Title	Ground state properties of the Kondo lattice model with electron-phonon interaction
Author(s)	冨永, 隼人
Citation	北海道大学. 博士(理学) 甲第15223号
Issue Date	2022-12-26
DOI	10.14943/doctoral.k15223
Doc URL	http://hdl.handle.net/2115/88173
Type	theses (doctoral)
File Information	Hayato_Tominaga.pdf

博士学位論文

Ground state properties of the Kondo lattice model with electron-phonon interaction
(電子格子相互作用をもつ近藤格子模型における基底状態の性質)

冨永隼人

北海道大学大学院理学院数学専攻

２０２２年１２月

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Hayato Tominaga

Abstract

It is known that heavy fermion systems exhibit a variety of orderings such as superconductivity, ferromagnetism, and antiferromagnetism. Therefore, heavy fermion systems have been actively studied both theoretically and experimentally. The Kondo lattice model(KLM) is one of the models for heavy fermion systems and describes the exchange interaction between localized spins and conduction electrons. Since the KLM has a wide range of applications, there have been various studies on this model. On the other hand, electron-phonon coupled systems have been extensively explored because the interaction between electrons and phonons causes intriguing physical phenomena.

In this thesis, we rigorously analyze the effect of electron-phonon interactions in heavy fermion systems. More specifically, the magnetic properties of the ground state of the half-filled KLM with the electron-phonon interaction term are examined in a rigorous manner. The spin reflection positivity introduced by Lieb is known to be very effective in analyzing the magnetic properties of the ground states of many electron systems. However, since the KLM does not have Coulomb interaction terms, the spin-reflection positivity cannot be directly applied to it. In this thesis, we show that this difficulty can be overcome by applying Miyao's operator inequality theory to the KLM. This enables us to prove that the ground state of the KLM with the electron-phonon interaction term is unique, and to determine the exact value of the total spin of the ground state.

Contents

1 Introduction

1.1 Background

Many-electron systems in which electrons strongly interact with each other are called strongly correlated electron systems. In strongly correlated electron systems, various physical phenomena emerge. Among strongly correlated electron systems, heavy fermion systems are those in which the effective mass of the electron is several hundred times heavier than the mass of the bare electron due to the strong repulsion between f electrons. In such a heavy fermion system, it has been experimentally observed that the effective mass of the conduction electron is tens to hundreds of times higher than that of the bare electron due to the strong coupling between the localized magnetic moment of the f electron and the conduction electron at low temperatures. This effect is known to cause various orders such as superconductivity, ferromagnetism, and antiferromagnetism in heavy fermion systems. For this reason, heavy fermion systems have been actively studied both theoretically and experimentally. The Kondo lattice model(KLM) is one of the models for heavy fermion systems and describes the exchange interaction between localized spins and conduction electrons. In particular, the half-filled KLM can be regarded as a model of Kondo insulators. The KLM has been actively studied because of its wide range of applications; see, for example,[4, 17, 21, 28]. There are many studies on the theoretical analysis of the KLM, but so far only a few rigorous results are available. Yanagisawa and Shimoi showed the ground state of the KLM with an extra on-site Coulomb repulsion is singlet if the strength of the Coulomb repulsion, U, is large [29]; in [27], Tsunetsugu provided a proof for $U = 0$; properties of the spin-spin correlations in the ground state were examined by Shen [22].

Interactions between electrons and phonons cause a variety of physical phenomena. For this reason, electron-lattice coupled systems have been actively studied both experimentally and theoretically. For example, when electrons and phonons interact, the electrons tend to form pairs. In the BCS theory [1], the starting point of the theory is the formation of the Cooper pair of two conduction electrons by electron-phonon interaction. The condensation of a huge number of Cooper pairs leads to an ordering. This mechanism can explain various properties of superconductors such as the Meissner effect.

The purpose of this doctoral thesis is to rigorously investigate the magnetic properties of the ground states of the half-filled KLM with electron-phonon interaction. More precisely, to prove the uniqueness of the ground states of this model, and to determine the exact value of the total spin of the ground states. To achieve the goals, we extend the method of spin-reflection positivity introduced by Lieb [7]. The concept of reflection positivity originates from the axiomatic quantum field theory [15, 16]. Lieb applied the concept of reflection positivity to the spin space of electrons in a simplified model for describing electrons in solids called the Hubbard model, and studied the magnetic properties of the ground states of the model. Yanagisawa and Shimoi first applied the method of the spin reflection positivity to the KLM [29]. Freericks and Lieb was the first to extend the spin reflection positivity to electron-phonon interacting systems [6]. Miyao further generalized the method of spin reflection positivity and applied it to more various systems including electron-phonon interacting systems. For reviews on the spin-reflection positivity, see, e.g., [23, 25, 26]. In the present paper, we apply the method of the spin reflection positivity to the KLM with the electron-phonon interaction by properly extending Miyao's idea.

The organization of this thesis is as follows. In Section 1, we define the KLM and the KLM with electron-phonon interaction, set the conditions that the model satisfies, and then describe the main theorems. We also present examples that satisfy the conditions and calculate the total spin of the ground states.

In Section 2, we first introduce the Hilbert cone to define operator inequalities. The Hilbert cone induces an order relation in the Hilbert space. From this order relation, an ordered structure is introduced for operators. Using this ordering structure, an extension of the Perron–Frobenius theorem holds for operators with a certain positivity. By applying this theorem, it becomes possible to show the uniqueness of the ground states of the KLM. In addition, we define in a general form Hilbert cones used in this doctoral thesis and introduce typical positive elements with respect to the induced order.

Section 3 is divided into two parts. In the first part, we prove the uniqueness of the ground state for the ordinary KLM and investigate the properties of the two-point correlation functions in the ground state. In the second part, we determine the total spin of the ground state. In order to apply the spin reflection positivity to the KLM, we perform the hole-particle transformation to the Hamiltonian. Then we show that the heat semigroup generated by the transformed Hamiltonian satisfies the conditions of the Perron–Frobenius–Faris theorem. In the proof of this part, we use the fact that the exchange interaction term in the KLM leads to an inequality similar to the one obtained by the Coulomb interaction. In the second part of this section, we determine the total spin of the ground state for the cases where the exchange interaction is ferromagnetic and antiferromagnetic, respectively. For this purpose, we use the results of the Hubbard model for the total spin of the ground state.

In Section 4, we analyze the ground states of the KLM with electron-phonon interaction, which is the main goal of this paper. In order to apply the spin-reflection positivity to this model, the hole-particle transformation is not sufficient, and we also need the Lang–Firsov transformation, which controls the electron-phonon interaction. In studying the total spin of the ground state, we use the results obtained in Section 3 for the KLM and the fact that spin operators are invariant under the Lang–Firsov transformation.

In Appendix A, we summarize the properties of the Lang–Firsov transformation that are needed in this thesis.

In Appendix B, we prove that the Hamiltonian of the KLM with electron-phonon interaction is a self-adjoint operator, bounded from below, using the Kato–Rellich theorem.

