Correlation inequalities for Schrödinger operators

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Abstract

The purpose of the present paper is to analyze correlation structures of the ground states of the Schrödinger operator. We construct Griffiths inequalities for the ground state expectations by applying operator-theoretic correlation inequalities. As an example of such an application, we study the ground state properties of Schrödinger operators.

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Schrödinger operator; Correlation, Ground state expectation; Griffiths inequalities; Operator inequalities; Self-dual cone.

1 Introduction

The so-called "Ising model" was introduced by Lenz [20] to study ferromagnetic properties of a magnet. This model was discussed in his PhD thesis by Ising [16], and has been actively studied by both mathematicians and physicists. The Ising model on $\Lambda = [-L, L)^d \cap \mathbb{Z}^d$ is defind as follows. For each spin configuration $\boldsymbol{\sigma} = \{\sigma_x\}_{x\in\Lambda} \in \Omega = \{-1, +1\}^\Lambda$ on Λ, the energy of the Ising system is

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

where J_{xy} is a nonnegative coupling constant. The thermal average is defined by

$$\langle\sigma_A\rangle = \sum_{\boldsymbol{\sigma}\in\Omega} \sigma_A e^{-\beta H(\boldsymbol{\sigma})}\Big/ Z_\beta, \quad Z_\beta = \sum_{\boldsymbol{\sigma}\in\Omega} e^{-\beta H(\boldsymbol{\sigma})}, \tag{1.2}$$

where $\sigma_A = \prod_{x\in A}\sigma_x$ for each $A \subseteq \Lambda$. In his study of Ising ferromagnets [12, 13, 14], Griffiths discovered the well-known *Griffiths inequalities*. Kelly and Sherman refined the Griffiths inequalities as follows [17]:

- First inequality:

$$\langle\sigma_A\rangle \ge 0, \qquad A \subseteq \Lambda; \tag{1.3}$$

- Second inequality:

$$\langle \sigma_A \sigma_B \rangle - \langle \sigma_A \rangle \langle \sigma_B \rangle \ge 0, \quad A, B \subseteq \Lambda. \tag{1.4}$$

These inequalities played an important role in the rigorous study of the Ising model [15]. Accordingly, we can expect that the Griffiths inequalities express the essential idea of correlation in the Ising system. Therefore, it is logical to ask whether similar inequalities hold for other models. An attempt to find a solution of this question can be regarded as an exploration of the model-independent structure of correlations. Ginibre's work [10] was a first important step toward understanding this model-independent structure. His framework of constructing the Griffiths inequalities still hold for several classical models [34]. However, we know of a few examples of quantum models that satisfy Griffiths inequalities; it has been actively studied to construct the inequalities for quantum models, see, e.g., [2, 19, 33].

In recent studies, Miyao established the Griffiths inequalities for both Bose and Fermi systems [29]. His theory was constructed from the veiwpoint of operator-theoretic correlation inequalities. According to this theory, we can unify the method of reflection positivity in the theory of phase transitions [5, 8, 9], Lieb's spin reflection positivity in the Hubbard model [22, 26, 30, 38, 40] and Griffiths inequalities. In this way, the new theory is expected to describe a universal aspect of the notion of correlation.

The Schrödinger operator is undoubtedly one of the most important models in quantum theory. Hence, we can expect that this model will provide a crucial clue, leading to better understanding of the universal aspects of correlation. Conversely, there has been little research on correlation structures of the ground states of this model.[1] The principal aim of the present paper is to analyze correlation properties of the ground states of the Schrödinger operator in terms of the operator-theoretic correlation inequalities. This kind of the study is expected to be useful, when we examine the entanglment structures of many-body systems. Through this analysis, we clarify the Griffiths inequalities for ground state expectations. As we will see, our correlation inequalities provide qualitative information on the shape of ground states. The forms of the obtained results are consistent with (1.3) and (1.4), as we will see in Section 2. This is more than coincidence because our construction is based on our previous work [29] which is a generalization of the Griffiths inequalities. Finally, remark that our method can be applied to many-body Schrödinger operators.

The remainder of this paper is as follows. In Section 2, we display results from the analysis of operator theoretic correlation inequalities.

In Section 3, we introduce several operator inequalities associated with self-dual cones. As we will see, these inequalities are very useful to study correlation structures of the ground states.

Sections 4-9 are devoted to the analysis of the ground states of Schrödinger operators in terms of the theory constructed in Section 3.

In Appendix A, we construct a general theory of correlation inequalities as operator inequalities associated with self-dual cones. Although many of the results in this section are already proved in previous studies [6, 11, 24, 26, 27, 28, 29, 30, 31], we have specified them here the for readers' convenience.

[1] For example, see [1, 21]. In [1], Hydrogen-like atoms in constant magnetic field are studied. In [21], the Born-Oppenheimer energy is investigated.

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2 Results

2.1 Definitions and assumptions

We will study the Schrödinger operator

$$H = -\Delta_x - V \tag{2.1}$$

acting on the Hilbert space $L^2(\mathbb{R}^d; dx)$. As usual, Δ_x is a self-adjoint realization of the d-dimensional Laplacian, and V is a potential.

To state our results, we need the assumptions **(A)**, **(B)**, and **(C)** below.

Our first assumption concerns the self-adjointness of H.

(A) The potential $V : \mathbb{R}^d \to \mathbb{R}$ is chosen such that H is self-adjoint on $\mathrm{dom}(-\Delta_x)$ and bounded from below. $\diamondsuit$

Example 1 If $V \in L^n(\mathbb{R}^d; dx) + L^\infty(\mathbb{R}^d; dx)$ with $n = 2$ for $d \leq 3$, $n > 2$ for $d = 4$ and $n = d/2$ for $d \geq 4$, then V satisfies **(A)**, see, e.g., [36, Theorem X. 29]. $\diamondsuit$

As usual, the Fourier transform of f is defined by

$$\hat{f}(p) := (2\pi)^{-d/2} \int_{\mathbb{R}^d} dx\, e^{-ip\cdot x} f(x). \tag{2.2}$$

Our second assumption is stated as follows.

(B) There exists an approximating sequence $V_n \neq 0$ for V such that (i)–(iii) hold:

(i) Let $H_n = -\Delta_x - V_n$. H_n converges to H in the strong resolvent sense as $n \to \infty$.[2]

(ii) For all $n \in \mathbb{N}$ and a.e. p, the Fourier transform $\hat{V}_n(p)$ exists and satisfies $\hat{V}_n \in L^1(\mathbb{R}^d; dp)$, $\hat{V}_n(p) \geq 0$ and $\hat{V}_n(-p) = \hat{V}_n(p)$ a.e. p. Moreover, there exists an $\varepsilon > 0$ such that $\mathrm{supp}\hat{V}_n \supset B_\varepsilon(0)$, where $\mathrm{supp}\hat{V}_n = \overline{\{p \in \mathbb{R}^d \,|\, \hat{V}_n(p) \neq 0\}}$ and $B_\varepsilon(0) = \{p \in \mathbb{R}^d \,|\, |p| < \varepsilon\}$.

(iii) $\hat{V}_n(p)$ is monotonically increasing in n, i.e., $\hat{V}_n(p) \leq \hat{V}_{n+1}(p)$ a.e. p for all $n \in \mathbb{N}$. $\diamondsuit$

Remark 2.1 In concrete applications, it often happens that $\hat{V}$ does not exist, or that $\hat{V}$ exists, but $\hat{V} \notin L^1(\mathbb{R}^d; dp)$. Even in these cases, we can apply our theory of operator-theoretic correlation inequalities on the basis of the assumption **(B)**. This is the principal reason for introducing $\{V_n\}_{n=1}^\infty$. $\diamondsuit$

[2]Let $\{A_n\}_{n=1}^\infty$ be a sequence of self-adjoint operators on $L^2(\mathbb{R}^d; dx)$. We say that A_n converges to A in the *strong resolvent sense* if $(A_n - z)^{-1}$ converges to $(A - z)^{-1}$ in the strong operator topology for all z with $\mathrm{Im}z \neq 0$.

Example 2 Let us consider the Yukawa potential, $V(x) = \dfrac{e^{-m|x|}}{|x|}$ with $m > 0$. In the three-dimensional case, we have $\hat{V}(p) = \dfrac{2^{1/2}}{p^2 + m^2}$. Clearly, $\hat{V}(p) \notin L^1(\mathbb{R}^3; dp)$. In this case, we set

$$V_n(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} e^{ip\cdot x} \hat{V}_n(p) dp, \tag{2.3}$$

where

$$\hat{V}_n(p) = \begin{cases} \hat{V}(p) & \text{if } |p| \le n \\ 0 & \text{if } |p| > n \end{cases}. \tag{2.4}$$

Then, V_n satisfies the assumption **(B)**.[3]

We can also deal with the case where $m = 0$ by extending the above arguments. In this case, we have $\hat{V}(p) = 2^{1/2}/p^2$. Set $\hat{V}_n(p) = \hat{V}(p)\chi_{I_n}(p)$, where χ_{I_n} is the indicator function of a set $I_n = B_n(0) \backslash B_{1/n}(0)$. Then we can readily confirm that $\hat{V}_n$ satisfies the assumption **(B)**. $\diamondsuit$

Example 3 We consider the three-dimensional case: $d = 3$. Let V be a potential such that $V \in \mathcal{S}(\mathbb{R}^3)$, the Schwartz class, and $V(-x) = V(x)$. We assume that $\hat{V}(p) \ge 0$ for all $p \in \mathbb{R}^3$. Then the following properties are readily obtained:

- $\hat{V}(0) > 0$;
- $\hat{V}(p)$ is continuous in p.

Therefore, there exists a number $\varepsilon > 0$ such that $\mathrm{supp}\hat{V} \supset B_\varepsilon(0)$. By setting $\hat{V}_n(p) = \hat{V}(p)$ for all $n \in \mathbb{N}$, we see that the assumption **(B)** is satisfied. A typical example is $V(x) = V_0 e^{-x^2/a^2}$ with $V_0 > 0$ and $a > 0$.

For a given linear operator A, we denote by $\sigma(A)$ spectrum of A. The following assumption concerns the least eigenvalue of H.

(C) There exists an $n_0 \in \mathbb{N}$ such that, for all $n \ge n_0$, $\inf \sigma(H_n)$ is an eigenvalue of H_n. In addition, $\inf \sigma(H)$ is an eigenvalue of H. $\diamondsuit$

Example 4 Let us consider the Yukawa potential given in Example 2. If m is small, then $\inf \sigma(H)$ is an eigenvalue. This is because $H^{(m)}$ converges to $H^{(m=0)}$, the Hamiltonian of the hydrogen-like atom, as $m \to +0$ in the strong resolvent sense. Here, we clarify the m-dependence of H by expressing H as $H^{(m)}$. Since H_n converges to H in the strong resolvent sense as $n \to \infty$, $\inf \sigma(H_n)$ must be an eigenvalue, provided that n is large enough. $\diamondsuit$

[3] *Proof.* (ii) and (iii) of the condition **(B)** are easy to check.

(i) Remark that $\|V_n - V\|_{L^2} = \|\hat{V}_n - \hat{V}\|_{L^2} \to 0$ as $n \to \infty$. Thus, for each $\varphi \in C_0^\infty(\mathbb{R}^3)$, we see that $\|(V_n - V)\varphi\|_{L^2} \le \|V_n - V\|_{L^2} \|\varphi\|_{L^\infty} \to 0$ as $n \to \infty$, which implies that $(-\Delta_x - V_n)\varphi$ converges to $(-\Delta_x - V)\varphi$ as $n \to \infty$. Because $C_0^\infty(\mathbb{R}^3)$ is a common core for $-\Delta_x - V_n$ and $-\Delta_x - V$, we can apply a general theorem [35, Theorem VIII. 25 (a)] and conclude that $-\Delta_x - V_n$ converges to $-\Delta_x - V$ in the strong resolvent sense. $\square$

Definition 2.2 We say that the potential V is *regular* if it satisfies **(A)**, **(B)**, and **(C)**. $\diamondsuit$

Example 5 (i) The Yukawa potential discussed in Example 2 is regular, if $m = 0$ or m is sufficiently small.

(ii) Let us consider the potential V concretely given in Example 3. Then V is regular provided that V_0 is large enough. $\diamondsuit$

Definition 2.3 Let A be a self-adjoint operator, bounded from below. If $\inf \sigma(A)$ is an eigenvalue, then the corresponding normalized eigenvectors are called *ground states* of A. $\diamondsuit$

The following proposition is a basic input.

Proposition 2.4 *Assume that V is regular. The ground state of H (resp., H_n) is unique. Let ψ (resp., ψ_n) be the unique ground state of H (resp., H_n). We have the following:*

(i) $\psi(x) > 0$ *and* $\psi_n(x) > 0$ *a.e.* x.

(ii) $\hat{\psi}(p) > 0$ *and* $\hat{\psi}_n(p) > 0$ *a.e.* p.

Remark 2.5 The property (i) is well-known, see, e.g., [37, Theorem XIII.45], however, as far as we know, the property (ii) is novel. $\diamondsuit$

We prove Proposition 2.4 in Section 4.

We denote by $\mathscr{B}(\mathfrak{H})$ the set of all bounded linear operators on a Hilbert space $\mathfrak{H}$.

Definition 2.6 Let ψ (resp., ψ_n) be the unique ground state of H (resp., H_n). For each $A \in \mathscr{B}(L^2(\mathbb{R}^d; dx))$, we define the *ground state expectation* $\langle A \rangle$ by

$$\langle A \rangle = \langle \psi | A\psi \rangle. \tag{2.5}$$

Similarly, we define $\langle A \rangle_n = \langle \psi_n | A\psi_n \rangle$. $\diamondsuit$

2.2 First inequalities

In this study, we write the operator M_f, for multiplication by the function f, simply as f, if no confusion occurs.

For each $f \in L^\infty(\mathbb{R}^d; dx)$, a linear operator $f(-i\nabla_x)$ is defined by

$$f(-i\nabla_x)\phi = \Big(f(p)\hat{\phi}\Big)^{\vee}, \quad \phi \in L^2(\mathbb{R}^d; dx), \tag{2.6}$$

where $\vee$ is the inverse Fourier transform.

Let

$$\mathfrak{A} = \big\{ f \in L^\infty(\mathbb{R}^d; dx) \cap L^2(\mathbb{R}^d; dx) \,\big|\, \hat{f}(p) \ge 0 \ \text{ a.e. } p \big\}. \tag{2.7}$$

The following theorem corresponds to the first Griffiths inequality (1.3).

Theorem 2.7 *Assume that V is regular.*

(i) *For all $f \in \mathfrak{A}$, $\langle f \rangle \ge 0$. The equality holds if and only if $f = 0$.*

(ii) *For all $f \in \mathfrak{A}$, $\big\langle f(-i\nabla_x) \big\rangle \ge 0$. The equality holds if and only if $f = 0$.*

We prove Theorem 2.7 in Section 4.

2.3 Second inequalities

Here, we state some results related to the second Griffiths inequality (1.4). For this purpose, we introduce the following:

$$\mathfrak{A}_{\rm e} = \left\{ f \in L^\infty(\mathbb{R}^d; dx) \cap L^2(\mathbb{R}^d; dx) \,\middle|\, \hat{f}(p) \ge 0 \ \text{ a.e. } p \text{ and } f(-x) = f(x) \text{ a.e. } x \right\}. \tag{2.8}$$

By the assumption (i) of **(B)**, we can readily expect that $\langle A \rangle_n$ converges to $\langle A \rangle$ as $n \to \infty$. The following theorem provides more detailed information on the convergence.

