|x\|}.$$
 (A.5)

Thus, $|x| \in \ker(A - E)$. Clearly, $|x| \ge 0$ w.r.t. \mathfrak{P} . \Box

Proposition A.7 A self-dual cone \mathfrak{P} has the following properties:

- (i) $\mathfrak{P} \cap (-\mathfrak{P}) = \{0\}.$
- (ii) There exists a unique antilinear involution J in \mathfrak{H} such that Jx = x for all $x \in \mathfrak{P}$.
- (iii) Each element $x \in \mathfrak{H}$ with Jx = x has a unique decomposition $x = x_+ x_-$ where $x_+, x_- \in \mathfrak{P}$ and $\langle x_+ | x_- \rangle = 0$.
- (iv) \mathfrak{H} is linearly spanned by \mathfrak{P} .

Proof. See, e.g., [5]. \Box

A.2 Reflection positive operators

To apply Theorem 3.11, it is crucial to show that $e^{-\beta H} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$ for all $\beta > 0$. The following proposition is often useful in proving this condition:

Proposition A.8 Let H_0 be a self-adjoint operator on $\mathscr{L}^2(\mathfrak{H})$ bounded from below. Let $V \in \mathscr{B}(\mathscr{L}^2(\mathfrak{H}))$ be self-adjoint. Assume the following:

- (i) $e^{-\beta H_0} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$ for all $\beta \ge 0$.
- (ii) $V \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$.

Let $H = H_0 - V$. We have $e^{-\beta H} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$ for all $\beta \ge 0$.

Proof. Note that

$$e^{\beta V} = \sum_{n \ge 0} \underbrace{\frac{\beta^n}{n!}}_{\ge 0} \underbrace{V^n}_{\succeq 0} \succeq 0 \quad \text{w.r.t. } \mathscr{L}^2(\mathfrak{H})_+.$$
(A.6)

Thus, by the Trotter-Kato product formula, we obtain

$$e^{-\beta H} = s - \lim_{n \to \infty} \left(\underbrace{e^{-\beta H_0/n}}_{\succeq 0} \underbrace{e^{\beta V/n}}_{\succeq 0} \right)^n \succeq 0 \quad \text{w.r.t. } \mathscr{L}^2(\mathfrak{H})_+ \text{ for all } \beta \ge 0, \tag{A.7}$$

where s- $\lim_{n \to \infty}$ means the strong limit. \Box

Corollary A.9 Let $H_0 = \mathcal{L}(A) + \mathcal{R}(A)$, where A is self-adjoint and bounded from below. Let

$$V = \sum_{j=1}^{\infty} \mathcal{L}(B_j) \mathcal{R}(B_j), \tag{A.8}$$

where $B_j \in \mathscr{B}(\mathfrak{H})$ is self-adjoint and the right hand side of (A.8) is a weak convergent sum. Define $H = H_0 - V$. Then we obtain $e^{-\beta H} \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$ for all $\beta \ge 0$.

Proof. Observe that $e^{-\beta H_0} = \mathcal{L}(e^{-\beta A})\mathcal{R}(e^{-\beta A}) \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$ for all $\beta \ge 0$. Since $V \succeq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$, we obtain the desired assertion by Proposition A.8. \Box

The following lemma will be often useful:

Lemma A.10 Let A_j , j = 1, ..., N be a bounded operator acting in \mathfrak{H} . Let $M = (M_{ij})$ be a positive semidefinite $N \times N$ matrix. Then we have

$$\sum_{i,j=1}^{N} M_{ij} \mathcal{L}(A_i^*) \mathcal{R}(A_j) \succeq 0 \quad w.r.t. \quad \mathscr{L}^2(\mathfrak{H})_+.$$
(A.9)

Proof. There exists a unitary matrix U such that $M = U^*DU$, where $D = \text{diag}(\lambda_j)$ is a diagonal matrix with $\lambda_j \ge 0$. Set $\tilde{A}_i = \sum_{j=1}^N U_{ij}A_j$. Then we see

LHS of (A.9) =
$$\sum_{j=1}^{N} \lambda_j \mathcal{L}(\tilde{A}_j^*) \mathcal{R}(\tilde{A}_j) \succeq 0 \text{ w.r.t. } \mathscr{L}^2(\mathfrak{H})_+.$$
 (A.10)

This completes the proof. \Box

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