In Appendix C, we prove the uniqueness of the ground state of the Hubbard model using the operator inequalities defined in Section 2. The idea of the proof of the uniqueness of the ground state of the KLM is to extend the proof of this appendix, and this is made explicit in Section 3 and Section 4 so that the reader does not lose the essence of the complex proof in the KLM case.

Acknowledgements

I would like to express my deepest gratitude to my advisor, Tadahiro Miyao, for his attentive supervision and advice in this research and in writing my thesis.

1.2 Definition of models

1.2.1 Definition of the Kondo lattice model

Let Λ and Ω be a lattice of conduction electrons and a lattice of localized electrons, respectively. The Hamiltonian of the Kondo lattice model(KLM) is given by

$$H_{\mathrm{KL}} = \mathbb{T} + \sum_{x\in\Lambda, u\in\Omega} J_{x,u} \boldsymbol{s}_x \cdot \boldsymbol{S}_u, \tag{1.1}$$

$$\mathbb{T} = -\sum_{x,y\in\Lambda} t_{x,y}(c^*_{x,\uparrow}c_{y,\uparrow} + c^*_{x,\downarrow}c_{y,\downarrow}), \tag{1.2}$$

where $c_{x,\sigma}$ is the conduction electron annihilation operator at site $x \in \Lambda$ with spin σ, $f_{u,\sigma}$ is the localized electron annihilation operator at site $u \in \Omega$ with spin σ and b_x is the phonon annihilation operator at site $x \in \Lambda$. These operators satisfy following relations:

$$\{c_{x,\sigma}, c^*_{y,\sigma'}\} = \delta_{x,y}\delta_{\sigma,\sigma'}, \quad \{c_{x,\sigma}, c_{y,\sigma'}\} = 0, \tag{1.3}$$

$$\{f_{u,\sigma}, f^*_{v,\sigma'}\} = \delta_{u,v}\delta_{\sigma,\sigma'}, \quad \{f_{u,\sigma}, f_{v,\sigma'}\} = 0, \tag{1.4}$$

$$\{c_{x,\sigma}, f_{u,\sigma'}\} = \{c_{x,\sigma}, f^*_{u,\sigma'}\} = 0. \tag{1.5}$$

The operator H_{KL} acts on $\mathcal{H}_{\mathrm{c}} \otimes \mathcal{H}_{\mathrm{f}}$, where

$$\mathcal{H}_{\mathrm{c}} = \mathscr{F}_{\mathrm{F}}(\ell^2(\Lambda)) \otimes \mathscr{F}_{\mathrm{F}}(\ell^2(\Lambda)), \tag{1.6}$$

$$\mathcal{H}_{\mathrm{f}} = \mathscr{F}_{\mathrm{F}}(\ell^2(\Omega)) \otimes \mathscr{F}_{\mathrm{F}}(\ell^2(\Omega)). \tag{1.7}$$

n^c_x and n^f_u stand for the electron number operators, and are respectively defined by $n^c_x = n^c_{x\uparrow} + n^c_{x\downarrow}$ and $n^f_u = n^f_{u\uparrow} + n^f_{u\downarrow}$, where $n^c_{x\sigma} = c^*_{x\sigma}c_{x\sigma}$ and $n^f_{u\sigma} = f^*_{u\sigma}f_{u\sigma}$. $\boldsymbol{s}_x$ and $\boldsymbol{S}_u$ denote spin operators of the conduction electrons and the localized spins, respectively. More precisely, the spin operators are defined by

$$s^+_x = (s^-_x)^* = c^*_{x\uparrow}c_{x\downarrow}, \quad s^{(3)}_x = \frac{1}{2}(c^*_{x\uparrow}c_{x\uparrow} - c^*_{x\downarrow}c_{x\downarrow}), \tag{1.8}$$

$$S^+_u = (S^-_u)^* = f^*_{u\uparrow}f_{u\downarrow}, \quad S^{(3)}_u = \frac{1}{2}(f^*_{u\uparrow}f_{u\uparrow} - f^*_{u\downarrow}f_{u\downarrow}) \tag{1.9}$$

and

$$\boldsymbol{s}_x \cdot \boldsymbol{S}_u = \frac{1}{2}(s^+_x S^-_u + s^-_x S^+_u) + s^{(3)}_x S^{(3)}_u. \tag{1.10}$$

$t_{x,y}$ is the hopping matrix element and $J_{x,u}$ is the strength of the exchange interaction. There is a local constraint such that every f orbital is always occupied by just one electron. Such a situation can be expressed in term of the projection given by

$$P_0 = \prod_{u\in\Omega}\left[n^f_{u\uparrow}(1 - n^f_{u\downarrow}) + (1 - n^f_{u\uparrow})n^f_{u\downarrow}\right]. \tag{1.11}$$

Note that

$$n^f_{u\uparrow} + n^f_{u\downarrow} = 1 \tag{1.12}$$

holds on $\mathrm{ran}(P_0)$, the range of P_0.

The total spin operators are defined by

$$S^{(3)}_{\rm tot} = s^{(3)}_\Lambda + S^{(3)}_\Omega, \quad S^\pm_{\rm tot} = s^\pm_\Lambda + S^\pm_\Omega, \tag{1.13}$$

where

$$s^{(3)}_\Lambda = \sum_{x\in\Lambda} s_x, \quad S^{(3)}_\Omega = \sum_{u\in\Omega} S^{(3)}_u, \quad s^\pm_\Lambda = \sum_{x\in\Lambda} s^\pm_x, \quad S^\pm_\Omega = \sum_{u\in\Omega} S^\pm_u. \tag{1.14}$$

In addition, we set

$$\boldsymbol{S}^2_{\rm tot} = \frac{1}{2}\big(S^+_{\rm tot}S^-_{\rm tot} + S^-_{\rm tot}S^+_{\rm tot}\big) + \big(S^{(3)}_{\rm tot}\big)^2. \tag{1.15}$$

Definition 1.1. In general, if a vector φ is an eigenvector with $\boldsymbol{S}^2_{\rm tot}\varphi = S(S+1)\varphi$, then we say that φ has *total spin* S.

Set $N = |\Lambda| + |\Omega|$. In the present paper, we are interested in the ground state properties at half-filling. For this reason, we introduce the subspace of $\mathcal{H}_{\rm c} \otimes \mathcal{H}_{\rm f}$ by

$$\mathcal{L}_N = \ker\Big(S^{(3)}_{\rm tot}\Big) \bigcap \ker\left(N_{\rm e} - N\right), \tag{1.16}$$

where $N_{\rm e} = N^c_{\rm e} + N^f_{\rm e}$ is the total electron number operator with $N^c_{\rm e} = \sum_{x\in\Lambda}(n^c_{x\uparrow} + n^c_{x\downarrow})$ and $N^f_{\rm e} = \sum_{u\in\Omega}(n^f_{u\uparrow} + n^f_{u\downarrow})$. Note that $S^{(3)}_{\rm tot} = 0$ on $\mathcal{L}_N$.