Theorem 2.8 *Assume that V is regular.*

- (i) *For all $f \in \mathfrak{A}_{\rm e}$, $\langle f \rangle_n$ is monotonically increasing in n and converges to $\langle f \rangle$.*
- (ii) *For all $f \in \mathfrak{A}_{\rm e}$, $\big\langle f(-i\nabla_x) \big\rangle_n$ is monotonically decreasing in n and converges to $\big\langle f(-i\nabla_x) \big\rangle$.*

We provide a proof of Theorem 2.8 in Section 5.

The following theorem is a generalization of the second Griffiths inequality (1.4).

Theorem 2.9 *Assume that V is regular. For all $f, g \in \mathfrak{A}_{\rm e}$, we have the following:*

- (i) $\langle fg \rangle - \langle f \rangle \langle g \rangle \ge 0$.
- (ii) $\big\langle f(-i\nabla_x) g(-i\nabla_x) \big\rangle - \big\langle f(-i\nabla_x) \big\rangle \big\langle g(-i\nabla_x) \big\rangle \ge 0$.
- (iii) $\big\langle f(-i\nabla_x) g \big\rangle - \big\langle f(-i\nabla_x) \big\rangle \big\langle g \big\rangle \le 0$.

Remark 2.10 In Section 4.3, we will show the following:

- (i) $\big\langle f(-i\nabla_x) g \big\rangle$ is a real number;
- (ii) if $f(x) \ge 0$ or $g(x) \ge 0$, then $\big\langle f(-i\nabla_x) g \big\rangle \ge 0$.

Thus, Theorem 2.9 (iii) is meanigful. $\diamondsuit$

We provide a proof of Theorem 2.9 in Section 6.

Definition 2.11 Let $V^{(1)}$ and $V^{(2)}$ be regular potentials. Let $\hat{V}_n^{(1)}$ and $\hat{V}_n^{(2)}$ be the corresponding approximating functions appearing in the condition **(B)**. We write $V^{(1)} \succeq V^{(2)}$, if there exists an $n_0 \in \mathbb{N}$ such that for all $n \ge n_0$, $\hat{V}_n^{(1)}(p) \ge \hat{V}_n^{(2)}(p)$ a.e. p. $\diamondsuit$

Example 6 Let W be a regular potential. Assume that λW is regular for all $\lambda \in I$, where I is an open subset of $(0, \infty)$. We set $V^{(1)} = \lambda_1 W$ and $V^{(2)} = \lambda_2 W$. If $\lambda_1, \lambda_2 \in I$ and $\lambda_1 \ge \lambda_2$, then $V^{(1)} \succeq V^{(2)}$.

As a typical example, we consider the following. Let W be a potential given in Example 3: $W(x) = W_0 e^{-x^2/a^2}$. The potential W is regular provided that W_0 is large enough. Let I be an open subset of $\mathbb{R}$ such that $I \subseteq [1, \infty)$. Then λW is regular for all $\lambda \in I$. $\diamondsuit$

Let $V^{(1)}$ and $V^{(2)}$ be regular potentials. We consider Schrödinger operators given by

$$H^{(1)} = -\Delta_x - V^{(1)}, \quad H^{(2)} = -\Delta_x - V^{(2)}. \tag{2.9}$$

Let $\psi^{(1)}$ (resp., $\psi^{(2)}$) be the unique ground state of $H^{(1)}$ (resp., $H^{(2)}$). We set

$$\langle A\rangle^{(1)} = \langle \psi^{(1)}|A\psi^{(1)}\rangle, \quad \langle A\rangle^{(2)} = \langle \psi^{(2)}|A\psi^{(2)}\rangle. \tag{2.10}$$

In Section 7, we demonstrate the following.

Theorem 2.12 *Assume that $V^{(1)}$ and $V^{(2)}$ are regular.*

(i) *If $V^{(1)} \succeq V^{(2)}$, then $\langle f\rangle^{(1)} \ge \langle f\rangle^{(2)}$ for all $f \in \mathfrak{A}_{\rm e}$.*

(ii) *If $V^{(1)} \succeq V^{(2)}$, then $\big\langle f(-i\nabla_x)\big\rangle^{(1)} \le \big\langle f(-i\nabla_x)\big\rangle^{(2)}$ for all $f \in \mathfrak{A}_{\rm e}$.*

2.4 Application I: Ground state properties

We study some properties of the ground states by the correlation inequalities. In Section 8, we will show the following theorems.

Theorem 2.13 *Assume that V is regular. Let ψ be the ground state of H. We set*

$$\mathcal{C}(V) = \{x \in \mathbb{R}^d \,|\, \psi \text{ is continuous at } x\}, \tag{2.11}$$
$$\hat{\mathcal{C}}(V) = \{p \in \mathbb{R}^d \,|\, \hat{\psi} \text{ is continuous at } p\}. \tag{2.12}$$

Assume that $0 \in \mathcal{C}(V)$ and $0 \in \hat{\mathcal{C}}(V)$. Then we have the following:

(i) *$\psi(0) \ge \psi(x)$ for all $x \in \mathcal{C}(V)$.*

(ii) *$\hat{\psi}(0) \ge \hat{\psi}(p)$ for all $p \in \hat{\mathcal{C}}(V)$.*

Taking the above theorem into consideration, we define

$$\delta\psi(x) = \sqrt{\psi(0)^2 - \psi(x)^2}. \tag{2.13}$$

Remark 2.14
1. Let us consider the hydrogen-like atom discussed in Example 2: $V(x) = 2^{1/2}/|x|$. Then we can confirm that all assumptions in Theorem 2.13 are satisfied.

2. Using [23, Theorem 11.7], we see that $0 \in \mathcal{C}(V)$ under additional assumptions on V. [4] We can also apply [39, Theorem C.1.1] to check that every potential given in Example 3 satisfies this condition. ♢

[4] For example, suppose that $V \in L^1(B_r)$, where $B_r = \{x \in \mathbb{R}^d \,|\, |x| < r\}$. Suppose that $d \ge 2$. If $V \in L^p(B_r)$ for $d \ge p > d/2$, then for all $\alpha < 2 - d/p$,

$$|\psi(x) - \psi(y)| \le C|x-y|^\alpha \tag{2.14}$$

for some $C > 0$ and all $x, y \in B_{r'}$ with $r' < r$. Hence, $\mathcal{C}(V) \supseteq B_{r'}$ in this case. Note that all potential given in Example 3 fulfill the assmptions.

Theorem 2.15 *Assume that* $V^{(1)}$ *and* $V^{(2)}$ *are regular. Assume that* $0 \in \mathcal{C}(V^{(1)}) \cap \mathcal{C}(V^{(2)})$. *If* $V^{(1)} \succeq V^{(2)}$, *then we have the following:*

(i) $\psi^{(1)}(0) \geq \psi^{(2)}(0)$.

(ii) $\delta\psi^{(1)}(x) \geq \delta\psi^{(2)}(x)$ *for all* $x \in \mathcal{C}(V^{(1)}) \cap \mathcal{C}(V^{(2)})$.

Next, we define

$$\delta\hat{\psi}(p) = \sqrt{\hat{\psi}(0)^2 - \hat{\psi}(p)^2}. \tag{2.15}$$

Theorem 2.16 *Assume that* $V^{(1)}$ *and* $V^{(2)}$ *are regular. Assume that* $0 \in \hat{\mathcal{C}}(V^{(1)}) \cap \hat{\mathcal{C}}(V^{(2)})$. *In addition, assume that* $\hat{\psi}^{(1)}$ *and* $\hat{\psi}^{(2)}$ *are bounded. If* $V^{(1)} \succeq V^{(2)}$, *then we have the following:*

(i) $\hat{\psi}^{(1)}(0) \leq \hat{\psi}^{(2)}(0)$.

(ii) $\delta\hat{\psi}^{(1)}(p) \leq \delta\hat{\psi}^{(2)}(p)$ *for all* $p \in \hat{\mathcal{C}}(V^{(1)}) \cap \hat{\mathcal{C}}(V^{(2)})$.

Example 7 Let W be a regular potential given in Example 6. Let ψ_λ be the unique ground state of $H_\lambda = -\Delta_x - \lambda W$. For simplicity, we assume that ψ_λ and $\hat{\psi}_\lambda$ are continuous on $\mathbb{R}^d$ for all $\lambda \in I$. We have the following:

(i) $\delta\psi_\lambda(x)$ is monotonically increasing in λ for all x.

(ii) $\delta\hat{\psi}_\lambda(p)$ is monotonically decreasing in λ for all p.

Roughly speaking, (i) and (ii) above mean that, as λ increases the shape of $\psi_\lambda(x)$ becomes sharper, while that of $\hat{\psi}_\lambda(p)$ becomes blunter. In other words, the wave function of the particle is more localized around the origin in the position space as λ increases, while in the momentum space, it is delocalized. These facts can be regarded as an expression of Heisenberg's uncertainty principle. $\diamondsuit$

2.5 Application II: Properties of $|\psi(x)|^2$

Let $\varrho(x) = |\psi(x)|^2$. In the context of quantum mechanics, $\varrho(x)$ is interpreted as the probability density that the particle is at x. We can apply the correlation inequalities to investigate properties of $\varrho(x)$. Here, we present some examples of applications.

Since $\varrho \in L^1(\mathbb{R}^d; dx)$, $\hat{\varrho}(p)$ exists for all $p \in \mathbb{R}^d$ and is continuous in p.

In Section 9, we prove the following three theorems:

Theorem 2.17 *Assume that* V *is regular.*

(i) $0 < \hat{\varrho}(p)$ *for all* p.

(ii) $\hat{\varrho}(p) \leq \hat{\varrho}(0) = (2\pi)^{-d/2}$ *for all* p. *There is equality if and only if* $p = 0$.

(iii) $(2\pi)^{d/2}\hat{\varrho}(p)\hat{\varrho}(p') \leq \frac{1}{2}\hat{\varrho}(p - p') + \frac{1}{2}\hat{\varrho}(p + p')$ *for all* p, p'.

Theorem 2.17 provides information about the shape of the function $\hat{\varrho}(p)$.

Let $\varrho_n(x) = |\psi_n(x)|^2$. By the assumption (i) of **(B)**, we readily confirm that $\hat{\varrho}_n(p)$ converges to $\hat{\varrho}(p)$ as $n \to \infty$. The correlation inequalities stated in this section enable us to obtain further information on the convergence:

Theorem 2.18 *Assume that V is regular. Then, $\hat{\varrho}_n(p)$ is monotonically increasing in n for all $p \in \mathbb{R}^d$.*

Theorem 2.19 *Assume that $V^{(1)}$ and $V^{(2)}$ are regular, and that $V^{(1)} \succeq V^{(2)}$. Let $\varrho^{(1)}(x) = |\psi^{(1)}(x)|^2$ and $\varrho^{(2)}(x) = |\psi^{(2)}(x)|^2$. Then, $\hat{\varrho}^{(1)}(p) \geq \hat{\varrho}^{(2)}(p)$ for all $p \in \mathbb{R}^d$.*

Theorem 2.19 suggests that, as the strength of V becomes larger, the probability density has a tendency to localized around the origin in the position space. This result is consistent with the results in Section 2.4.

Example 8 Let W be a regular potential given in Example 6. Let ψ_λ be the unique ground state of $H_\lambda = -\Delta_x - \lambda W$, and let $\varrho_\lambda(x) = |\psi_\lambda(x)|^2$. Then, $\hat{\varrho}_\lambda(p)$ is monotonically increasing in $\lambda \in I$ for all $p \in \mathbb{R}^d$. $\diamondsuit$

3 Preliminaries

In order to prove the theorems in Section 2, we must introduce several operator inequalities associated with self-dual cones.

3.1 Self-dual cones

Let $\mathfrak{H}$ be a complex Hilbert space. By a *convex cone*, we understand a closed convex set $\mathfrak{P} \subset \mathfrak{H}$ such that $t\mathfrak{P} \subseteq \mathfrak{P}$ for all $t \geq 0$ and $\mathfrak{P} \cap (-\mathfrak{P}) = \{0\}$. In what follows, we always assume that $\mathfrak{P} \neq \{0\}$.

Definition 3.1 The *dual cone of* $\mathfrak{P}$ is defined by

$$\mathfrak{P}^\dagger = \{\eta \in \mathfrak{H} \,|\, \langle \eta|\xi\rangle \geq 0 \ \forall \xi \in \mathfrak{P}\}. \tag{3.1}$$

We say that $\mathfrak{P}$ is *self-dual* if $\mathfrak{P} = \mathfrak{P}^\dagger$. $\diamondsuit$

Definition 3.2 ([6]) Let $\mathfrak{H}$ be a complex Hilbert space. A convex cone $\mathfrak{P}$ in $\mathfrak{H}$ is called a *Hilbert cone*, if it satisfies the following:

(i) $\langle \xi|\eta\rangle \geq 0$ for all $\xi, \eta \in \mathfrak{P}$.

(ii) Let $\mathfrak{H}_\mathbb{R}$ be a real closed subspace of $\mathfrak{H}$ generated by $\mathfrak{P}$. Then for all $\xi \in \mathfrak{H}_\mathbb{R}$, there exist $\xi_+, \xi_- \in \mathfrak{P}$ such that $\xi = \xi_+ - \xi_-$ and $\langle \xi_+|\xi_-\rangle = 0$.

(iii) $\mathfrak{H} = \mathfrak{H}_\mathbb{R} + i\mathfrak{H}_\mathbb{R} = \{\xi + i\eta \,|\, \xi, \eta \in \mathfrak{H}_\mathbb{R}\}$. $\diamondsuit$

Remark 3.3 Let $\mathfrak{P}$ be a Hilbert cone in $\mathfrak{H}$. For each $\xi \in \mathfrak{H}$, we have the following expression:

$$\xi = (\xi_1 - \xi_2) + i(\xi_3 - \xi_4), \tag{3.2}$$

where ξ_1, ξ_2, ξ_3 and ξ_4 satisfy $\xi_1, \xi_2, \xi_3, \xi_4 \in \mathfrak{P}$, $\langle \xi_1|\xi_2\rangle = 0$ and $\langle \xi_3|\xi_4\rangle = 0$. $\diamondsuit$

Theorem 3.4 *Let $\mathfrak{P}$ be a convex cone in $\mathfrak{H}$. The following are equivalent:*

(i) *$\mathfrak{P}$ is a self-dual cone.*

(ii) $\mathfrak{P}$ *is a Hilbert cone.*

Proof. For (i) $\Rightarrow$ (ii), see, e.g., [4] or [3, Proof of Proposition 2.58].