Taking the above requirements into account, we introduce the following Hilbert space:

$$\mathcal{H}_{\rm KL} = P_0\mathcal{L}_N. \tag{1.17}$$

In what follows, we will examine ground state properties of the restricted Hamiltonian $H_{\rm KL} \restriction \mathcal{H}_{\rm KL}$. To simplify notation, we also denote the restriction of $H_{\rm KL}$ to the subspace $\mathcal{H}_{\rm KL}$ by $H_{\rm KL}$.

1.2.2 Definition of the Kondo lattice model with electron-phonon interaction

The Hamiltonian of the Kondo lattice model with an electron-phonon interaction is given by

$$H = H_{\rm KL} + \mathbb{U} + \sum_{x,y\in\Lambda} g_{x,y} n^c_x (b^*_y + b_y) + \omega_0 \sum_{x\in\Lambda} b^*_x b_x, \tag{1.18}$$

$$\mathbb{U} = \sum_{x,y\in\Lambda} U_{x,y}(n^c_x - 1)(n^c_y - 1). \tag{1.19}$$

b_x and b^*_x are the bosonic annihilation and creation operators at site $x \in \Lambda$ satisfying the standard commutation relations:

$$[b_x, b^*_y] = \delta_{x,y}, \quad [b_x, b_y] = 0. \tag{1.20}$$

The operator H acts on

$$\mathcal{H} = \mathcal{H}_{\rm KL} \otimes \mathcal{H}_{\rm ph}, \tag{1.21}$$

where

$$\mathcal{H}_{\rm ph} = L^2(\mathbb{R}^{|\Lambda|}). \tag{1.22}$$

By Theorem B.6, H is a self-adjoint operator on $\mathcal{H}_{\rm KL} \otimes {\rm dom}(N_{\rm p})$, where $N_{\rm p} = \sum_{x\in\Lambda} b_x^* b_x$. Furthermore, H is bounded from below.

$U_{x,y}$ is the energy of the Coulomb interaction and $g_{x,y}$ is the strength of the conductive electron-phonon interaction. The phonons are assumed to be dispersionless with energy $\omega_0 > 0$. Throughout the present study, we assume the following:

1. $g_{x,y}, t_{x,y}, J_{x,u}, U_{x,y} \in \mathbb{R}$ for all $x, y \in \Lambda, u \in \Omega$.

2. $g_{x,y} = g_{y,x}, t_{x,y} = t_{y,x}$ and $U_{x,y} = U_{y,x}$ for all $x, y \in \Lambda, u \in \Omega$.

Our principal assumptions are stated as follows:

(C.1) Let $E = \{\{x, y\} \in \Lambda \times \Lambda \,|\, t_{x,y} \neq 0\}$. The graph (Λ, E) is connected and bipartite. More precisely,

- for any $x, y \in \Lambda$, there is a path $p = \{\{x_j, y_j\}\}_{j=1}^n \subset E$ such that $x_1 = x$ and $y_n = y$;
- there are disjoint sublattices Λ_1 and Λ_2 with $\Lambda = \Lambda_1 \cup \Lambda_2$ such that $t_{x,y} = 0$, whenever $x, y \in \Lambda_1$ or $x, y \in \Lambda_2$.

(C.2) For any $u \in \Omega$, there exists a $x \in \Lambda$ such that $J_{x,u} \neq 0$. In addition, for any $x \in \Lambda$, there exists a $u \in \Omega$ such that $J_{x,u} \neq 0$. If $J_{x,u} \neq 0$, then ${\rm sgn} J_{x,u}$, the sign of $J_{x,u}$, is independent of x for each $u \in \Omega$.

(C.3) There are disjoint subsets Ω_1 and Ω_2 such that

- $\Omega = \Omega_1 \cup \Omega_2$;[1]
- $J_{x,u} = 0$ ($x \in \Lambda_1, u \in \Omega_1$ *or* $x \in \Lambda_2, u \in \Omega_2$).

(C.4) $|\Lambda|$ and $|\Omega|$ are even numbers.

(C.5) $\displaystyle\sum_{x\in\Lambda} g_{x,y}$ is independent of $y \in \Lambda$.

Definition 1.2. (i) We collectively denote (C.1), (C.2), (C.3) and (C.4) as **(C$_0$)**.

(ii) Conditions (C.1), (C.2), (C.3), (C.4) and (C.5) are collectively referred to as **(C)**.

In what follows, we will examine ground state properties of the restricted Hamiltonian $H \restriction \mathcal{H}$. To simplify notation, we also denote the restriction of H to the subspace $\mathcal{H}$ by H.

1.3 Main results

To state the main theorem, we introduce one terminology.

Definition 1.3. Let A be a self-adjoint operator on $\mathcal{X}$. Assume that $\inf {\rm spec}(A)$ is an eigenvalue of A. We call $\psi \in \mathcal{X}$ a *ground state* of A if ψ is an eigenvector corresponding to the minimum eigenvalue of A.

[1]Note that this condition does not necessarily mean that Ω is bipartite.

The magnetic properties of the ground states of the Kondo lattice model can be characterized by the following theorem:

Theorem 1.4. *Assume* **(C$_0$)**. *Then we obtain the following* (i) *and* (ii)*:*

(i) *The ground state of $H_{\rm KL}$ is unique.*

(ii) *We denote by ψ the ground state of $H_{\rm KL}$. Then ψ satisfies the following:*

$$\gamma_x\gamma_y\langle\psi, s_x^+ s_y^-\psi\rangle > 0, \quad \gamma_u\gamma_v \mathrm{sgn} J_{x,u} \mathrm{sgn} J_{y,v}\langle\psi, S_u^+ S_v^-\psi\rangle > 0 \tag{1.23}$$

for every $x, y \in \Lambda$ and $u, v \in \Omega$, where $\gamma_z = -1$ for $z \in \Lambda_1$ or Ω_1, $\gamma_z = 1$ for $z \in \Lambda_2$ or Ω_2.

In addition, we assume one of the following conditions:

(C.6) $J_{x,u} \geq 0$ *for every $x \in \Lambda$ and $u \in \Omega$, the antiferromagnetic coupling.*

(C.7) $J_{x,u} \leq 0$ *for every $x \in \Lambda$ and $u \in \Omega$, the ferromagnetic coupling.*

Then ψ has total spin S given by

$$S = \begin{cases} \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|, & \text{if (C.6) holds,} \\ \frac{1}{2}\big||\Lambda_1| + |\Omega_2| - |\Lambda_2| - |\Omega_1|\big|, & \text{if (C.7) holds.} \end{cases} \tag{1.24}$$

Remark 1.5. Theorem 1.4 means as follows; The ground state properties change whether the coupling is ferromagnetic or antiferromagnetic. See Section 1.4.