Suppose that $\mathfrak{P}$ is a Hilbert cone. We easily see that $\mathfrak{P} \subseteq \mathfrak{P}^\dagger$ by Definition 3.2 (i). We will show the inverse. Let $\xi \in \mathfrak{P}^\dagger$. By (3.2), we can write ξ as $\xi = (\xi_{R,+} - \xi_{R,-}) + i(\xi_{I,+} - \xi_{I,-})$ with $\xi_{R,\pm}, \xi_{I,\pm} \in \mathfrak{P}$, $\langle \xi_{R,+} | \xi_{R,-} \rangle = 0$ and $\langle \xi_{I,+} | \xi_{I,-} \rangle = 0$. Assume that $\xi_{I,+} \neq 0$. Then $\langle \xi | \xi_{I,+} \rangle$ is a complex number, which contradicts with the fact that $\langle \xi | \eta \rangle \geq 0$ for all $\eta \in \mathfrak{P}$. Thus, $\xi_{I,+} = 0$. Similarly, we have $\xi_{I,-} = 0$. Next, assume that $\xi_{R,-} \neq 0$. Because $\xi_{R,-} \in \mathfrak{P}$, we have

$$0 \leq \langle \xi | \xi_{R,-} \rangle = -\|\xi_{R,-}\|^2 < 0, \tag{3.3}$$

which is a contradiction. Hence, we conclude that $\xi = \xi_{R,+} \in \mathfrak{P}$. $\square$

Definition 3.5

- A vector ξ is said to be *positive w.r.t.* $\mathfrak{P}$ if $\xi \in \mathfrak{P}$. We write this as $\xi \geq 0$ w.r.t. $\mathfrak{P}$.
- A vector $\eta \in \mathfrak{P}$ is called *strictly positive w.r.t.* $\mathfrak{P}$ whenever $\langle \xi | \eta \rangle > 0$ for all $\xi \in \mathfrak{P} \backslash \{0\}$. We write this as $\eta > 0$ w.r.t. $\mathfrak{P}$. $\diamondsuit$

Example 9 For each $d \in \mathbb{N}$, we set

$$L^2(\mathbb{R}^d; du)_+ = \{ f \in L^2(\mathbb{R}^d; du) \,|\, f(u) \geq 0 \ \text{ a.e. } u \}. \tag{3.4}$$

$L^2(\mathbb{R}^d; du)_+$ is a self-dual cone in $L^2(\mathbb{R}^d; du)$. $f \geq 0$ w.r.t. $L^2(\mathbb{R}^d; du)_+$ if and only if $f(u) \geq 0$ a.e. u. On the other hand, $f > 0$ w.r.t. $L^2(\mathbb{R}^d; du)_+$ if and only if $f(u) > 0$ a.e. u. $\diamondsuit$

3.2 Operator inequalities associated with self-dual cones

In subsequent sections, we use the following operator inequalities.

Definition 3.6 Let $A, B \in \mathscr{B}(\mathfrak{H})$. Let $\mathfrak{P}$ be a self-dual cone in $\mathfrak{H}$.

If $A\mathfrak{P} \subseteq \mathfrak{P}$,[5] we then write this as $A \trianglerighteq 0$ w.r.t. $\mathfrak{P}$.[6] In this case, we say that A *preserves the positivity w.r.t.* $\mathfrak{P}$. Suppose that $A\mathfrak{H}_\mathbb{R} \subseteq \mathfrak{H}_\mathbb{R}$ and $B\mathfrak{H}_\mathbb{R} \subseteq \mathfrak{H}_\mathbb{R}$. If $(A - B)\mathfrak{P} \subseteq \mathfrak{P}$, then we write this as $A \trianglerighteq B$ w.r.t. $\mathfrak{P}$. $\diamondsuit$

Remark 3.7

(i) $A \trianglerighteq 0$ w.r.t. $\mathfrak{P} \iff \langle \xi | A\eta \rangle \geq 0$ for all $\xi, \eta \in \mathfrak{P}$.

(ii) Let $A \in \mathscr{B}(\mathfrak{H})$. If $A\mathfrak{H}_\mathbb{R} \subseteq \mathfrak{H}_\mathbb{R}$, we say that A *preserves the reality w.r.t.* $\mathfrak{P}$. The following fact will be often used: if A preserves the positivity w.r.t. $\mathfrak{P}$, then A preserves the reality w.r.t. $\mathfrak{P}$. $\diamondsuit$

The following proposition is fundamental to this paper.

Proposition 3.8 *Let $A, B, C, D \in \mathscr{B}(\mathfrak{H})$ and let $a, b \in \mathbb{R}$.*

(i) *If $A \trianglerighteq 0, B \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ and $a, b \geq 0$, then $aA + bB \trianglerighteq 0$ w.r.t. $\mathfrak{P}$.*

[5] For each subset $\mathfrak{C} \subseteq \mathfrak{H}$, $A\mathfrak{C}$ is defined by $A\mathfrak{C} = \{Ax \,|\, x \in \mathfrak{C}\}$.

[6] This symbol was introduced by Miura [32], see also [18].

(ii) *If* $A \trianglerighteq B \trianglerighteq 0$ *and* $C \trianglerighteq D \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}$*, then* $AC \trianglerighteq BD \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}$*.*

(iii) *If* $A \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}$*, then* $A^* \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}$*.*

Proof. (i) is trivial.

(ii) If $X \trianglerighteq 0$ and $Y \trianglerighteq 0$ w.r.t. $\mathfrak{P}$, we have $XY\mathfrak{P} \subseteq X\mathfrak{P} \subseteq \mathfrak{P}$. Hence, it holds that $XY \trianglerighteq 0$ w.r.t. $\mathfrak{P}$. Hence, we have

$$AC - BD = \underbrace{A}_{\trianglerighteq 0}\underbrace{(C-D)}_{\trianglerighteq 0} + \underbrace{(A-B)}_{\trianglerighteq 0}\underbrace{D}_{\trianglerighteq 0} \trianglerighteq 0 \quad \text{w.r.t. } \mathfrak{P}.$$

(iii) For each $\xi, \eta \in \mathfrak{P}$, we know that

$$\langle \xi | A^* \eta \rangle = \langle \underbrace{A}_{\trianglerighteq 0}\underbrace{\xi}_{\geq 0} | \underbrace{\eta}_{\geq 0} \rangle \geq 0. \tag{3.5}$$

Thus, by Remark 3.7 (i), we conclude (iii). $\square$

Definition 3.9 Let $A \in \mathscr{B}(\mathfrak{H})$. We write $A \triangleright 0$ w.r.t. $\mathfrak{P}$, if $A\xi > 0$ w.r.t. $\mathfrak{P}$ for all $\xi \in \mathfrak{P}\backslash\{0\}$. In this case, we say that A *improves the positivity w.r.t.* $\mathfrak{P}$. $\diamondsuit$

Definition 3.10 Let $A \in \mathscr{B}(\mathfrak{H})$. Assume that $A \trianglerighteq 0$ w.r.t. $\mathfrak{P}$. We say that A is *ergodic w.r.t.* $\mathfrak{P}$ if for each $\xi, \eta \in \mathfrak{P}\backslash\{0\}$, there exists an $n \in \{0\} \cup \mathbb{N}$ such that $\langle \xi | A^n \eta \rangle > 0$. Note that the number n could depend on ξ and η. $\diamondsuit$

3.3 A canonical cone in $\mathscr{L}^2(\mathfrak{H})$

Let $\mathfrak{H}$ be a complex Hilbert space. The set of all Hilbert–Schmidt class operators on $\mathfrak{H}$ is denoted by $\mathscr{L}^2(\mathfrak{H})$, i.e., $\mathscr{L}^2(\mathfrak{H}) = \{\xi \in \mathscr{B}(\mathfrak{H}) \,|\, \mathrm{Tr}[\xi^*\xi] < \infty\}$. $\mathscr{L}^2(\mathfrak{H})$ is a two-sided ideal in $\mathscr{B}(\mathfrak{H})$. Henceforth, we regard $\mathscr{L}^2(\mathfrak{H})$ as a Hilbert space equipped with the inner product $\langle \xi | \eta \rangle_{\mathscr{L}^2} = \mathrm{Tr}[\xi^*\eta]$, $\xi, \eta \in \mathscr{L}^2(\mathfrak{H})$.

Definition 3.11 For each $A \in \mathscr{B}(\mathfrak{H})$, the *left multiplication operator* is defined by

$$\mathcal{L}(A)\xi = A\xi, \quad \xi \in \mathscr{L}^2(\mathfrak{H}). \tag{3.6}$$

Similarly, the *right multiplication operator* is defined by

$$\mathcal{R}(A)\xi = \xi A, \quad \xi \in \mathscr{L}^2(\mathfrak{H}). \tag{3.7}$$

Note that $\mathcal{L}(A)$ and $\mathcal{R}(A)$ belong to $\mathscr{B}(\mathscr{L}^2(\mathfrak{H}))$, where $\mathscr{B}(\mathscr{L}^2(\mathfrak{H}))$ is the set of all bounded linear operators on $\mathscr{L}^2(\mathfrak{H})$. $\diamondsuit$

It is not difficult to check that

$$\mathcal{L}(A)\mathcal{L}(B) = \mathcal{L}(AB), \quad \mathcal{R}(A)\mathcal{R}(B) = \mathcal{R}(BA), \quad A, B \in \mathscr{B}(\mathfrak{H}). \tag{3.8}$$

Let ϑ be an antiunitary operator on $\mathfrak{H}$.[7] Let Φ_ϑ be an isometric isomorphism from $\mathscr{L}^2(\mathfrak{H})$ onto $\mathfrak{H} \otimes \mathfrak{H}$ defined by

$$\Phi_\vartheta(|x\rangle\langle y|) = x \otimes \vartheta y \quad \forall x, y \in \mathfrak{H}, \tag{3.9}$$

[7] We say that a bijective map ϑ on $\mathfrak{H}$ is *antiunitary* if $\langle \vartheta x | \vartheta y \rangle = \overline{\langle x | y \rangle}$ for all $x, y \in \mathfrak{H}$.

where the linear operator $|x\rangle\langle y|$ is defined by $|x\rangle\langle y|z = \langle y|z\rangle x$ for all $z \in \mathfrak{H}$. Then,

$$\mathcal{L}(A) = \Phi_\vartheta^{-1} A \otimes \mathbb{1}\Phi_\vartheta, \quad \mathcal{R}(\vartheta A^* \vartheta) = \Phi_\vartheta^{-1} \mathbb{1} \otimes A\Phi_\vartheta \tag{3.10}$$

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

$$\mathfrak{H} \otimes \mathfrak{H} = \mathscr{L}^2(\mathfrak{H}), \quad A \otimes \mathbb{1} = \mathcal{L}(A), \quad \mathbb{1} \otimes A = \mathcal{R}(\vartheta A^* \vartheta), \tag{3.11}$$

if no confusion arises.

The left and right multiplication operators can be extended to unbounded operators by (3.10) as follows. Let A be a densely defined closed operator on $\mathfrak{H}$. The left multiplication operator $\mathcal{L}(A)$ and the right multiplication operator $\mathcal{R}(A)$ are defined as $\mathcal{L}(A) = \Phi_\vartheta^{-1} A \otimes \mathbb{1}\Phi_\vartheta$ and $\mathcal{R}(A) = \Phi_\vartheta^{-1} \mathbb{1} \otimes \vartheta A^* \vartheta \Phi_\vartheta$, respectively.

Remark 3.12 (i) Both $\mathcal{L}(A)$ and $\mathcal{R}(A)$ are closed operators on $\mathscr{L}^2(\mathfrak{H})$.

(ii) If A is self-adjoint, then $\mathcal{L}(A)$ and $\mathcal{R}(A)$ are self-adjoint.

(iii) We will also use the conventional identification (3.11). $\diamondsuit$

Recall that a linear operator A on $\mathfrak{H}$ is said to be *positive* if $\langle \xi | A\xi \rangle_{\mathfrak{H}} \geq 0$ for all $\xi \in \mathfrak{H}$. We write this as $A \geq 0$.

Definition 3.13 A canonical cone in $\mathscr{L}^2(\mathfrak{H})$ is given by

$$\mathscr{L}^2(\mathfrak{H})_+ = \Big\{ \xi \in \mathscr{L}^2(\mathfrak{H}) \,\Big|\, \xi \text{ is self-adjoint and } \xi \geq 0 \text{ as an operator on } \mathfrak{H} \Big\}. \quad \diamondsuit \tag{3.12}$$

Theorem 3.14 *$\mathscr{L}^2(\mathfrak{H})_+$ is a self-dual cone in $\mathscr{L}^2(\mathfrak{H})$.*

Proof. We now check the conditions (i)–(iii) in Definition 3.2.

(i) Let $\xi, \eta \in \mathscr{L}^2(\mathfrak{H})_+$. Since $\xi^{1/2}\eta\xi^{1/2} \geq 0$, we have $\langle \xi | \eta \rangle_{\mathscr{L}^2} = \mathrm{Tr}[\xi\eta] = \mathrm{Tr}[\xi^{1/2}\eta\xi^{1/2}] \geq 0$.

(ii) Note that $\mathscr{L}^2(\mathfrak{H})_\mathbb{R} = \{\xi \in \mathscr{L}^2(\mathfrak{H}) \,|\, \xi \text{ is self-adjoint }\}$. Let $\xi \in \mathscr{L}^2(\mathfrak{H})_\mathbb{R}$. By the spectral theorem, there is a projection valued measure $\{E(\cdot)\}$ such that $\xi = \int_\mathbb{R} \lambda dE(\lambda)$. Denote $\xi_+ = \int_0^\infty \lambda dE(\lambda)$ and $\xi_- = \int_{-\infty}^0 (-\lambda) dE(\lambda)$. Clearly, it holds that $\xi_+\xi_- = 0, \xi_\pm \in \mathscr{L}^2(\mathfrak{H})_+$ and $\xi = \xi_+ - \xi_-$. Thus, (ii) is satisfied.

(iii) For each $\xi \in \mathscr{L}^2(\mathfrak{H})$, we have $\xi = \xi_R + i\xi_I$, where $\xi_R = (\xi + \xi^*)/2$ and $\xi_I = (\xi - \xi^*)/2i$. Trivially, $\xi_R, \xi_I \in \mathscr{L}^2(\mathfrak{H})_\mathbb{R}$. Hence, $\mathscr{L}^2(\mathfrak{H})_+$ is a Hilbert cone. By Theorem 3.4, we conclude that $\mathscr{L}^2(\mathfrak{H})_+$ is a self-dual cone. $\square$

Proposition 3.15 *Let $A \in \mathscr{B}(\mathfrak{H})$. We have $\mathcal{L}(A^*)\mathcal{R}(A) \trianglerighteq 0$ w.r.t. $\mathscr{L}^2(\mathfrak{H})_+$.*

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

Remark 3.16 As we noted in references [29, 31], Proposition 3.15 is closely related to spin reflection positivity [22]; see also references [6, 11]. $\diamondsuit$

4 Proof of Proposition 2.4 and Theorem 2.7

4.1 Proof of Proposition 2.4

Let $\mathcal{F}$ be the Fourier transformation on $L^2(\mathbb{R}^d; dx)$:

$$(\mathcal{F}f)(p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{-ip\cdot x} f(x) dx, \quad f \in L^2(\mathbb{R}^d; dx). \tag{4.1}$$

It is known that $\mathcal{F}$ is a unitary operator from $L^2(\mathbb{R}^d; dx)$ onto $L^2(\mathbb{R}^d; dp)$.

Let $H_n = -\Delta_x - V_n$ and let $\hat{H}_n = \mathcal{F} H_n \mathcal{F}^{-1}$. We have

$$\hat{H}_n = p^2 - V_n(-i\nabla_p), \tag{4.2}$$

where p^2 stands for the multiplication operator. Of course, $\hat{H}_n$ acts on $L^2(\mathbb{R}^d; dp)$.

Remark 4.1 By the condition **(B)**, $\hat{V}_n \in L^1(\mathbb{R}^d; dp)$, which implies that $V_n \in L^\infty(\mathbb{R}^d; dx)$. Thus, the linear operator $V_n(-i\nabla_p)$ can be defined by (2.6). $\diamondsuit$

Lemma 4.2 *For all $n \in \mathbb{N}$, we have the following:*

- (i) $V_n(-i\nabla_p) \trianglerighteq 0$ *w.r.t.* $L^2(\mathbb{R}^d; dp)_+$*, where* $L^2(\mathbb{R}^d; dp)_+$ *is defined in Example 9.*
- (ii) $\exp(-\beta \hat{H}_n) \trianglerighteq 0$ *w.r.t.* $L^2(\mathbb{R}^d; dp)_+$ *for all* $\beta \geq 0$*.*

Proof. Let $\nabla_p = (D_{p_1}, \ldots, D_{p_d})$, where D_{p_j} is the (generalized) differential operator on $L^2(\mathbb{R}^d; dp)$.

(i) Since $e^{ik\cdot(-i\nabla_p)}$ is a translation, we see that $e^{ik\cdot(-i\nabla_p)} \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$ for all $k \in \mathbb{R}^d$. Thus, by (ii) of **(B)** and the fact $\mathcal{F} e^{ik\cdot x} \mathcal{F}^{-1} = e^{ik\cdot(-i\nabla_p)}$, we have

$$V_n(-i\nabla_p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{e^{ik\cdot(-i\nabla_p)}}_{\trianglerighteq 0} \underbrace{\hat{V}_n(k)}_{\geq 0} dk \trianglerighteq 0 \quad \text{w.r.t. } L^2(\mathbb{R}^d; dp)_+. \tag{4.3}$$

(ii) We know that the multiplication operator $e^{-\beta p^2}$ satisfies $e^{-\beta p^2} \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$. Thus, applying Theorem A.3, we conclude (ii). $\square$

Before we proceed, we take note of the following fact.

Lemma 4.3 *Let $\mathbb{B}^d$ be the Borel algebra on $\mathbb{R}^d$. Let $B_1, B_2 \in \mathbb{B}^d$ with $|B_1| > 0$ and $|B_2| > 0$, where $|\cdot|$ is the Lebesgue measure. For any $\varepsilon > 0$, we set*

$$\mathcal{S}_\varepsilon^{(\ell)} = \Big\{ (p, p_1, \ldots, p_\ell) \in \mathbb{R}^{d\times(\ell+1)} \,\Big|\, p \in B_2,\, p + p_1 + \cdots + p_\ell \in B_1,\, p_1, \ldots, p_\ell \in B_\varepsilon(0) \Big\}. \tag{4.4}$$

Then, for each $\varepsilon > 0$, there exists an $\ell \in \mathbb{N}_0 := \{0\} \cup \mathbb{N}$ such that $\big|\mathcal{S}_\varepsilon^{(\ell)}\big| > 0$.

Proof. Without loss of generality, we may assume that B_1 and B_2 are connected sets. For each $p_1, \dots, p_\ell \in \mathbb{R}^d$ and $\varepsilon > 0$, we set

$$\mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell) = \Big\{ p \in \mathbb{R}^d \,\Big|\, p \in B_2,\, p + p_1 + \cdots + p_\ell \in B_1 \Big\}. \tag{4.5}$$

Note that $\mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell)$ could be empty. For each $\varepsilon > 0$, there exist an $\ell \in \mathbb{N}_0$ and $p_1, \dots, p_\ell \in B_\varepsilon(0)$ such that $\Big| B_2 \cap (B_1 - p_1 - \cdots - p_\ell) \Big| > 0$, where $B_1 - p_1 - \cdots - p_\ell = \{ p - p_1 - \cdots - p_\ell \,|\, p \in B_1 \}$. Thus, for these $\ell \in \mathbb{N}_0$ and $p_1, \dots, p_\ell \in B_\varepsilon(0)$, $\big| \mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell) \big| > 0$. Because $\big| \mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell) \big|$ is continuous in $p_1, \dots, p_\ell$, we have

$$\big| \mathcal{S}_\varepsilon^{(\ell)} \big| = \int_{(B_\varepsilon(0))^{\times \ell}} dp_1 \cdots dp_\ell \big| \mathcal{S}_\varepsilon^{(\ell)}(p_1, \dots, p_\ell) \big| > 0. \tag{4.6}$$

This completes the proof. □

Proposition 4.4 *For each $n \in \mathbb{N}$, $V_n(-i\nabla_p)$ is ergodic w.r.t. $L^2(\mathbb{R}^d; dp)_+$ (see Definition 3.10).*

Proof. Recall that, by (ii) of the assumption **(B)**, there exists an $\varepsilon > 0$ such that $\mathrm{supp} \hat{V}_n \supset B_\varepsilon(0)$.

Let $f_1, f_2 \in L^2(\mathbb{R}^d; dp)_+ \backslash \{0\}$. Because f_1 and f_2 are non-zero, there exist $B_1, B_2 \in \mathbb{B}^d$ such that $|B_1| > 0$, $|B_2| > 0$, and $f_1(p) > 0$ on B_1, $f_2(p) > 0$ on B_2. By Lemma 4.3, there exists an $\ell \in \mathbb{N}_0$ such that $\big| \mathcal{S}_\varepsilon^{(\ell)} \big| > 0$. In addition, we have

$$f_2(p) \Big(e^{i(p_1 + \cdots + p_\ell) \cdot (-i\nabla_p)} f_1 \Big)(p) = f_2(p) f_1(p + p_1 + \cdots + p_\ell) > 0 \tag{4.7}$$

for all $p, p_1, \dots, p_\ell \in \mathbb{R}^d$ such that $(p, p_1, \dots, p_\ell) \in \mathcal{S}_\varepsilon^{(\ell)}$. Therefore, we obtain

$$\begin{aligned}
&\langle f_2 | V_n^\ell(-i\nabla_p) f_1 \rangle \\
=&(2\pi)^{-nd/2} \int_{\mathbb{R}^d} dp \int_{(\mathbb{R}^d)^{\times \ell}} dp_1 \cdots dp_\ell \underbrace{\hat{V}_n(p_1) \cdots \hat{V}_n(p_\ell)}_{\geq 0} \underbrace{f_2(p) f_1(p + p_1 + \cdots + p_\ell)}_{\geq 0} \\
\geq&(2\pi)^{-nd/2} \int_{\mathcal{S}_\varepsilon^{(\ell)}} dp dp_1 \cdots dp_\ell \underbrace{\hat{V}_n(p_1) \cdots \hat{V}_n(p_\ell)}_{>0} \underbrace{f_2(p) f_1(p + p_1 + \cdots + p_\ell)}_{>0} \\
>&0.
\end{aligned} \tag{4.8}$$

This completes the proof. □

Proposition 4.5 *We have* $\exp(-\beta \hat{H}) \rhd 0$ *w.r.t.* $L^2(\mathbb{R}^d; dp)_+$ *for all* $\beta > 0$.

Proof. By Lemma 4.2 (ii), Theorem A.6 and Proposition 4.4, we have $\exp(-\beta \hat{H}_n) \rhd 0$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$ for all $\beta > 0$ and $n \in \mathbb{N}$.

For each $m, n \in \mathbb{N}$ with $n \geq m$, we have, by the assumption (iii) of **(B)**,

$$V_n(-i\nabla_p) - V_m(-i\nabla_p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{(\hat{V}_n(k) - \hat{V}_m(k))}_{\geq 0} \underbrace{e^{ik \cdot (-i\nabla_p)}}_{\trianglerighteq 0} dk \trianglerighteq 0 \tag{4.9}$$

w.r.t. $L^2(\mathbb{R}^d; dp)_+$. By Theorem A.4, we obtain that $\exp(-\beta\hat{H}_n) \trianglerighteq \exp(-\beta\hat{H}_m)$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$ for all $\beta \geq 0$. Taking $n \to \infty$, we conclude that $\exp(-\beta\hat{H}) \trianglerighteq \exp(-\beta\hat{H}_m)$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$ for all $\beta \geq 0$, where $\hat{H} = \mathcal{F}H\mathcal{F}^{-1}$. Since $\exp(-\beta\hat{H}_m) \triangleright 0$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$ for all $\beta > 0$, we finally arrive at

$$\exp(-\beta\hat{H}) \trianglerighteq \exp(-\beta\hat{H}_m) \triangleright 0 \quad \text{w.r.t. } L^2(\mathbb{R}^d; dp)_+ \text{ for all } \beta > 0. \tag{4.10}$$

Thus we are done. □

Proof of Proposition 2.4

It is well-known that $\exp(-\beta H) \triangleright 0$ and $\exp(-\beta H_n) \triangleright 0$ w.r.t. $L^2(\mathbb{R}^d; dx)_+$ for all $\beta > 0$, see, e.g., [37, Theorem XIII. 45]. Thus, we conclude the uniqueness of ground states by [37, Theorem XIII. 4.4]. Simultaneously, we obtain (i).

By [37, Theorem XIII. 45] and Proposition 4.5 , we conclude (ii). □

4.2 Proof of Theorem 2.7

Lemma 4.6 *Let $f \in \mathfrak{A}$.*

- (i) *$\mathcal{F}f\mathcal{F}^{-1} \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$.*
- (ii) *$f(-i\nabla_x) \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dx)_+$.*

Proof. (i) Because $\mathcal{F}f\mathcal{F}^{-1} = f(-i\nabla_p)$ and $\mathcal{F}e^{ik\cdot x}\mathcal{F}^{-1} = e^{ik\cdot(-i\nabla_p)} \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$, we have

$$\mathcal{F}f\mathcal{F}^{-1} = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{\hat{f}(k)}_{\geq 0} \underbrace{e^{ik\cdot(-i\nabla_p)}}_{\trianglerighteq 0} dk \trianglerighteq 0 \quad \text{w.r.t. } L^2(\mathbb{R}^d; dp)_+. \tag{4.11}$$

(ii) Because $e^{ik\cdot(-i\nabla_x)} \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dx)_+$, we have

$$f(-i\nabla_x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \underbrace{\hat{f}(k)}_{\geq 0} \underbrace{e^{ik\cdot(-i\nabla_x)}}_{\trianglerighteq 0} dk \trianglerighteq 0 \quad \text{w.r.t. } L^2(\mathbb{R}^d; dx)_+. \tag{4.12}$$

This completes the proof. □

Proof of Theorem 2.7

(i) By Proposition 2.4 (ii) and Lemma 4.6 (i),

$$\langle f \rangle = \langle \underbrace{\hat{\psi}}_{>0} | \underbrace{\mathcal{F}f\mathcal{F}^{-1}}_{\trianglerighteq 0} \underbrace{\hat{\psi}}_{>0} \rangle \geq 0. \tag{4.13}$$

By Theorem A.7, the equality holds if and only if $f = 0$.

(ii) By Proposition 2.4 (i) and Lemma 4.6 (ii),

$$\langle f(-i\nabla_x) \rangle = \langle \underbrace{\psi}_{>0} | \underbrace{f(-i\nabla_x)}_{\trianglerighteq 0} \underbrace{\psi}_{>0} \rangle \geq 0. \tag{4.14}$$

By Theorem A.7, the equality holds if and only if $f = 0$. □

4.3 Proof of Remark 2.10

(i) Let J be a natural involution defined by $J\psi = \overline{\psi}$ for each $\psi \in L^2(\mathbb{R}^d; dx)$. Thus, we have

$$\langle J\chi | J\varphi\rangle = \overline{\langle \chi | \varphi\rangle}, \quad \chi, \varphi \in L^2(\mathbb{R}^d; dx). \tag{4.15}$$

Because g is in $\mathfrak{A}_{\mathrm{e}}$, we have $\overline{g(x)} = g(-x) = g(x)$, that is, g is real-valued, which implies that $JgJ = g$. Because $Je^{ik\cdot(-i\nabla_x)}J = e^{ik\cdot(-i\nabla_x)}$, we have $Jf(-i\nabla_x)J = f(-i\nabla_x)$. Therefore, since $J\psi = \psi$ by Proposition 2.4 (i), we have

$$\overline{\langle \psi | f(-i\nabla_x) g\psi\rangle} = \langle J\psi | Jf(-i\nabla_x)g\psi\rangle = \langle J\psi | Jf(-i\nabla_x)JJgJJ\psi\rangle = \langle \psi | f(-i\nabla_x)g\psi\rangle. \tag{4.16}$$

Thus, we conclude (i).

(ii) First, assume that $g(x) \ge 0$. Then $g \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dx)_+$. Thus, $f(-i\nabla_x)g \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dx)_+$ by Lemma 4.6 (ii), which implies that

$$\langle \underbrace{\psi}_{>0} | \underbrace{f(-i\nabla_x)g}_{\trianglerighteq 0} \underbrace{\psi}_{>0} \rangle \ge 0. \tag{4.17}$$

Next, assume that $f(x) \ge 0$. Remark that $f(p) \trianglerighteq 0$ and $g(-i\nabla_p) = \mathcal{F} g \mathcal{F}^{-1} \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dp)_+$ by Lemma 4.6 (i). Hence, by Proposition 2.4 (ii),

$$\langle \psi | f(-i\nabla_x) g\psi\rangle = \langle \underbrace{\hat{\psi}}_{>0} | \underbrace{f(p)g(-i\nabla_p)}_{\trianglerighteq 0} \underbrace{\hat{\psi}}_{>0} \rangle \ge 0. \tag{4.18}$$

Thus we are done. □

5 Proof of Theorem 2.8

5.1 Extended Hamiltonian

Consider the extended Hamiltonian

$$\mathbb{H}_n = H_n \otimes \mathbb{1} + \mathbb{1} \otimes H_n \tag{5.1}$$

acting on the doubled Hilbert space $\mathfrak{H}_{\mathrm{ext}} := \mathfrak{H} \otimes \mathfrak{H} \cong L^2(\mathbb{R}^d \times \mathbb{R}^d; dx_1 dx_2)$.

Let us introduce a new coordinate system (X_1, X_2) by

$$X_1 = \frac{x_2 - x_1}{\sqrt{2}}, \quad X_2 = \frac{x_2 + x_1}{\sqrt{2}}. \tag{5.2}$$

Trivially,

$$\nabla_{x_1} = -\frac{1}{\sqrt{2}}\nabla_{X_1} + \frac{1}{\sqrt{2}}\nabla_{X_2}, \quad \nabla_{x_2} = \frac{1}{\sqrt{2}}\nabla_{X_1} + \frac{1}{\sqrt{2}}\nabla_{X_2}, \tag{5.3}$$

implying

$$-\Delta_{x_1} - \Delta_{x_2} = -\Delta_{X_1} - \Delta_{X_2}. \tag{5.4}$$

We define an antiunitary operator ϑ on $L^2(\mathbb{R}^d; dX)$ by

$$(\vartheta\phi)(X) = \overline{\phi(X)} \quad \text{a.e. } X \tag{5.5}$$

for each $\phi \in L^2(\mathbb{R}^d; dX)$. Using ϑ, we obtain the following identifications:

$$\begin{aligned}
\mathfrak{H}_{\mathrm{ext}} &= L^2(\mathbb{R}^d; dx) \otimes L^2(\mathbb{R}^d; dx) \\
&\cong L^2(\mathbb{R}^d \times \mathbb{R}^d; dx_1 dx_2) \\
&= L^2(\mathbb{R}^d \times \mathbb{R}^d; dX_1 dX_2) \\
&\cong L^2(\mathbb{R}^d; dX) \otimes L^2(\mathbb{R}^d; dX) \\
&= \mathscr{L}^2(L^2(\mathbb{R}^d; dX)).
\end{aligned} \tag{5.6}$$

In the last equality, we use the identification (3.11) with ϑ given by (5.5). Taking the identifications (5.6) into account, we introduce a self-dual cone $\mathfrak{P}_{\mathrm{ext}}$ in $\mathfrak{H}_{\mathrm{ext}}$ by

$$\mathfrak{P}_{\mathrm{ext}} = \mathscr{L}^2(L^2(\mathbb{R}^d; dX))_+. \tag{5.7}$$

Lemma 5.1 *Under the identifications (5.6), we have the following:*

(i) $V_n \otimes \mathbb{1} + \mathbb{1} \otimes V_n \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}_{\mathrm{ext}}$.