Next, we consider the case that the phonons interacts with the conduction electrons. We want to consider whether the properties of the ground state are affected by the interaction or not in this case. The answer to this question is given by the following theorem:

Theorem 1.6. *Assume* **(C)**. *Let $U_{{\rm eff},x,y}$ be the energy of the effective Coulomb interaction:*

$$U_{{\rm eff},x,y} = U_{x,y} - \omega_0^{-1}\sum_{z\in\Lambda} g_{x,z}g_{y,z}. \tag{1.25}$$

Suppose that $U_{\rm eff}$ is positive semi-definite.[2] *Notice that the critical case where $U_{\rm eff} = O$, the zero matrix, satisfies this condition. Then we obtain the following* (i) *and* (ii)*:*

(i) *The ground state of H is unique.*

(ii) *We denote by ψ the ground state of H. Then ψ satisfies the following:*

$$\gamma_x\gamma_y\langle\psi, s_x^+ s_y^-\psi\rangle > 0, \quad \gamma_u\gamma_v \mathrm{sgn} J_{x,u} \mathrm{sgn} J_{y,v}\langle\psi, S_u^+ S_v^-\psi\rangle > 0 \tag{1.26}$$

for every $x, y \in \Lambda$ and $u, v \in \Omega$, where $\gamma_z = -1$ for $z \in \Lambda_1$ or Ω_1, $\gamma_z = 1$ for $z \in \Lambda_2$ or Ω_2.

In addition, we assume one of **(C.6)** *and* **(C.7)**. *Then ψ has total spin S given by*

$$S = \begin{cases} \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|, & \text{if (C.6) holds,} \\ \frac{1}{2}\big||\Lambda_1| + |\Omega_2| - |\Lambda_2| - |\Omega_1|\big|, & \text{if (C.7) holds.} \end{cases} \tag{1.27}$$

Remark 1.7. Theorem 1.6 means as follows; If the electron-phonon coupling is not strong, we obtain similar results as Theorem 1.4.

[2]More precisely, $U_{\rm eff}$ is *positive semi-definite*, if $\sum_{x,y\in\Lambda} U_{{\rm eff},x,y} z_x^* z_y \geq 0$ for all $\boldsymbol{z} = \{z_x\}_{x\in\Lambda} \in \mathbb{C}^\Lambda$.

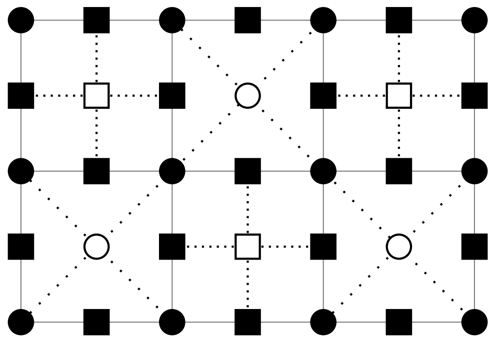

Figure 1: Filled circles and boxes respectively indicate the sites of Λ_1 and Λ_2. Open circles and boxes respectively indicate the sites of Ω_2 and Ω_1.

1.4 Examples

In this section, we will give some examples for better understanding of Theorems 1.4 and 1.6.

Example 1

Let us consider the case where $\Omega = \Lambda$ with $\Omega_1 = \Lambda_2$ and $\Omega_2 = \Lambda_1$. By choosing $g_{x,y}$, $J_{x,u}$ and $U_{x,y}$ as

$$J_{x,u} = J\delta_{x,u}, \quad g_{x,y} = g\delta_{x,y}, \quad U_{x,y} = U\delta_{x,y} \tag{1.28}$$

with $U \geq 0$, we can reproduce the standard Kondo lattice model with the electron-phonon interaction:

$$\begin{aligned}\mathbf{H} = &-\sum_{x,y\in\Lambda}\sum_{\sigma=\uparrow,\downarrow} t_{x,y} c_{x\sigma}^* c_{y\sigma} + J\sum_{x\in\Lambda} \boldsymbol{s}_x \cdot \boldsymbol{S}_x + U\sum_{x\in\Lambda}(n_x^c - 1)^2 \\ &+ g\sum_{x\in\Lambda} n_x^c (b_x^* + b_x) + \omega_0 \sum_{x\in\Lambda} b_x^* b_x. \end{aligned} \tag{1.29}$$

Assume that (C.1) is satisfied and $|\Lambda|$ is even. In this case, the assumptions (C.2)–(C.5) are automatically fulfilled. If $|g| \leq \sqrt{\omega_0 U}$, then U_{eff} is positive semi-definite. Notice that the case where $g = \pm\sqrt{\omega_0 U}$ is allowed. It is noteworthy that, if $J > 0$, then the total spin of the ground state is always equal to zero: $S = 0$. In contrast to this, if $J < 0$, then we have $S = \big||\Lambda_1| - |\Lambda_2|\big|$.

Example 2

Let us consider a two-dimensional lattice given by Figure 1. For each $x, y \in \Lambda$ and $u \in \Omega$, we set

$$t_{x,y} = \begin{cases} t & |x-y| = \frac{1}{2} \\ 0 & \text{otherwise,} \end{cases} \qquad J_{x,u} = \begin{cases} J & u \in \Omega_1, |x-u| = \frac{1}{2} \text{ or } u \in \Omega_2, |x-u| = \frac{1}{\sqrt{2}} \\ 0 & \text{otherwise,} \end{cases} \tag{1.30}$$

where $t \neq 0$. The conditions (C.1)–(C.4) are satisfied. In this example, we simply assume (C.5). First, let us consider the case where $J > 0$. Then (C.6) is satisfied. Because $|\Lambda_2| = 2|\Lambda_1|$ and $|\Omega_1| = |\Omega_2| = |\Lambda_1|/2$, the ground state has total spin $S = |\Lambda_1|/2 = N/8$. Similarly, if $J < 0$, then (C.7) is fulfilled and $S = |\Lambda_1|/2 = N/8$.

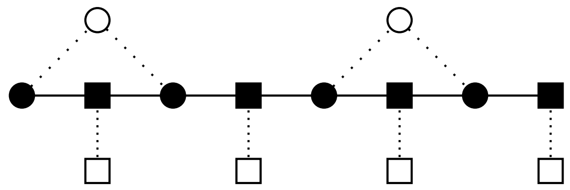

Figure 2: Filled circles and boxes respectively indicate the sites of Λ_1 and Λ_2. Open circles and boxes respectively indicate the sites of Ω_2 and Ω_1.

Example 3

In this example, let us consider a chain given by Figure 2. We set

$$t_{x,y} = \begin{cases} t & |x-y| = \frac{1}{2} \\ 0 & \text{otherwise,} \end{cases} \qquad J_{x,u} = \begin{cases} J & u \in \Omega_1, |x-u| = \frac{1}{2} \text{ or } u \in \Omega_2, |x-u| = \frac{1}{\sqrt{2}} \\ 0 & \text{otherwise,} \end{cases} \tag{1.31}$$

where $t \neq 0$. With regard to $g_{x,y}$, we simply assume (C.5). Then we readily confirm that $|\Lambda_1| = |\Lambda_2| = |\Lambda|/2$ and $|\Omega_1| = |\Lambda|/2, |\Omega_2| = |\Lambda|/4$. Hence, if $J \neq 0$, then the ground state has total spin $S = |\Lambda|/8 = N/14$, i.e., the value of S is independent of the sign of J.

2 General theory of operator inequalities

2.1 Operator inequalities and the Perron–Frobenius–Faris theorem

In this section, we will introduce operator inequalities, which will play an essential role in the analysis of this paper. It should be emphasized that the inequalities introduced here are different from the usual operator inequalities found in textbooks on functional analysis. To define the operator inequalities, we introduce Hilbert cones.

Let $\mathcal{X}$ be a Hilbert space and $\mathscr{B}(\mathcal{X})$ be the set of all bounded operators on $\mathcal{X}$. Let $\mathcal{C} \subset \mathcal{X}$ be a nonempty set.

Definition 2.1. $\mathcal{C}$ is said to be a *cone*, if the following (i) and (ii) hold:

(i) $u, v \in \mathcal{C}, a, b \geq 0 \Rightarrow au + bv \in \mathcal{C}$,

(ii) $u, -u \in \mathcal{C} \Rightarrow u = 0$.

Definition 2.2. $\mathcal{C}$ is a *Hilbert cone*, if the following (i), (ii) and (iii) hold:

(i) $\mathcal{C}$ is a closed cone,

(ii) $u, v \in \mathcal{C} \Rightarrow \langle u, v \rangle \geq 0$,

(iii) for any $w \in \mathcal{X}$, there exists $u, v, u', v' \in \mathcal{C}$ s.t. $w = u - v + i(u' - v')$ and $\langle u, v \rangle = \langle u', v' \rangle = 0$.

We write $u \geq 0$ w.r.t. $\mathcal{C}$ if $u \in \mathcal{C}$ and this u is called *positive* w.r.t. $\mathcal{C}$. A vector $v \in \mathcal{X}$ is said to be *strictly positive* w.r.t. $\mathcal{C}$, whenever $\langle u, v\rangle > 0$ for all $u \in \mathcal{C} \setminus \{0\}$ and we write this as $v > 0$ w.r.t. $\mathcal{C}$. In this way, if we fix a Hilbert cone in the Hilbert space, the vectors are naturally ordered. As we will see below, the ordering structure of the vectors induces ordering relations for the operators.

Definition 2.3. Let $A \in \mathscr{B}(\mathcal{X})$.

(i) A is *reality preserving w.r.t.* $\mathcal{C}$ if for all $u, v \in \mathcal{C}$, $\langle u, Av\rangle \in \mathbb{R}$.

(ii) A is *positivity preserving w.r.t.* $\mathcal{C}$ if $A\mathcal{C} \subset \mathcal{C}$ and we write this as $A \trianglerighteq 0$ w.r.t. $\mathcal{C}$.

(iii) A is *positivity improving w.r.t.* $\mathcal{C}$ if for any $u \in \mathcal{C} \setminus \{0\}$, $Au > 0$ w.r.t. $\mathcal{C}$ holds and we write this as $A \triangleright 0$ w.r.t. $\mathcal{C}$.

We prove some fundamental properties of positivity preserving operators.

Lemma 2.4. *Let $A, B \in \mathscr{B}(\mathcal{X}), a, b \geq 0$. Assume that $A \trianglerighteq 0$ w.r.t. $\mathcal{C}$ and $B \trianglerighteq 0$ w.r.t. $\mathcal{C}$. Then we have the following:*

(i) *$aA + bB \trianglerighteq 0$ w.r.t. $\mathcal{C}$.*

(ii) *$AB \trianglerighteq 0$ w.r.t. $\mathcal{C}$.*

Proof. (i) For any $A, B \in \mathscr{B}(\mathcal{X}), a, b \geq 0$ and $\varphi, \psi \in \mathcal{C}$, we have $\langle \varphi, (aA + bB)\psi\rangle \geq 0$. Hence, $aA + bB \trianglerighteq 0$ w.r.t. $\mathcal{C}$ holds.

(ii) Because $B\psi \in \mathcal{C}$, $AB\psi \in \mathcal{C}$ holds, which implies that $\langle \varphi, AB\psi\rangle \geq 0$. Hence, $AB \trianglerighteq 0$ w.r.t. $\mathcal{C}$ holds. □

Definition 2.5. Let A, B be reality preserving w.r.t. $\mathcal{C}$. We write $A \trianglerighteq B$ w.r.t. $\mathcal{C}$ if $A - B \trianglerighteq 0$ w.r.t. $\mathcal{C}$.

Unlike ordinary operator inequalities, the order is preserved even for products.

Proposition 2.6 ([10])**.** *Let $A, B, C, D \in \mathscr{B}(\mathcal{X})$. Assume $A \trianglerighteq B \trianglerighteq 0$ w.r.t. $\mathcal{C}$ and $C \trianglerighteq D \trianglerighteq 0$ w.r.t. $\mathcal{C}$ Then we have $AC \trianglerighteq BD \trianglerighteq 0$ w.r.t. $\mathcal{C}$.*

Proof. Because $A \trianglerighteq B \trianglerighteq 0$ w.r.t. $\mathcal{C}$ and $C \trianglerighteq D \trianglerighteq 0$ w.r.t. $\mathcal{C}$, we have $BD \trianglerighteq 0$ w.r.t. $\mathcal{C}$ and

$$(A - B)(C + D) \trianglerighteq 0, \quad (A + B)(C - D) \trianglerighteq 0 \text{ w.r.t. } \mathcal{C}. \tag{2.1}$$

Therefore, we have

$$(A - B)(C + D) + (A + B)(C - D) = 2AC - 2BD \trianglerighteq 0 \text{ w.r.t. } \mathcal{C}. \tag{2.2}$$

Hence, we obtain $AC \trianglerighteq BD \trianglerighteq 0$ w.r.t. $\mathcal{C}$. □

Lemma 2.7. *Let A, B be self-adjoint operators on $\mathcal{X}$. Suppose that A is bounded from below and $B \in \mathscr{B}(\mathcal{X})$. Assume that*

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

(ii) *$B \trianglerighteq 0$ w.r.t. $\mathcal{C}$.*

Then we have $e^{-\beta(A-B)} \trianglerighteq e^{-\beta A}$ w.r.t. $\mathcal{C}$.

Proof. Because $B \trianglerighteq 0$ w.r.t. $\mathcal{C}$, we have $e^{tB} = \sum_{n=0}^{\infty} \frac{t^n}{n!} B^n \trianglerighteq 1$ w.r.t. $\mathcal{C}$ for all $t \geq 0$. By the Trotter product formula [20, Theorem S. 20], for all $t \geq 0$, we obtain

$$e^{-t(A-B)} = \lim_{n\to\infty} \left(e^{-\frac{t}{n}A} e^{\frac{t}{n}B}\right)^n \trianglerighteq e^{-tA} \text{ w.r.t. } \mathcal{C}. \tag{2.3}$$

□

Remark 2.8. By Lemma 2.7, we see that the mapping on $\mathscr{B}(\mathcal{X}) : A \mapsto \exp(-\beta A)$ reverses the order of the operators.