(ii) $f \otimes \mathbb{1} \pm \mathbb{1} \otimes f \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}_{\mathrm{ext}}$ *for each* $f \in \mathfrak{A}_{\mathrm{e}}$.

Proof. We apply Ginibre's idea [10].

(i) By the elementary fact

$$\cos a + \cos b = 2 \cos \frac{a+b}{2} \cos \frac{a-b}{2}, \tag{5.8}$$

we have

$$\begin{aligned}
V_n \otimes \mathbb{1} + \mathbb{1} \otimes V_n &= V_n(x_1) + V_n(x_2) \\
&= V_n\Big(\frac{X_2 - X_1}{\sqrt{2}}\Big) + V_n\Big(\frac{X_1 + X_2}{\sqrt{2}}\Big) \\
&= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \hat{V}_n(p) \Big\{ \cos\Big(p \cdot \frac{X_2 - X_1}{\sqrt{2}}\Big) + \cos\Big(p \cdot \frac{X_2 + X_1}{\sqrt{2}}\Big) \Big\} dp \\
&= (2\pi)^{-d/2} \int_{\mathbb{R}^d} 2\, \underbrace{\hat{V}_n(p)}_{\geq 0} \underbrace{\mathcal{L}\Big[\cos\Big(p \cdot \frac{X}{\sqrt{2}}\Big)\Big] \mathcal{R}\Big[\cos\Big(p \cdot \frac{X}{\sqrt{2}}\Big)\Big]}_{\trianglerighteq 0 \text{ by Proposition 3.15}} dp \\
&\trianglerighteq 0 \quad \text{w.r.t.} \quad \mathfrak{P}_{\mathrm{ext}}.
\end{aligned} \tag{5.9}$$

(ii) By (5.8) and

$$\cos a - \cos b = 2 \sin \frac{b+a}{2} \sin \frac{b-a}{2}, \tag{5.10}$$

we have

$$f \otimes 1\!\!1 + 1\!\!1 \otimes f = (2\pi)^{-d/2} \int_{\mathbb{R}^d} 2\underbrace{\hat{f}(p)}_{\geq 0} \underbrace{\mathcal{L}\Big[\cos\Big(p \cdot \frac{X}{\sqrt{2}}\Big)\Big]\mathcal{R}\Big[\cos\Big(p \cdot \frac{X}{\sqrt{2}}\Big)\Big]}_{\unrhd 0 \text{ by Proposition 3.15}} dp \unrhd 0, \tag{5.11}$$

$$f \otimes 1\!\!1 - 1\!\!1 \otimes f = (2\pi)^{-d/2} \int_{\mathbb{R}^d} 2\underbrace{\hat{f}(p)}_{\geq 0} \underbrace{\mathcal{L}\Big[\sin\Big(p \cdot \frac{X}{\sqrt{2}}\Big)\Big]\mathcal{R}\Big[\sin\Big(p \cdot \frac{X}{\sqrt{2}}\Big)\Big]}_{\unrhd 0 \text{ by Proposition 3.15}} dp \unrhd 0 \tag{5.12}$$

w.r.t. $\mathfrak{P}_{\rm ext}$. □

Theorem 5.2 *Assume that V is regular. We have $e^{-\beta \mathbb{H}_n} \unrhd 0$ w.r.t. $\mathfrak{P}_{\rm ext}$ for all $\beta \geq 0$.*

Proof. We set $\mathbb{H}_n = \mathbb{H}_0 - \mathbb{V}_n$, where $\mathbb{H}_0 = (-\Delta_x) \otimes 1\!\!1 + 1\!\!1 \otimes (-\Delta_x)$ and $\mathbb{V}_n = V_n \otimes 1\!\!1 + 1\!\!1 \otimes V_n$. Note that, by Lemma 5.1, we know that $\mathbb{V}_n \unrhd 0$ w.r.t. $\mathfrak{P}_{\rm ext}$. By (5.4) and the identifications (5.6), we have

$$\mathbb{H}_0 = -\Delta_{X_1} - \Delta_{X_2} = \mathcal{L}\Big(-\Delta_X\Big) + \mathcal{R}\Big(-\Delta_X\Big). \tag{5.13}$$

Thus, by Proposition 3.15,

$$e^{-\beta \mathbb{H}_0} = \mathcal{L}\big[e^{\beta \Delta_X}\big]\mathcal{R}\big[e^{\beta \Delta_X}\big] \unrhd 0 \tag{5.14}$$

w.r.t. $\mathfrak{P}_{\rm ext}$. (Remark that, because $e^{\beta \Delta_x}$ is bounded, the RHS of (5.14) is bounded as well.) Now, we can apply Theorem A.3 and conclude the theorem. □

Lemma 5.3 *Let $f \in \mathfrak{A}_{\rm e}$. Under the identifications (5.6), we have the following:*

(i) $f(-i\nabla_x) \otimes 1\!\!1 + 1\!\!1 \otimes f(-i\nabla_x) \unrhd 0$ *w.r.t.* $\mathfrak{P}_{\rm ext}$.

(ii) $f(-i\nabla_x) \otimes 1\!\!1 - 1\!\!1 \otimes f(-i\nabla_x) \unlhd 0$ *w.r.t.* $\mathfrak{P}_{\rm ext}$.

Proof. Note that

$$\vartheta(-i\nabla_X)\vartheta^{-1} = +i\nabla_X. \tag{5.15}$$

(i) Since $f(-x) = f(x)$, we have

$$f(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \hat{f}(p) \cos(p \cdot x) dp. \tag{5.16}$$

By (5.3), (5.8) and (5.16),

$$
\begin{aligned}
&f(-i\nabla_x)\otimes \mathbb{1} + \mathbb{1}\otimes f(-i\nabla_x)\\
&= f(-i\nabla_{x_1}) + f(-i\nabla_{x_2})\\
&\underset{(5.3)}{=} f\Big(\frac{i}{\sqrt{2}}\nabla_{X_1} - \frac{i}{\sqrt{2}}\nabla_{X_2}\Big) + f\Big(-\frac{i}{\sqrt{2}}\nabla_{X_1} - \frac{i}{\sqrt{2}}\nabla_{X_2}\Big)\\
&\underset{(5.16)}{=} (2\pi)^{-d/2}\int_{\mathbb{R}^d}\hat{f}(p)\Big\{\cos\Big[p\cdot\Big(\frac{i}{\sqrt{2}}\nabla_{X_1} - \frac{i}{\sqrt{2}}\nabla_{X_2}\Big)\Big] +\\
&\qquad\qquad + \cos\Big[p\cdot\Big(-\frac{i}{\sqrt{2}}\nabla_{X_1} - \frac{i}{\sqrt{2}}\nabla_{X_2}\Big)\Big]\Big\}dp\\
&\underset{(5.8)}{=} 2(2\pi)^{-d/2}\int_{\mathbb{R}^d}\hat{f}(p)\cos\Big(\frac{-ip\cdot\nabla_{X_1}}{\sqrt{2}}\Big)\cos\Big(\frac{-ip\cdot\nabla_{X_2}}{\sqrt{2}}\Big)dp\\
&= 2(2\pi)^{-d/2}\int_{\mathbb{R}^d}\underbrace{\hat{f}(p)}_{\ge 0}\underbrace{\mathcal{L}\Big[\cos\Big(\frac{-ip\cdot\nabla_X}{\sqrt{2}}\Big)\Big]\mathcal{R}\Big[\cos\Big(\frac{-ip\cdot\nabla_X}{\sqrt{2}}\Big)\Big]}_{\trianglerighteq 0 \text{ by Proposition 3.15}}dp\\
&\trianglerighteq 0 \quad \text{w.r.t. } \mathfrak{P}_{\mathrm{ext}}.
\end{aligned}
\tag{5.17}
$$

This proves (i). Similarly, by (5.3), (5.10) and (5.16),

$$
\begin{aligned}
&f(-i\nabla_x)\otimes \mathbb{1} - \mathbb{1}\otimes f(-i\nabla_x)\\
&\underset{(5.3)}{=} f\Big(\frac{i}{\sqrt{2}}\nabla_{X_1} - \frac{i}{\sqrt{2}}\nabla_{X_2}\Big) - f\Big(-\frac{i}{\sqrt{2}}\nabla_{X_1} - \frac{i}{\sqrt{2}}\nabla_{X_2}\Big)\\
&\underset{(5.16)}{=} (2\pi)^{-d/2}\int_{\mathbb{R}^d}\hat{f}(p)\Big\{\cos\Big[p\cdot\Big(\frac{i}{\sqrt{2}}\nabla_{X_1} - \frac{i}{\sqrt{2}}\nabla_{X_2}\Big)\Big] -\\
&\qquad\qquad - \cos\Big[p\cdot\Big(-\frac{i}{\sqrt{2}}\nabla_{X_1} - \frac{i}{\sqrt{2}}\nabla_{X_2}\Big)\Big]\Big\}dp\\
&\underset{(5.10)}{=} 2(2\pi)^{-d/2}\int_{\mathbb{R}^d}\hat{f}(p)\sin\Big(\frac{-ip\cdot\nabla_{X_1}}{\sqrt{2}}\Big)\sin\Big(\frac{-ip\cdot\nabla_{X_2}}{\sqrt{2}}\Big)dp\\
&= 2(2\pi)^{-d/2}\int_{\mathbb{R}^d}\hat{f}(p)\mathcal{L}\Big[\sin\Big(\frac{-ip\cdot\nabla_X}{\sqrt{2}}\Big)\Big]\mathcal{R}\Big[\underbrace{\vartheta\sin\Big(\frac{-ip\cdot\nabla_X}{\sqrt{2}}\Big)\vartheta^{-1}}_{=-\sin\left(\frac{-ip\cdot\nabla_X}{\sqrt{2}}\right) \text{ by (5.15)}}\Big]dp\\
&\trianglelefteq 0 \quad \text{w.r.t. } \mathfrak{P}_{\mathrm{ext}}.
\end{aligned}
\tag{5.18}
$$

This proves (ii). □

5.2 Duhamel expansion

Let $\Omega(x) = \pi^{-d/4}\exp(-|x|^2/2) \in L^2(\mathbb{R}^d; dx)$ and let $Z_{\beta,n} = \|e^{-\beta H_n}\Omega\|^2$. We introduce a vector $\phi_{\beta,n} \in L^2(\mathbb{R}^d; dx)$ by

$$
\phi_{\beta,n} = \frac{e^{-\beta H_n}\Omega}{\sqrt{Z_{\beta,n}}}. \tag{5.19}
$$

Lemma 5.4 $\langle A\rangle_n = \lim_{\beta\to\infty} \langle \phi_{\beta,n}|A\phi_{\beta,n}\rangle$.

Proof. By Proposition 2.4, we have $\langle\Omega|\psi_n\rangle > 0$. Hence, we obtain

$$\psi_n = \text{strong} \lim_{\beta\to\infty} \phi_{\beta,n}. \tag{5.20}$$

Thus we are done. □

Lemma 5.5 *Under the identifications (5.6), we have $\Omega\otimes\Omega \ge 0$ w.r.t. $\mathfrak{P}_{\rm ext}$.*

Proof. By (5.2) and (5.6),

$$\Omega\otimes\Omega = \pi^{-d/2}\exp\big\{-(X_1^2+X_2^2)/2\big\} = \tilde{\Omega}\otimes\tilde{\Omega} = |\tilde{\Omega}\rangle\langle\tilde{\Omega}|, \tag{5.21}$$

where $\tilde{\Omega}(X) = \pi^{-d/4}\exp(-|X|^2/2) \in L^2(\mathbb{R}^d; dX)$. The RHS of (5.21) ≥ 0 w.r.t. $\mathfrak{P}_{\rm ext}$, because the projection $|\tilde{\Omega}\rangle\langle\tilde{\Omega}|$ is positive as a linear operator on $L^2(\mathbb{R}^d; dX)$. □

Theorem 5.6 *Let $A \in \mathscr{B}(L^2(\mathbb{R}^d; dx))$.*

(i) *If $A\otimes 1\!\!1 - 1\!\!1\otimes A \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$, then $\langle A\rangle_n$ is monotonically increasing in n.*

(ii) *If $A\otimes 1\!\!1 - 1\!\!1\otimes A \trianglelefteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$, then $\langle A\rangle_n$ is monotonically decreasing in n.*

Proof. Suppose that $n \ge m$. Note that

$$\langle A\rangle_n - \langle A\rangle_m = \lim_{\beta\to\infty} \frac{Z_{\beta,m}}{Z_{\beta,n}} \mathscr{I}_\beta, \tag{5.22}$$

where

$$\mathscr{I}_\beta = \frac{\big\langle e^{-\beta H_n}\Omega\big|Ae^{-\beta H_n}\Omega\big\rangle}{Z_{\beta,m}} - \frac{\big\langle e^{-\beta H_m}\Omega\big|Ae^{-\beta H_m}\Omega\big\rangle}{Z_{\beta,m}}\frac{Z_{\beta,n}}{Z_{\beta,m}}. \tag{5.23}$$

Let $\delta = V_n - V_m$. By the Duhamel formula,

$$e^{-\beta H_n} = e^{-\beta(H_m-\delta)} = \sum_{j\ge 0}\int_{\mathcal{T}_j(\beta)} \delta(s_1)\cdots\delta(s_n)e^{-\beta H_m} ds_1\cdots ds_n, \tag{5.24}$$

where $\delta(s) = e^{-sH_m}\delta e^{sH_m}$ and $\mathcal{T}_j(\beta) = \{(s_1,\dots,s_j)\,|\,0\le s_1\le\cdots\le s_j\le\beta\}$. The RHS of (5.24) converges in the operator norm topology.

For each $A \in \mathscr{B}(L^2(\mathbb{R}^d; dx))$, we set

$$\omega(A) = \langle \phi_{\beta,m}|A\phi_{\beta,m}\rangle. \tag{5.25}$$

The following formula is useful:

Lemma 5.7 *We have*

$$\mathscr{I}_\beta = \sum_{i,j\ge 0}\int_{\mathcal{T}_i(\beta)}\int_{\mathcal{T}_j(\beta)} \Big\{\omega\big(X_i(\boldsymbol{s})AY_j(\boldsymbol{t})\big) - \omega(A)\omega\big(X_i(\boldsymbol{s})Y_j(\boldsymbol{t})\big)\Big\} ds_1\cdots ds_i dt_1\cdots dt_j, \tag{5.26}$$

where $X_i(\boldsymbol{s}) = \delta(s_i)\delta(s_{i-1})\cdots\delta(s_1)$ and $Y_j(\boldsymbol{t}) = \delta(t_1)\cdots\delta(t_{j-1})\delta(t_j)$.