To characterize the Hilbert cone, we prepare the following lemma:

Lemma 2.9. *Let $\psi \in \mathcal{X}$. If $\langle \psi, \varphi \rangle \geq 0$ for all $\varphi \in \mathcal{C}$, then we have $\psi \in \mathcal{C}$.*

Proof. By the definition of the Hilbert cone, there exist $u, u', v, v' \in \mathcal{C}$ such that $\psi = u - v + i(u' - v')$. Since $\langle \psi, \varphi \rangle \geq 0$ for all $\varphi \in \mathcal{C}$, we see that $\langle u' - v', \varphi \rangle = 0$ and $\langle u - v, \varphi \rangle \geq 0$ for all $\varphi \in \mathcal{C}$. Because $\operatorname{span} \mathcal{C} = \mathcal{X}$, $u' = v'$ holds. Since $u + \alpha v \in \mathcal{C}$ for any $\alpha \geq 0$, we have $\langle u - v, u + \alpha v \rangle = \|u\|^2 - \alpha \|v\|^2 \geq 0$, which implies $v = 0$. Hence, we conclude $\psi = u \in \mathcal{C}$. □

Definition 2.10. Let $\mathcal{D} \subset \mathcal{X}$ be a cone. The dual cone of $\mathcal{D}$ is defined by

$$\mathcal{D}^\dagger = \{\varphi \in \mathcal{X} \,|\, \langle \psi, \varphi \rangle \geq 0 \text{ for any } \psi \in \mathcal{D}\}. \tag{2.4}$$

We call $\mathcal{D}$ a self-dual cone when $\mathcal{D}$ satisfies $\mathcal{D} = \mathcal{D}^\dagger$.

The following proposition shows that the self-dual cone and the Hilbert cone are equivalent

Proposition 2.11. *Let $\mathcal{D} \subset \mathcal{X}$ be a nonempty set. $\mathcal{D}$ is a Hilbert cone if and only if $\mathcal{D}$ is a self-dual cone.*

Proof. Assume that $\mathcal{D}$ is a Hilbert cone. By using Lemma 2.9 and Definition 2.2 (ii), we see that $\mathcal{D}$ is a self-dual cone. Conversely, if $\mathcal{D}$ is a self-dual cone, then $\mathcal{D}$ is a closed cone and $\langle \varphi, \psi \rangle \geq 0$ holds for any $\varphi, \psi \in \mathcal{D}$. Let $\varphi \in (\overline{\operatorname{span}} \mathcal{D})^\perp$. We see $\varphi \in \mathcal{D}^\dagger = \mathcal{D} \subset \overline{\operatorname{span}} \mathcal{D}$ because $\langle \varphi, \psi \rangle = 0$ for any $\psi \in \mathcal{D}$. Hence we have $\varphi = 0$, which implies $\overline{\operatorname{span}} \mathcal{D} = \mathcal{X}$. Therefore, for all $\varphi \in \mathcal{X}$, there are $\psi_1, \psi_2, \psi_3, \psi_4 \in \mathcal{D}$ with $\varphi = \psi_1 - \psi_2 + i(\psi_3 - \psi_4)$. Set $\varphi_r = \psi_1 - \psi_2$ and $\varphi_i = \psi_3 - \psi_4$. We choose $\varphi_1 \in \mathcal{D}$ with $\inf_{\psi \in \mathcal{D}} \|\varphi_r - \psi\| = \|\varphi_r - \varphi_1\|$. For any $t \geq 0$ and $\psi \in \mathcal{D}$, we obtain

$$\begin{aligned} \|\varphi_r - \varphi_1\|^2 &\leq \|\varphi_r - \varphi_1 - t\psi\|^2 \\ &= \|\varphi_r - \varphi_1\|^2 - 2t\langle \varphi_r - \varphi_1, \psi \rangle + t^2 \|\psi\|^2, \end{aligned} \tag{2.5}$$

which implies that

$$\langle \varphi_r - \varphi_1, \psi \rangle \leq \frac{t}{2} \|\psi\|^2 \to 0 \quad (t \to 0). \tag{2.6}$$

Set $\varphi_2 = \varphi_1 - \varphi_r$. By using (2.6), we have $\langle \varphi_2, \psi \rangle \geq 0$, which implies $\varphi_2 \in \mathcal{D}$. For any $0 \leq t \leq 1$, we see

$$\begin{aligned} \|\varphi_r - \varphi_1\|^2 &\leq \|\varphi_r - t\varphi_1\|^2 \\ &= \|\varphi_r - \varphi_1\|^2 + 2(1-t)\langle \varphi_r - \varphi_1, \varphi_1 \rangle + (1-t)^2 \|\varphi_1\|^2. \end{aligned} \tag{2.7}$$

Thus, $\langle \varphi_2, \varphi_1 \rangle \leq 0$ holds. Since $\varphi_1, \varphi_2 \in \mathcal{D}$, we obtain $\langle \varphi_2, \varphi_1 \rangle = 0$. By applying the similar arguments to φ_i, we can show that there are $\varphi_3, \varphi_4 \in \mathcal{D}$ with $\varphi_i = \varphi_3 - \varphi_4$, $\langle \varphi_3, \varphi_4 \rangle = 0$. From the above, $\mathcal{D}$ is a Hilbert cone. □

Remark 2.12. The fact that the Hilbert cone is a self dual cone is essential to the following sections.

We prepare two technical lemmas for later convenience.

Lemma 2.13 ([12])**.** *Let $A \in \mathscr{B}(\mathcal{X}), \varphi \in \mathcal{C}$. Assume that $A \neq 0, A \trianglerighteq 0$ w.r.t. $\mathcal{C}$ and $\varphi > 0$ w.r.t. $\mathcal{C}$. Then we have $A\varphi \neq 0$.*

Proof. Suppose that $A\varphi = 0$. For any $\psi \in \mathcal{C}$, we see $\langle A^*\psi, \varphi\rangle = 0$. Since $A^* \trianglerighteq 0$ w.r.t. $\mathcal{C}$, $A^*\psi = 0$ holds for all $\psi \in \mathcal{C}$. This shows $A^* = 0$, which contradicts with $A \neq 0$. This completes the proof. □

Lemma 2.14. *Let P be a projection on $\mathcal{X}$ with $P \trianglerighteq 0$ w.r.t. $\mathcal{C}$. Then $P\mathcal{C} \subset P\mathcal{X}$ is a Hilbert cone.*

Proof. Let $\psi \in \mathcal{C}$. Because $P \trianglerighteq 0$ w.r.t. $\mathcal{C}$, $\langle P\psi, P\varphi\rangle \geq 0$ holds for any $\varphi \in \mathcal{C}$. Hence, we have $P\psi \in (P\mathcal{C})^\dagger$, which implies $P\mathcal{C} \subset (P\mathcal{C})^\dagger$. Let $\varphi \in (P\mathcal{C})^\dagger$. Then we obtain $\langle P\psi, \varphi\rangle \geq 0$ for all $\psi \in \mathcal{C}$. Since $\varphi \in \mathrm{ran}(P)$, it follows that $\langle P\psi, \varphi\rangle = \langle \psi, \varphi\rangle \geq 0$ holds. This shows $\varphi \in P\mathcal{C}$. Hence, $P\mathcal{C}$ is a self-dual cone. By Proposition 2.11, $P\mathcal{C}$ is a Hilbert cone. □

The aim of this paper is to analyze the properties of ground states of some specific Hamiltonians. A general theory for this purpose is given below.

Definition 2.15. Let A be a self-adjoint operator on $\mathcal{X}$ which is bounded from below. Assume that $e^{-tA} \trianglerighteq 0$ w.r.t. $\mathcal{C}$ for all $t \geq 0$. The semigroup $\{e^{-tA}\}_{t\geq 0}$ is said to be ergodic w.r.t. $\mathcal{C}$ if for each $u, v \in \mathcal{C} \setminus \{0\}$, there is a $t \geq 0$ such that $\langle u, e^{-tA}v\rangle > 0$.

The relationship between the positivity improvingness and the ergodicity is as shown in the following lemma:

Lemma 2.16. *Let A be a self-adjoint operator on $\mathcal{X}$, bounded from below. If $e^{-tA} \triangleright 0$ w.r.t. $\mathcal{C}$ for all $t > 0$, then $\{e^{-tA}\}_{t\geq 0}$ is ergodic w.r.t. $\mathcal{C}$.*

Proof. Since $e^{-tA} \triangleright 0$ w.r.t. $\mathcal{C}$, we have $\langle \varphi, e^{-tA}\psi\rangle > 0$ for any $\varphi, \psi \in \mathcal{C} \setminus \{0\}$ and $t > 0$. Therefore, $\{e^{-tA}\}_{t\geq 0}$ is ergodic w.r.t. $\mathcal{C}$. □

The following theorem is important in demonstrating the uniqueness of ground states of Hamiltonians.

Theorem 2.17 (Perron–Frobenius–Faris)**.** *Let A be a self-adjoint operator on $\mathcal{X}$, bounded from below. Assume that $\lambda = \inf \mathrm{spec}(A)$ is an eigenvalue of A. Let $\mathcal{V}$ be the eigenspace corresponding to λ. If $\{e^{-tA}\}_{t\geq 0}$ is ergodic w.r.t. $\mathcal{C}$, then $\dim \mathcal{V} = 1$ and $\mathcal{V}$ is spanned by a strictly positive vector w.r.t. $\mathcal{C}$.*

Proof. See [5].

Remark 2.18. By Lemma 2.16, if $e^{-tA} \triangleright 0$ w.r.t. $\mathcal{C}$ for all $t > 0$, the self-adjoint operator A satisfies the assumptions of Theorem 2.17.

The uniqueness of ground states can be proved by using Theorem 2.17. In general, it is difficult to prove that some bounded operators are positivity improving. The following proposition is useful in proving that heat semigroups are positivity improving.

Proposition 2.19. *Let A be a self-adjoint operator on $\mathcal{X}$ which is bounded from below. Let B be a self-adjoint operator on $\mathcal{X}$. Suppose that $B \trianglerighteq 0$ w.r.t. $\mathcal{C}$. Assume that $e^{-tA} \trianglerighteq 0$ w.r.t. $\mathcal{C}$ for all $t \geq 0$. Let $\mathcal{I}$ be a subset of $\mathcal{C} \setminus \{0\}$. Suppose that for all $u \in \mathcal{C} \setminus \{0\}$ there exist $n \in \mathbb{N}$ and $\psi \in \mathcal{I}$ with $B^n u \geq \psi$ w.r.t. $\mathcal{C}$. Let $\beta > 0$. If*

$$\langle \varphi, e^{-\beta(A-B)}\psi \rangle > 0 \tag{2.8}$$

holds for any $\varphi, \psi \in \mathcal{I}$, then we have $e^{-\beta(A-B)} \triangleright 0$ w.r.t. $\mathcal{C}$.

Proof. By using the Duhamel formula, we have

$$e^{-\beta(A-B)} = \sum_{n\geq 0} \beta^n \int_{0\leq s_1\leq\cdots\leq s_n\leq 1} E^n_\beta(s_1,\dots,s_n)\, ds_n \cdots ds_1, \tag{2.9}$$

$$E^n_\beta(s_1,\dots,s_n) = e^{-s_1\beta A} B \cdots B e^{(1-s_n)\beta A}. \tag{2.10}$$

Since $E^n_\beta(s_1,\dots,s_n) \trianglerighteq 0$ w.r.t. $\mathcal{C}$ and $\langle \varphi, e^{-\beta(A-B)}\psi\rangle > 0$ for all $\varphi, \psi \in \mathcal{I}$, there exists an $m \in \mathbb{N}$ such that

$$\left\langle \varphi, \int_{0\leq s_1\leq\cdots\leq s_m\leq 1} E^m_\beta(s_1,\dots,s_m)\, ds_m \cdots ds_1 \psi \right\rangle > 0. \tag{2.11}$$

Because $\langle \varphi, E^m_\beta(s_1,\dots,s_m)\psi\rangle$ is continuous in $s_1,\dots,s_m$, there exist $0 \leq t_1 \leq \cdots \leq t_m \leq 1$ such that

$$\langle \varphi, E^m_\beta(t_1,\dots,t_m)\psi\rangle > 0. \tag{2.12}$$

For any $u, v \in \mathcal{C} \setminus \{0\}$, there exist $\varphi, \psi \in \mathcal{I}$ and $k, l \in \mathbb{N}$ such that $B^k u \geq \varphi$ w.r.t. $\mathcal{C}$ and $B^l v \geq \psi$ w.r.t. $\mathcal{C}$. Set $n = k + l + m$. Since

$$E^n_\beta(0,\dots,0,t_1,\dots,t_m,1,\dots,1) = B^k E^m_\beta(t_1,\dots,t_m) B^l, \tag{2.13}$$

we have

$$\begin{aligned}
&\langle u, E^n_\beta(0,\dots,0,t_1,\dots,t_m,1,\dots,1)v\rangle \\
&= \langle u, B^k E^m_\beta(t_1,\dots,t_m) B^l v\rangle \\
&\geq \langle \varphi, E^m_\beta(t_1,\dots,t_m)\psi\rangle \\
&> 0.
\end{aligned} \tag{2.14}$$

Hence, by (2.14),

$$\int_{0\leq s_1\leq\cdots\leq s_n\leq 1} \langle u, E^n_\beta(s_1,\dots,s_n)v\rangle\, ds_n \cdots ds_1 > 0 \tag{2.15}$$

holds. Therefore, we have

$$\langle u, e^{-\beta(A-B)}v\rangle \geq \beta^n \int_{0\leq s_1\leq\cdots\leq s_n\leq 1} \langle u, E^n_\beta(s_1,\dots,s_n)v\rangle\, ds_n \cdots ds_1 > 0, \tag{2.16}$$

which implies that $e^{-\beta(A-B)} \triangleright 0$ w.r.t. $\mathcal{C}$. □

2.2 Some useful Hilbert cones

In this section, we introduce some Hilbert cones and prove basic operator inequalities for each Hilbert cone. In addition, we define some specific Hilbert cones to be used when analyzing the KLM.