Proof. By (5.19) and (5.24), we have

$$
\begin{aligned}
&\frac{\left\langle e^{-\beta H_n}\Omega \middle| A e^{-\beta H_n}\Omega\right\rangle}{Z_{\beta,m}}\\
&=\sum_{i,j\ge 0}\int_{\mathcal{T}_i(\beta)}\int_{\mathcal{T}_j(\beta)} Z_{\beta,m}^{-1}\left\langle e^{-\beta H_m}\Omega \middle| X_i(\boldsymbol{s})AY_j(\boldsymbol{t})e^{-\beta H_m}\Omega\right\rangle ds_1\cdots ds_i dt_1\cdots dt_j\\
&=\sum_{i,j\ge 0}\int_{\mathcal{T}_i(\beta)}\int_{\mathcal{T}_j(\beta)} \omega\big(X_i(\boldsymbol{s})AY_j(\boldsymbol{t})\big) ds_1\cdots ds_i dt_1\cdots dt_j. \qquad (5.27)
\end{aligned}
$$

As for the term $Z_{\beta,n}/Z_{\beta,m}$, we have, by (5.27),

$$
\begin{aligned}
\frac{Z_{\beta,n}}{Z_{\beta,m}} &= \frac{\left\langle e^{-\beta H_n}\Omega \middle| \mathbb{1} e^{-\beta H_n}\Omega\right\rangle}{Z_{\beta,m}}\\
&=\sum_{i,j\ge 0}\int_{\mathcal{T}_i(\beta)}\int_{\mathcal{T}_j(\beta)} \omega\big(X_i(\boldsymbol{s})Y_j(\boldsymbol{t})\big) ds_1\cdots ds_i dt_1\cdots dt_j. \qquad (5.28)
\end{aligned}
$$

Inserting these formulas into (5.23), we obtain the desired identity. □

Thus, to prove the theorem, it suffices to prove the following proposition.

Proposition 5.8 *Let* $A \in \mathscr{B}(L^2(\mathbb{R}^d; dx))$.

(i) *If* $A\otimes \mathbb{1} - \mathbb{1}\otimes A \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}_{\rm ext}$, *then we have*

$$
\omega\big(X_i(\boldsymbol{s})AY_j(\boldsymbol{t})\big) - \omega\big(X_i(\boldsymbol{s})Y_j(\boldsymbol{t})\big)\omega(A) \ge 0 \qquad (5.29)
$$

for all $\boldsymbol{s}\in\mathcal{T}_i(\beta)$ *and* $\boldsymbol{t}\in\mathcal{T}_j(\beta)$.

(ii) *If* $A\otimes \mathbb{1} - \mathbb{1}\otimes A \trianglelefteq 0$ *w.r.t.* $\mathfrak{P}_{\rm ext}$, *then we have*

$$
\omega\big(X_i(\boldsymbol{s})AY_j(\boldsymbol{t})\big) - \omega\big(X_i(\boldsymbol{s})Y_j(\boldsymbol{t})\big)\omega(A) \le 0 \qquad (5.30)
$$

for all $\boldsymbol{s}\in\mathcal{T}_i(\beta)$ *and* $\boldsymbol{t}\in\mathcal{T}_j(\beta)$.

Proof. (i) For each $B\in\mathscr{B}(L^2(\mathbb{R}^d; dx))$, we set

$$
B_\pm = B\otimes\mathbb{1} \pm \mathbb{1}\otimes B. \qquad (5.31)
$$

By (5.8),

$$
\delta_+ = 2(2\pi)^{-d/2}\int_{\mathbb{R}^d} \underbrace{(\hat V_n(p)-\hat V_m(p))}_{\ge 0}\underbrace{\mathcal{L}\Big[\cos\Big(\frac{p\cdot X}{\sqrt{2}}\Big)\Big]\mathcal{R}\Big[\cos\Big(\frac{p\cdot X}{\sqrt{2}}\Big)\Big]}_{\trianglerighteq 0} dp \trianglerighteq 0 \quad \text{w.r.t. } \mathfrak{P}_{\rm ext}. \qquad (5.32)
$$

Similarly, $\delta_- \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$. In addition, $A_- \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$ by the assumption.

We define

$$
X_\pm(\boldsymbol{s}) = \left[\overleftarrow{\prod_{\alpha=1}^{i}}\delta(s_\alpha)\right]\otimes\mathbb{1} \pm \mathbb{1}\otimes\left[\overleftarrow{\prod_{\alpha=1}^{i}}\delta(s_\alpha)\right], \qquad (5.33)
$$

where $\overset{\longleftarrow}{\prod_{\alpha=1}^{i}} B_\alpha = B_i B_{i-1} \cdots B_2 B_1$, an ordered product. Let

$$\delta_\pm[s] = e^{-s\mathbb{H}_m} \delta_\pm e^{s\mathbb{H}_m}. \tag{5.34}$$

Since $\delta \otimes \mathbb{1} = \frac{1}{2}(\delta_+ + \delta_-)$ and $\mathbb{1} \otimes \delta = \frac{1}{2}(\delta_+ - \delta_-)$, we obtain

$$X_\pm(\boldsymbol{s}) = 2^{-i} \overset{\longleftarrow}{\prod_{\alpha=1}^{i}} \Big\{ \delta_+[s_\alpha] + \delta_-[s_\alpha] \Big\} \pm 2^{-i} \overset{\longleftarrow}{\prod_{\alpha=1}^{i}} \Big\{ \delta_+[s_\alpha] - \delta_-[s_\alpha] \Big\}. \tag{5.35}$$

For each $\boldsymbol{\varepsilon} = \{\varepsilon_1, \dots, \varepsilon_i\} \in \{+,-\}^i$, we define

$$\boldsymbol{\delta}_{\boldsymbol{\varepsilon}}[\boldsymbol{s}] = \overset{\longleftarrow}{\prod_{\alpha=1}^{i}} \delta_{\varepsilon_\alpha}[s_\alpha]. \tag{5.36}$$

In terms of this notation,

$$\overset{\longleftarrow}{\prod_{\alpha=1}^{i}} \Big\{ \delta_+[s_\alpha] + \delta_-[s_\alpha] \Big\} = \sum_{\boldsymbol{\varepsilon} \in \{+,-\}^i} \boldsymbol{\delta}_{\boldsymbol{\varepsilon}}[\boldsymbol{s}], \tag{5.37}$$

$$\overset{\longleftarrow}{\prod_{\alpha=1}^{i}} \Big\{ \delta_+[s_\alpha] - \delta_-[s_\alpha] \Big\} = \sum_{\boldsymbol{\varepsilon} \in \{+,-\}^i} \sigma(\boldsymbol{\varepsilon}) \boldsymbol{\delta}_{\boldsymbol{\varepsilon}}[\boldsymbol{s}], \tag{5.38}$$

where $\sigma(\boldsymbol{\varepsilon}) = (\varepsilon_1 1)(\varepsilon_2 1) \cdots (\varepsilon_i 1) = +1$ if the number of $\varepsilon_\alpha = -$ is even, $\sigma(\boldsymbol{\varepsilon}) = -1$ if the number of $\varepsilon_\alpha = -$ is odd. Thus, we have

$$X_+(\boldsymbol{s}) = 2^{-(i-1)} \sum_{\sigma(\boldsymbol{\varepsilon})=+1} \boldsymbol{\delta}_{\boldsymbol{\varepsilon}}[\boldsymbol{s}], \quad X_-(\boldsymbol{s}) = 2^{-(i-1)} \sum_{\sigma(\boldsymbol{\varepsilon})=-1} \boldsymbol{\delta}_{\boldsymbol{\varepsilon}}[\boldsymbol{s}]. \tag{5.39}$$

Because, for each $\boldsymbol{s} \in \mathcal{T}_i(\beta)$,

$$e^{-\beta\mathbb{H}_m} \boldsymbol{\delta}_{\boldsymbol{\varepsilon}}[\boldsymbol{s}] = \underbrace{e^{-(\beta - s_i)\mathbb{H}_m}}_{\trianglerighteq 0} \underbrace{\delta_{\varepsilon_i}}_{\trianglerighteq 0} \underbrace{e^{-(s_i - s_{i-1})\mathbb{H}_m}}_{\trianglerighteq 0} \cdots \underbrace{e^{-(s_2 - s_1)\mathbb{H}_m}}_{\trianglerighteq 0} \underbrace{\delta_{\varepsilon_1}}_{\trianglerighteq 0} \underbrace{e^{-s_1\mathbb{H}_m}}_{\trianglerighteq 0} \trianglerighteq 0 \tag{5.40}$$

w.r.t. $\mathfrak{P}_{\text{ext}}$, we conclude that $e^{-\beta\mathbb{H}_m} X_\pm(\boldsymbol{s}) \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\text{ext}}$ by (5.39). Similarly, we can prove that $Y_\pm(\boldsymbol{t}) e^{-\beta\mathbb{H}_m} \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\text{ext}}$.

Because

$$\underbrace{e^{-\beta\mathbb{H}_m} X_+(\boldsymbol{s})}_{\trianglerighteq 0} \underbrace{A_-}_{\trianglerighteq 0} \underbrace{Y_-(\boldsymbol{t}) e^{-\beta\mathbb{H}_m}}_{\trianglerighteq 0} \trianglerighteq 0 \tag{5.41}$$

w.r.t. $\mathfrak{P}_{\text{ext}}$, we have, by Lemma 5.5,

$$\begin{aligned} &\Big\langle \phi_{\beta,m} \otimes \phi_{\beta,m} \Big| X_+(\boldsymbol{s}) A_- Y_-(\boldsymbol{t}) \phi_{\beta,m} \otimes \phi_{\beta,m} \Big\rangle \\ &= Z_{\beta,n}^{-2} \Big\langle \underbrace{\Omega \otimes \Omega}_{\geq 0} \Big| \underbrace{e^{-\beta\mathbb{H}_m} X_+(\boldsymbol{s}) A_- Y_-(\boldsymbol{t}) e^{-\beta\mathbb{H}_m}}_{\trianglerighteq 0} \underbrace{\Omega \otimes \Omega}_{\geq 0} \Big\rangle \geq 0, \end{aligned} \tag{5.42}$$

implying that

$$\omega\big(X_i(\boldsymbol{s})AY_j(\boldsymbol{t})\big) - \omega\big(X_i(\boldsymbol{s})Y_j(\boldsymbol{t})\big)\omega(A)$$
$$+\,\omega\big(AY_j(\boldsymbol{t})\big)\omega\big(X_i(\boldsymbol{s})\big) - \omega\big(Y_j(\boldsymbol{t})\big)\omega\big(X_i(\boldsymbol{s})A\big) \geq 0. \tag{5.43}$$

On the other hand, we have $e^{-\beta\mathbb{H}_m}X_-(\boldsymbol{s})A_-Y_+(\boldsymbol{t})e^{-\beta\mathbb{H}_m} \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$, which implies

$$\omega\big(X_i(\boldsymbol{s})AY_j(\boldsymbol{t})\big) - \omega\big(X_i(\boldsymbol{s})Y_j(\boldsymbol{t})\big)\omega(A)$$
$$-\,\omega\big(AY_j(\boldsymbol{t})\big)\omega\big(X_i(\boldsymbol{s})\big) + \omega\big(Y_j(\boldsymbol{t})\big)\omega\big(X_i(\boldsymbol{s})A\big) \geq 0. \tag{5.44}$$

Combining (5.43) and (5.44), we obtain the desired result. We can prove (ii) similarly. □

Proof of Theorem 2.8

By Lemma 5.3 and Theorem 5.6, we conclude Theorem 2.8. □

6 Proof of Theorem 2.9

We begin with the following proposition.

Proposition 6.1 *If $n > m$, then $e^{-\beta\mathbb{H}_n} \trianglerighteq e^{-\beta\mathbb{H}_m} \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$ for all $\beta \geq 0$.*

Proof. By (5.32), we already know that $\delta_+ = \mathbb{V}_n - \mathbb{V}_m \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$. Because $\mathbb{H}_n = \mathbb{H}_m - \delta_+$, we conclude the assertion by using Theorem A.4. □

Let

$$\mathbb{H} = H \otimes \mathbb{1} + \mathbb{1} \otimes H. \tag{6.1}$$

Theorem 6.2 *$e^{-\beta\mathbb{H}} \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$ for all $\beta \geq 0$.*

Proof. By Proposition 6.1, we know that $e^{-\beta\mathbb{H}_n} \trianglerighteq e^{-\beta\mathbb{H}_m} \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$ for all $\beta \geq 0$, provided that $n > m$. Since $e^{-\beta\mathbb{H}_n}$ strongly converges to $e^{-\beta\mathbb{H}}$ by the assumption **(B)**, we obtain $e^{-\beta\mathbb{H}} \trianglerighteq e^{-\beta\mathbb{H}_m} \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$ for all $\beta \geq 0$ by Proposition A.1. □

Corollary 6.3 *Let ψ be the unique ground state of H. Under the identifications (5.6), $\psi \otimes \psi \geq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$.*

Proof. Let $\Psi = \psi \otimes \psi$. Since the ground state of H is unique, Ψ is the unique ground state of $\mathbb{H}$. Thus, by Proposition A.2 and Theorem 6.2, we conclude the assertion. □

Theorem 6.4 *Let $A, B \in \mathscr{B}(L^2(\mathbb{R}^d; dx))$. Under the identifications (5.6), we have the following:*

(i) *If $A \otimes \mathbb{1} - \mathbb{1} \otimes A \trianglerighteq 0$ and $B \otimes \mathbb{1} - \mathbb{1} \otimes B \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$, then $\langle AB\rangle - \langle A\rangle\langle B\rangle \geq 0$.*

(ii) *If $A \otimes \mathbb{1} - \mathbb{1} \otimes A \trianglelefteq 0$ and $B \otimes \mathbb{1} - \mathbb{1} \otimes B \trianglelefteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$, then $\langle AB\rangle - \langle A\rangle\langle B\rangle \geq 0$.*

(iii) *If $A \otimes \mathbb{1} - \mathbb{1} \otimes A \trianglelefteq 0$ and $B \otimes \mathbb{1} - \mathbb{1} \otimes B \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$, then $\langle AB\rangle - \langle A\rangle\langle B\rangle \leq 0$.*

Proof. (i) By Corollary 6.3,

$$2(\langle AB\rangle - \langle A\rangle\langle B\rangle) = \Big\langle \underbrace{\psi\otimes\psi}_{\geq 0} \Big| \underbrace{(A\otimes 1\!\!1 - 1\!\!1\otimes A)}_{\trianglerighteq 0} \underbrace{(B\otimes 1\!\!1 - 1\!\!1\otimes B)}_{\trianglerighteq 0} \underbrace{\psi\otimes\psi}_{\geq 0} \Big\rangle \geq 0. \quad (6.2)$$

Thus, we obtain (i). We can prove (ii) and (iii) similarly. □

Proof of Theorem 2.9

By Lemmas 5.1, 5.3 and Theorem 6.4, we conclude Theorem 2.9. □

7 Proof of Theorem 2.12

Let $V_n^{(1)}$ (resp., $V_n^{(2)}$) be an approximating sequence of $V^{(1)}$ (resp., $V^{(2)}$) in condition **(B)**. Let

$$H_n^{(1)} = -\Delta_x - V_n^{(1)}, \quad H_n^{(2)} = -\Delta_x - V_n^{(2)}. \quad (7.1)$$

Then,

$$H_n^{(1)} = H_n^{(2)} - W_n, \quad W_n = V_n^{(1)} - V_n^{(2)}. \quad (7.2)$$

As previously, we study the extended Hamiltonian

$$\mathbb{H}_n^{(1)} = H_n^{(1)}\otimes 1\!\!1 + 1\!\!1\otimes H_n^{(1)}, \quad \mathbb{H}_n^{(2)} = H_n^{(2)}\otimes 1\!\!1 + 1\!\!1\otimes H_n^{(2)}. \quad (7.3)$$

By (7.2),

$$\mathbb{H}_n^{(1)} = \mathbb{H}_n^{(2)} - \mathbb{W}_n, \quad \mathbb{W}_n = W_n\otimes 1\!\!1 + 1\!\!1\otimes W_n. \quad (7.4)$$

Lemma 7.1 $\mathbb{W}_n \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}_{\rm ext}$.

Proof. In a similar manner as in the proof of Lemma 5.1 (i), we see that

$$\mathbb{W}_n = 2(2\pi)^{-d/2}\int_{\mathbb{R}^d} \underbrace{(\hat{V}_n^{(1)}(k) - \hat{V}_n^{(2)}(k))}_{\geq 0} \underbrace{\mathcal{L}\Big[\cos\Big(\frac{k\cdot X}{\sqrt{2}}\Big)\Big]\mathcal{R}\Big[\cos\Big(\frac{k\cdot X}{\sqrt{2}}\Big)\Big]}_{\trianglerighteq 0} dk \trianglerighteq 0 \quad (7.5)$$

w.r.t. $\mathfrak{P}_{\rm ext}$. □

Theorem 7.2 *Let* $A\in\mathscr{B}(L^2(\mathbb{R}^d;dx))$.

(i) *If* $A\otimes 1\!\!1 - 1\!\!1\otimes A \trianglerighteq 0$ *w.r.t.* $\mathfrak{P}_{\rm ext}$, *then* $\langle A\rangle^{(1)} \geq \langle A\rangle^{(2)}$.

(ii) *If* $A\otimes 1\!\!1 - 1\!\!1\otimes A \trianglelefteq 0$ *w.r.t.* $\mathfrak{P}_{\rm ext}$, *then* $\langle A\rangle^{(1)} \leq \langle A\rangle^{(2)}$.

Proof. The proof of this theorem is similar to that of Theorem 5.6. Hence, we provide only a sketch of the proof. Let $\psi_n^{(1)}$ (resp., $\psi_n^{(2)}$) be the unique ground state of $H_n^{(1)}$ (resp., $H_n^{(2)}$). For each $A\in\mathscr{B}(L^2(\mathbb{R}^d;dx))$, we set

$$\langle A\rangle_n^{(1)} = \langle\psi_n^{(1)}|A\psi_n^{(1)}\rangle, \quad \langle A\rangle_n^{(2)} = \langle\psi_n^{(2)}|A\psi_n^{(2)}\rangle. \quad (7.6)$$

Corresponding to (5.22), we obtain

$$\langle A\rangle_n^{(1)} - \langle A\rangle_n^{(2)} = \lim_{\beta\to\infty} \frac{Z_\beta^{(2)}}{Z_\beta^{(1)}} \mathscr{I}_\beta, \tag{7.7}$$

where $Z_\beta^{(j)} = \left\|e^{-\beta H_n^{(j)}}\Omega\right\|^2$ $(j = 1, 2)$ and

$$\mathscr{I}_\beta = \frac{\left\langle e^{-\beta H_n^{(1)}}\Omega \middle| Ae^{-\beta H_n^{(1)}}\Omega\right\rangle}{Z_\beta^{(2)}} - \frac{\left\langle e^{-\beta H_n^{(2)}}\Omega \middle| Ae^{-\beta H_n^{(2)}}\Omega\right\rangle}{Z_\beta^{(2)}} \frac{Z_\beta^{(1)}}{Z_\beta^{(2)}}. \tag{7.8}$$

Since $\langle A\rangle^{(\alpha)} = \lim_{n\to\infty} \langle A\rangle_n^{(\alpha)}$ for each $\alpha = 1, 2$, it suffices to prove that $\mathscr{I}_\beta \ge 0$ for all $\beta > 0$.

Let $\phi_n^{(2)} = e^{-\beta H_n^{(2)}}\Omega \Big/ \sqrt{Z_\beta^{(2)}}$. We set

$$\tilde{\omega}(A) = \left\langle \phi_n^{(2)} \middle| A\phi_n^{(2)}\right\rangle, \quad A \in \mathscr{B}(L^2(\mathbb{R}^d; dx)). \tag{7.9}$$

By the Duhamel formula, we obtain

$$\mathscr{I}_\beta = \sum_{i,j\ge 0} \int_{\mathcal{T}_i(\beta)} \int_{\mathcal{T}_j(\beta)} \left\{\tilde{\omega}\Big(\mathcal{X}_i(\boldsymbol{s})A\mathcal{Y}_j(\boldsymbol{t})\Big) - \tilde{\omega}(A)\tilde{\omega}\Big(\mathcal{X}_i(\boldsymbol{s})\mathcal{Y}_j(\boldsymbol{t})\Big)\right\} ds_1\cdots ds_i dt_1\cdots dt_j, \tag{7.10}$$

where $\mathcal{X}_i(\boldsymbol{s}) = W_n(s_i)W_n(s_{i-1})\cdots W_n(s_1)$ and $\mathcal{Y}_j(\boldsymbol{t}) = W_n(t_1)\cdots W_n(t_{j-1})W_n(t_j)$. By Proposition 7.3 below, the RHS of (7.10) is positive. □

Proposition 7.3 *Let $A \in \mathscr{B}(L^2(\mathbb{R}^d; dx))$.*

(i) *If $A\otimes \mathbb{1} - \mathbb{1}\otimes A \trianglerighteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$, then we have*

$$\tilde{\omega}\big(\mathcal{X}_i(\boldsymbol{s})A\mathcal{Y}_j(\boldsymbol{t})\big) - \tilde{\omega}\big(\mathcal{X}_i(\boldsymbol{s})\mathcal{Y}_j(\boldsymbol{t})\big)\tilde{\omega}(A) \ge 0 \tag{7.11}$$

for all $\boldsymbol{s} \in \mathcal{T}_i(\beta)$ and $\boldsymbol{t} \in \mathcal{T}_j(\beta)$.

(ii) *If $A\otimes \mathbb{1} - \mathbb{1}\otimes A \trianglelefteq 0$ w.r.t. $\mathfrak{P}_{\rm ext}$, then we have*

$$\tilde{\omega}\big(\mathcal{X}_i(\boldsymbol{s})A\mathcal{Y}_j(\mathbf{t})\big) - \tilde{\omega}\big(\mathcal{X}_i(\boldsymbol{s})\mathcal{Y}_j(\boldsymbol{t})\big)\tilde{\omega}(A) \le 0 \tag{7.12}$$

for all $\boldsymbol{s} \in \mathcal{T}_i(\beta)$ and $\boldsymbol{t} \in \mathcal{T}_j(\beta)$.

Proof. We can prove Proposition 7.3 in a manner similar to that in the proof of Proposition 5.8. □

Proof of Theorem 2.12

By Lemmas 5.1, 5.3 and Theorem 7.2, we conclude Theorem 2.12. □

8 Proof of Theorems 2.13, 2.15 and 2.16

8.1 Proof of Theorem 2.13

For each $f \in \mathfrak{A}$ and $a \in \mathbb{R}^d$, we set

$$\mathscr{C}_a^+[f] = f + \frac{1}{2}\{f(\cdot - a) + f(\cdot + a)\}, \tag{8.1}$$

$$\mathscr{C}_a^-[f] = f - \frac{1}{2}\{f(\cdot - a) + f(\cdot + a)\}. \tag{8.2}$$

Proposition 8.1 *$\mathscr{C}_a^\pm$ maps $\mathfrak{A}$ into $\mathfrak{A}$.*

Proof. Let $\hat{\mathscr{C}_a^\pm}[f]$ be the Fourier transform of $\mathscr{C}_a^\pm[f]$. We have

$$\hat{\mathscr{C}_a^\pm}[f](p) = \{1 \pm \cos(p \cdot a)\}\hat{f}(p) \geq 0. \tag{8.3}$$

Thus we are done. □

Proof of Theorem 2.13

(i) Choose $a \in \mathcal{C}(V)$ arbitrarily. By Theorem 2.7 (i) and Proposition 8.1, we have $\langle \mathscr{C}_a^-[f] \rangle \geq 0$. By a limiting argument,[8] we have

$$\psi(0)^2 - \frac{1}{2}\{\psi(a)^2 + \psi(-a)^2\} \geq 0. \tag{8.5}$$

Because $\psi(-a) = \psi(a)$, we obtain the desired result.

(ii) Let $p \in \hat{\mathcal{C}}(V)$. By Theorem 2.7 (ii) and Proposition 8.1, we have $\langle \mathscr{C}_p^-[f](-i\nabla_x) \rangle \geq 0$. Since $\langle f(-i\nabla_x) \rangle = \langle \hat{\psi} | f \hat{\psi} \rangle$, we have $\langle \hat{\psi} | \mathscr{C}_p^-[f] \hat{\psi} \rangle \geq 0$. By a limiting argument, we have

$$\hat{\psi}(0)^2 - \frac{1}{2}\{\hat{\psi}(p)^2 + \hat{\psi}(-p)^2\} \geq 0. \tag{8.6}$$

Because $\hat{\psi}(-p) = \hat{\psi}(p)$, we conclude the assertion. □

8.2 Proof of Theorems 2.15 and 2.16

Proposition 8.2 *$\mathscr{C}_a^\pm$ maps $\mathfrak{A}_{\mathrm{e}}$ into $\mathfrak{A}_{\mathrm{e}}$.*

Proof. It is easy to check that $\mathscr{C}_a^\pm[f](-x) = \mathscr{C}_a^\pm[f](x)$. Thus, the assertion follows from Proposition 8.1. □

Proof of Theorem 2.15

[8] To be precise, take $f \in C_0^\infty(\mathbb{R}^d)$ with $\|f\|_{L^2} = 1$. Set $f_\varepsilon(x) = \varepsilon^{-d/2} f(x/\varepsilon)$. Then we have, by the dominated convergence theorem,

$$\int_{\mathbb{R}^d} \psi(x)^2 f_\varepsilon(x) dx \to \psi(0)^2 \tag{8.4}$$

as $\varepsilon \to +0$. Thus, $\langle \mathscr{C}_a^-[f] \rangle \geq 0$ implies (8.5).

Let $a \in \mathcal{C}(V^{(1)}) \cap \mathcal{C}(V^{(2)})$. By Theorem 2.12 and Proposition 8.2, we have $\big\langle \mathscr{C}_a^{\pm}[f] \big\rangle^{(1)} \ge \big\langle \mathscr{C}_a^{\pm}[f] \big\rangle^{(2)}$. By a limiting argument, we obtain that

$$\psi^{(1)}(0)^2 \pm \frac{1}{2}\{\psi^{(1)}(a)^2 + \psi^{(1)}(-a)^2\} \ge \psi^{(2)}(0)^2 \pm \frac{1}{2}\{\psi^{(2)}(a)^2 + \psi^{(2)}(-a)^2\}. \tag{8.7}$$

Because $\psi^{(j)}(-x) = \psi^{(j)}(x)$, we have

$$\psi^{(1)}(0)^2 \pm \psi^{(1)}(a)^2 \ge \psi^{(2)}(0)^2 \pm \psi^{(2)}(a)^2. \tag{8.8}$$

Thus we are done. □

Proof of Theorem 2.16

Choose $p \in \hat{\mathcal{C}}(V^{(1)}) \cap \hat{\mathcal{C}}(V^{(2)})$ arbitrarily. By Theorem 2.12 and Proposition 8.2, we have $\big\langle \mathscr{C}_p^{\pm}[f](-i\nabla_x) \big\rangle^{(1)} \le \big\langle \mathscr{C}_p^{\pm}[f](-i\nabla_x) \big\rangle^{(2)}$. Because $\langle f(-i\nabla_x)\rangle^{(j)} = \langle \hat{\psi}^{(j)} | f \hat{\psi}^{(j)} \rangle$, $j = 1, 2$, we have $\langle \hat{\psi}^{(1)} | \mathscr{C}_p^{\pm}[f] \hat{\psi}^{(1)} \rangle \le \langle \hat{\psi}^{(2)} | \mathscr{C}_p^{\pm}[f] \hat{\psi}^{(2)} \rangle$. By a limiting argument, we obtain that

$$\hat{\psi}^{(1)}(0)^2 \pm \frac{1}{2}\{\hat{\psi}^{(1)}(p)^2 + \hat{\psi}^{(1)}(-p)^2\} \le \hat{\psi}^{(2)}(0)^2 \pm \frac{1}{2}\{\hat{\psi}^{(2)}(p)^2 + \hat{\psi}^{(2)}(-p)^2\}. \tag{8.9}$$

Because $\hat{\psi}^{(j)}(-p) = \hat{\psi}^{(j)}(p)$, we have

$$\hat{\psi}^{(1)}(0)^2 \pm \hat{\psi}^{(1)}(p)^2 \le \hat{\psi}^{(2)}(0)^2 \pm \hat{\psi}^{(2)}(p)^2. \tag{8.10}$$

This completes the proof. □

9 Proof of Theorems 2.17, 2.18 and 2.19

9.1 Proof of Theorem 2.17

(i) By Theorem 2.7 (i),

$$\langle f \rangle = (2\pi)^{-d/2} \int_{\mathbb{R}} dp \hat{f}(p) \langle \psi | e^{ip\cdot x} \psi \rangle = \int_{\mathbb{R}^d} dp \hat{f}(p) \hat{\varrho}(p) > 0 \tag{9.1}$$

for all $f \in \mathfrak{A} \cap L^1(\mathbb{R}^d; dx)$ with $f \neq 0$. Thus, we conclude (i).

(ii) Since $V(-x) = V(x)$ a.e. x by the assumption (ii) of **(B)**, we know that $\psi(-x) = \psi(x)$ a.e. x, which implies

$$\langle \psi | \sin(p \cdot x) \psi \rangle = 0. \tag{9.2}$$

Using the elementary fact that $1 - \cos\theta = 2\Big\{\sin(\theta/2)\Big\}^2$, we have, by (9.2),

$$1 - (2\pi)^{d/2} \hat{\varrho}(p) = \langle \psi | (\mathbb{1} - e^{-ip\cdot x}) \psi \rangle = 2\Big\langle \psi \Big| \Big\{ \sin\Big(\frac{p \cdot x}{2}\Big) \Big\}^2 \psi \Big\rangle. \tag{9.3}$$

Note that the multiplication operator $\Big\{\sin\Big(\frac{p\cdot x}{2}\Big)\Big\}^2$ satisfies $\Big\{\sin\Big(\frac{p\cdot x}{2}\Big)\Big\}^2 \trianglerighteq 0$ w.r.t. $L^2(\mathbb{R}^d; dx)_+$, and is nonzero if and only if $p \neq 0$. Hence, by Proposition 2.4 (i) and Theorem A.7, the RHS of (9.3) is strictly positive if and only if $p \neq 0$.

(iii) Note that if $f \in \mathfrak{A}_{\rm e}$, then $\overline{f} \in \mathfrak{A}_{\rm e}$ as well. Thus, by Theorem 2.9 (i), we have

$$\langle fg\rangle \geq \langle f\rangle\langle g\rangle, \quad \langle f\overline{g}\rangle \geq \langle f\rangle\langle \overline{g}\rangle. \tag{9.4}$$

Since $\langle \overline{g}\rangle = \langle g\rangle$,

$$\langle fg\rangle + \langle f\overline{g}\rangle \geq 2\langle f\rangle\langle g\rangle. \tag{9.5}$$

Let $C_0(\mathbb{R}^d)$ be the set of all continuous functions on $\mathbb{R}^d$ with compact support. Observe that, for all $f, g \in \mathfrak{A}_{\rm e} \cap C_0(\mathbb{R}^d)$,

$$\langle fg\rangle = (2\pi)^{-d/2} \int_{\mathbb{R}^d\times\mathbb{R}^d} dpdp' \hat{f}(p)\hat{g}(p')\hat{\varrho}(p+p'), \tag{9.6}$$

$$\langle f\overline{g}\rangle = (2\pi)^{-d/2} \int_{\mathbb{R}^d\times\mathbb{R}^d} dpdp' \hat{f}(p)\hat{g}(p')\hat{\varrho}(p-p') \tag{9.7}$$

and

$$\langle f\rangle\langle g\rangle = \int_{\mathbb{R}^d\times\mathbb{R}^d} dpdp' \hat{f}(p)\hat{g}(p')\hat{\varrho}(p)\hat{\varrho}(p'). \tag{9.8}$$

Since $\hat{\varrho}(p) > 0$, $\hat{f}(p) \geq 0$ and $\hat{g}(p) \geq 0$ for all $f, g \in \mathfrak{A}_{\rm e} \cap C_0(\mathbb{R}^d)$, we arrive at

$$(2\pi)^{-d/2}\{\hat{\varrho}(p+p') + \hat{\varrho}(p-p')\} \geq 2\hat{\varrho}(p)\hat{\varrho}(p'). \tag{9.9}$$

This completes the proof of (iii). $\Box$

9.2 Proof of Theorems 2.18 and 2.19

These theorems follow immediately from Theorems 2.8 and 2.12. $\Box$

A General theory of correlation inequalities

In this appendix, we will review some basic results concerning the operator inequalities introduced in Section 3. Almost all results are taken from the author's previous works [24, 26, 27, 28, 29, 30, 31].

Proposition A.1 *Let $\{A_n\}_{n=1}^\infty \subseteq \mathscr{B}(\mathfrak{H})$ and let $A \in \mathscr{B}(\mathfrak{H})$. Suppose that A_n converges to A in the weak operator topology. If $A_n \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ for all $n \in \mathbb{N}$, then $A \trianglerighteq 0$ w.r.t. $\mathfrak{P}$.*

Proof. By Remark 3.7 (i), $\langle \xi | A_n \eta\rangle \geq 0$ for all $\xi, \eta \in \mathfrak{P}$. Thus, $\langle \xi | A\eta\rangle = \lim_{n\to\infty} \langle \xi | A_n\eta\rangle \geq 0$ for all $\xi, \eta \in \mathfrak{P}$. By Remark 3.7 (i) again, we conclude that $A \trianglerighteq 0$ w.r.t. $\mathfrak{P}$. $\Box$

Proposition A.2 *Let A be a self-adjoint positive operator on $\mathfrak{H}$. Assume that $e^{-\beta A} \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ for all $\beta \geq 0$. Assume that $E = \inf \sigma(A)$ is an eigenvalue of A. Then there exists a nonzero vector $\xi \in \ker(A - E)$ such that $\xi \geq 0$ w.r.t. $\mathfrak{P}$.*

Proof. Let $\eta \in \mathfrak{H}$. By Theorem 3.4, we can express η as $\eta = \eta_R + i\eta_I$ with $\eta_R, \eta_I \in \mathfrak{H}_{\mathbb{R}}$. Now, we define an antilinear involution J by $J\eta = \eta_R - i\eta_I$. Clearly,

$$\eta_R = \frac{1}{2}(\eta + J\eta), \quad \eta_I = \frac{1}{2i}(\eta - J\eta). \tag{A.1}$$

Moreover, $\mathfrak{H}_{\mathbb{R}} = \{\eta \in \mathfrak{H} \,|\, J\eta = \eta\}$. Because $e^{-\beta A}\mathfrak{P} \subseteq \mathfrak{P}$, we see that $e^{-\beta A}\mathfrak{H}_{\mathbb{R}} \subseteq \mathfrak{H}_{\mathbb{R}}$ for all $\beta \geq 0$, see Remark 3.7 (i). Hence, for all $\beta \geq 0$, we obtain

$$Je^{-\beta A} = e^{-\beta A}J. \tag{A.2}$$

Let $\xi \in \ker(A-E)$ with $\xi \neq 0$. ξ can be expressed as $\xi = \xi_R + i\xi_I$ with $\xi_R, \xi_I \in \mathfrak{H}_{\mathbb{R}}$. Because $\xi \neq 0$, we have $\xi_R \neq 0$ or $\xi_I \neq 0$. By (A.1) and (A.2), we know that $\xi_R, \xi_I \in \ker(A-E) \cap \mathfrak{H}_{\mathbb{R}}$. Without loss of generality, we may assume that $\xi_R \neq 0$. By Definition 3.2 (ii) and Theorem 3.4, we have a unique decomposition $\xi_R = \xi_{R,+} - \xi_{R,-}$, where $\xi_{R,\pm} \in \mathfrak{P}$ with $\langle \xi_{R,+} | \xi_{R,-}\rangle = 0$. Let $|\xi_R| = \xi_{R,+} + \xi_{R,-}$. Because $\|\xi_R\| = \||\xi_R|\|$, we have

$$e^{-\beta E}\|\xi_R\|^2 = \langle \xi_R | e^{-\beta A}\xi_R\rangle \leq \langle |\xi_R| | e^{-\beta A}|\xi_R|\rangle \leq e^{-\beta E}\|\xi_R\|^2. \tag{A.3}$$

Thus, $|\xi_R| \in \ker(A-E)$. Clearly, $|\xi_R| \geq 0$ w.r.t. $\mathfrak{P}$. □

Theorem A.3 *Let A be a self-adjoint positive operator on $\mathfrak{H}$ and $B \in \mathscr{B}(\mathfrak{H})$. Suppose that*

(i) *$e^{-\beta A} \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ for all $\beta \geq 0$;*

(ii) *$B \trianglerighteq 0$ w.r.t. $\mathfrak{P}$.*

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

Proof. By (ii) and Proposition A.1,

$$e^{\beta B} = \sum_{n\geq 0} \underbrace{\frac{\beta^n}{n!}}_{\geq 0} \underbrace{B^n}_{\trianglerighteq 0} \trianglerighteq 0 \quad \text{w.r.t. } \mathfrak{P} \text{ for all } \beta \geq 0. \tag{A.4}$$

Hence, by (i) and Proposition 3.8 (ii),

$$\Big(\underbrace{e^{-\beta A/n}}_{\trianglerighteq 0}\underbrace{e^{\beta B/n}}_{\trianglerighteq 0}\Big)^n \trianglerighteq 0 \quad \text{w.r.t. } \mathfrak{P} \text{ for all } \beta \geq 0. \tag{A.5}$$

Using the Trotter–Kato product formula(e.g., [35, Theorem S. 21]) and Proposition A.1, we arrive at the desired assertion. □

Theorem A.4 *Let A, B be self-adjoint positive operators on $\mathfrak{H}$. Assume that $B = A - C$ with $C \in \mathscr{B}(\mathfrak{H})$. Suppose that*

(i) *$e^{-\beta A} \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ for all $\beta \geq 0$;*

(ii) *$C \trianglerighteq 0$ w.r.t. $\mathfrak{P}$.*

Then we have $e^{-\beta B} \trianglerighteq e^{-\beta A}$ w.r.t. $\mathfrak{P}$ for all $\beta \geq 0$.

Proof. By the Duhamel formula, we have the norm-convergent expansion

$$e^{-\beta B} = \sum_{n=0}^{\infty} D_n(\beta), \tag{A.6}$$

$$D_n(\beta) = \int_{S_n(\beta)} e^{-s_1 A} C e^{-s_2 A} C \cdots e^{-s_n A} C e^{-(\beta - \sum_{j=1}^n s_j)A}, \tag{A.7}$$

where $\int_{S_n(\beta)} = \int_0^\beta ds_1 \int_0^{\beta - s_1} ds_2 \cdots \int_0^{\beta - \sum_{j=1}^{n-1} s_j} ds_n$ and $D_0(\beta) = e^{-\beta A}$. Since $C \trianglerighteq 0$ and $e^{-tA} \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ for all $t \geq 0$, it holds that, by Proposition 3.8 (ii),

$$\underbrace{e^{-s_1 A}}_{\trianglerighteq 0} \underbrace{C}_{\trianglerighteq 0} \underbrace{e^{-s_2 A}}_{\trianglerighteq 0} \cdots \underbrace{e^{-s_n A}}_{\trianglerighteq 0} \underbrace{C}_{\trianglerighteq 0} \underbrace{e^{-(\beta - \sum_{j=1}^n s_j)A}}_{\trianglerighteq 0} \trianglerighteq 0 \tag{A.8}$$

provided that $s_1 \geq 0, \ldots, s_n \geq 0$ and $\beta - s_1 - \cdots - s_n \geq 0$. Thus, by Proposition A.1, we obtain $D_n(\beta) \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ for all $n \geq 0$. Accordingly, by (A.6) and Proposition A.1 again, we have $e^{-\beta B} \trianglerighteq D_{n=0}(\beta) = e^{-\beta A}$ w.r.t. $\mathfrak{P}$ for all $\beta \geq 0$. $\square$

Remark A.5 By (i), there exists a unique $\xi \in \mathfrak{H}$ such that $\xi > 0$ w.r.t. $\mathfrak{P}$ and $P_A = |\xi\rangle\langle\xi|$. Of course, ξ satisfies $A\xi = \inf \sigma(A)\xi$. $\diamondsuit$

Theorem A.6 *Let A be a self-adjoint positive operator on $\mathfrak{H}$, and let $B \in \mathscr{B}(\mathfrak{H})$. Suppose the following:*

(i) *$e^{-\beta A} \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ for all $\beta \geq 0$.*

(ii) *B is ergodic w.r.t. $\mathfrak{P}$.*

Then, $e^{-\beta(A-B)} \triangleright 0$ w.r.t. $\mathfrak{P}$ for all $\beta > 0$.

Proof. Set $H = A - B$. We apply Fröhlich's idea [7] and use the Duhamel expansion:

$$e^{-\beta H} = \sum_{n \geq 0} \mathscr{D}_n(\beta), \tag{A.9}$$

$$\mathscr{D}_n(\beta) = \int_{S_n(\beta)} e^{-s_1 A} B e^{-s_2 A} \cdots e^{-s_n A} B e^{-(\beta - \sum_{j=1}^n s_j)A}. \tag{A.10}$$

In a manner similar to that used in the proof of Theorem A.4, we know that

$$\mathscr{D}_n(\beta) \trianglerighteq 0, \tag{A.11}$$

$$e^{-s_1 A} B e^{-s_2 A} \cdots e^{-s_n A} B e^{-(\beta - \sum_{j=1}^n s_j)A} \trianglerighteq 0 \tag{A.12}$$

w.r.t. $\mathfrak{P}$, provided that $s_1 \geq 0, \ldots, s_n \geq 0$ and $\beta - s_1 - \cdots - s_n \geq 0$.

Let $\xi, \eta \in \mathfrak{P} \backslash \{0\}$. Since $e^{-\beta A} \trianglerighteq 0$ w.r.t. $\mathfrak{P}$ for all $\beta \geq 0$, we have $e^{-\beta A}\eta \in \mathfrak{P} \backslash \{0\}$. Let $\beta > 0$ be fixed arbitrarily. Because B is ergodic w.r.t. $\mathfrak{P}$, there exists an $n \in \{0\} \cup \mathbb{N}$ such that $\langle \xi | B^n e^{-\beta A} \eta \rangle > 0$. Now, let

$$F(s_1, \ldots, s_n) = \left\langle \xi \middle| e^{-s_1 A} B e^{-s_2 A} \cdots e^{-s_n A} B e^{-(\beta - \sum_{j=1}^n s_j)A} \eta \right\rangle. \tag{A.13}$$

By (A.12), it holds that $F(s_1, \ldots, s_n) \geq 0$. In addition, we have $F(0, \ldots, 0) = \langle \xi | B^n e^{-\beta A} \eta \rangle > 0$. Because $F(s_1, \ldots, s_n)$ is continuous in $s_1, \ldots, s_n$, we obtain

$$\langle \xi | \mathscr{D}_n(\beta) \eta \rangle = \int_{S_n(\beta)} F(s_1, \ldots, s_n) > 0. \tag{A.14}$$

By (A.9) and (A.11), we see that $e^{-\beta H} \trianglerighteq \mathscr{D}_n(\beta)$, which implies

$$\langle \xi | e^{-\beta H} \eta \rangle \geq \langle \xi | \mathscr{D}_n(\beta) \eta \rangle > 0. \tag{A.15}$$

Since ξ and η are in $\mathfrak{P} \backslash \{0\}$, we conclude that $e^{-\beta H} \eta > 0$ w.r.t. $\mathfrak{P}$. Since β is arbitrary, we obtain that $e^{-\beta H} \triangleright 0$ w.r.t. $\mathfrak{P}$ for all $\beta > 0$. □

Theorem A.7 *Let $A \in \mathscr{B}(\mathfrak{H})$. Assume that $u > 0$ w.r.t. $\mathfrak{P}$ and $A \trianglerighteq 0$ w.r.t. $\mathfrak{P}$. Then, $\langle u | Au \rangle = 0$ if and only if $A = 0$.*

Proof. We will divide the proof into several steps.

Step 1. *Let $A \in \mathscr{B}(\mathfrak{H})$. If $Au = 0$ for all $u \in \mathfrak{P}$, then $A = 0$.*

Proof. By Remark 3.3, each $u \in \mathfrak{H}$ can be written as $u = v_1 - v_2 + i(w_1 - w_2)$, where $v_1, v_2, w_1, w_2 \in \mathfrak{P}$ such that $\langle v_1 | v_2 \rangle = 0$ and $\langle w_1 | w_2 \rangle = 0$. Thus, the assumption implies that $Au = 0$ for *all* $u \in \mathfrak{H}$. □

Step 2. *Let $A \in \mathscr{B}(\mathfrak{H})$ with $A \neq 0$. Assume that $u > 0$ w.r.t. $\mathfrak{P}$. If $A \trianglerighteq 0$ w.r.t. $\mathfrak{P}$, then $Au \neq 0$.*

Proof. Assume that $Au = 0$. Then, $\langle v | Au \rangle = 0$ for all $v \in \mathfrak{P}$, implying that $\langle A^* v | u \rangle = 0$. Since $u > 0$ and $A^* v \geq 0$ w.r.t. $\mathfrak{P}$, we conclude that $A^* v$ must be zero. Because v is arbitrary, $A^* = 0$ by **Step 1**. □

Completion of the proof.

Suppose that $\langle u | Au \rangle = 0$. Assume that $A \neq 0$. Since $Au \geq 0$ and $u > 0$ w.r.t. $\mathfrak{P}$, Au must be zero. However, this contradicts with **Step 2**. □

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