2.2.1 A Hilbert cone in $\mathscr{I}_2(\mathcal{X})$

Let

$$\mathscr{I}_2(\mathcal{X}) = \{A \in \mathscr{B}(\mathcal{X}) \,|\, \mathrm{Tr}[A^*A] < \infty\}. \tag{2.17}$$

$\mathscr{I}_2(\mathcal{X})$ is the set of all Hilbert-Schmidt class operators on $\mathcal{X}$. In what follows, we regard $\mathscr{I}_2(\mathcal{X})$ as a Hilbert space with the inner product given by $\langle A, B\rangle_2 = \mathrm{Tr}[A^*B]$.

Definition 2.20. We define $\mathscr{I}_+(\mathcal{X}) \subset \mathscr{I}_2(\mathcal{X})$ by

$$\mathscr{I}_+(\mathcal{X}) = \{A \in \mathscr{I}_2(\mathcal{X}) \,|\, A \geq 0\}. \tag{2.18}$$

Proposition 2.21. *$\mathscr{I}_+(\mathcal{X})$ is a Hilbert cone in $\mathscr{I}_2(\mathcal{X})$.*

Proof. Let $B, C \in \mathscr{I}_+(\mathcal{X})$. Since $B \geq 0$, there is a $D \in \mathscr{I}_2(\mathcal{X})$ with $B = D^*D$. Because $DCD^* \geq 0$, we have

$$\langle B, C\rangle_2 = \mathrm{Tr}[DCD^*] \geq 0. \tag{2.19}$$

For any $A \in \mathscr{I}_2(\mathcal{X})$, we set

$$A_{\mathrm{re}} = \frac{1}{2}(A + A^*), \tag{2.20}$$
$$A_{\mathrm{im}} = \frac{1}{2i}(A - A^*). \tag{2.21}$$

Then we have $A = A_{\mathrm{re}} + iA_{\mathrm{im}}$. Define

$$A_1 = \frac{1}{2}(|A_{\mathrm{re}}| + A_{\mathrm{re}}), \tag{2.22}$$
$$A_2 = \frac{1}{2}(|A_{\mathrm{re}}| - A_{\mathrm{re}}), \tag{2.23}$$
$$A_3 = \frac{1}{2}(|A_{\mathrm{im}}| + A_{\mathrm{im}}), \tag{2.24}$$
$$A_4 = \frac{1}{2}(|A_{\mathrm{im}}| - A_{\mathrm{im}}). \tag{2.25}$$

Then A_1, A_2, A_3 and A_4 are positive operators. We readily confirm that $A = A_1 - A_2 + i(A_3 - A_4)$ and $A_1A_2 = A_3A_4 = 0$. Thus, $\mathscr{I}_+(\mathcal{X})$ is a Hilbert cone. □

$\mathscr{I}_+(\mathcal{X})$ is the most fundamental Hilbert cone for the spin reflection positivity.

Definition 2.22. Let $A \in \mathscr{B}(\mathcal{X})$ and $B \in \mathscr{I}_2(\mathcal{X})$. We define the left multiplication operator $\mathcal{L}(A)$ on $\mathscr{I}_2(\mathcal{X})$ and the right multiplication operator $\mathcal{R}(A)$ on $\mathscr{I}_2(\mathcal{X})$ by

$$\mathcal{L}(A)B = AB, \tag{2.26}$$
$$\mathcal{R}(A)B = BA. \tag{2.27}$$

Lemma 2.23. *Let $A, B \in \mathscr{B}(\mathcal{X})$. Then we have*

$$\mathcal{L}(AB) = \mathcal{L}(A)\mathcal{L}(B), \quad \mathcal{R}(AB) = \mathcal{R}(B)\mathcal{R}(A). \tag{2.28}$$

Proof. Let $C \in \mathscr{I}_2(\mathcal{X})$. Then we see that

$$\mathcal{L}(A)\mathcal{L}(B)C = ABC = \mathcal{L}(AB)C, \tag{2.29}$$
$$\mathcal{R}(B)\mathcal{R}(A)C = CAB = \mathcal{R}(AB)C. \tag{2.30}$$

□

Remark 2.24. Note that in (2.28), the order of the products is different for $\mathcal{L}$ and $\mathcal{R}$.

Proposition 2.25. *Let $A \in \mathscr{B}(\mathcal{X})$. We have $\mathcal{L}(A^*)\mathcal{R}(A) \trianglerighteq 0$ w.r.t. $\mathscr{I}_+(\mathcal{X})$.*

Proof. Take $\xi, \nu \in \mathscr{I}_+(\mathcal{X})$, arbitrarily. Then there exist sequences of positive numbers, $\{\xi_n\}_n$ and $\{\nu_n\}_n$, and complete orthonormal systems(CONSs) $\{x_n\}_n$ and $\{y_n\}_n$ in $\mathcal{X}$ such that $\xi = \sum_n \xi_n |x_n\rangle\langle x_n|$ and $\nu = \sum_n \nu_n |y_n\rangle\langle y_n|$ hold. Because

$$\mathcal{L}(A)\mathcal{R}(A^*)\nu = \sum_n \nu_n |Ay_n\rangle\langle Ay_n|, \tag{2.31}$$

we have

$$\langle \xi, \mathcal{L}(A)\mathcal{R}(A^*)\nu\rangle = \sum_{m,n} \xi_m \nu_n |\langle x_m, Ay_n\rangle|^2 \ge 0. \tag{2.32}$$

Hence, we have $\mathcal{L}(A)\mathcal{R}(A^*) \trianglerighteq 0$ w.r.t. $\mathscr{I}_+(\mathcal{X})$. □

The operator inequality in the above proposition is fundamental in this paper.

2.2.2 A Hilbert cone in $\mathcal{X} \otimes \mathcal{X}$

Let ϑ ba an antiunitary operator on $\mathcal{X}$. We define the map $\Psi_\vartheta : \mathcal{X} \otimes \mathcal{X} \to \mathscr{I}_2(\mathcal{X})$ by

$$\Psi_\vartheta(\varphi \otimes \vartheta\psi) = |\varphi\rangle\langle\psi|, \quad \varphi, \psi \in \mathcal{X}. \tag{2.33}$$

Lemma 2.26. *Ψ_ϑ is a unitary operator.*

Proof. We readily confirm that Ψ_ϑ is surjective. Let $\{e_i\}_i \subset \mathcal{X}$ be a CONS. Then $\{e_i \otimes \vartheta e_j\}_{i,j}$ is a CONS in $\mathcal{X} \otimes \mathcal{X}$ as well. Therefore, we have

$$\begin{aligned}\Big\langle \Psi_\vartheta(e_i \otimes \vartheta e_j), \Psi_\vartheta(e_k \otimes \vartheta e_l)\Big\rangle &= \Big\langle |e_i\rangle\langle e_j|, |e_k\rangle\langle e_l|\Big\rangle_2 \\ &= \delta_{i,k}\delta_{j,l} \\ &= \langle e_i \otimes \vartheta e_j, e_k \otimes \vartheta e_l\rangle. \end{aligned} \tag{2.34}$$

Thus, Ψ_ϑ is a unitary operator. □

By Lemma 2.26, we can naturally identify $\mathcal{X} \otimes \mathcal{X}$ with $\mathscr{I}_2(\mathcal{X})$. We write this identification as

$$\mathcal{X} \otimes \mathcal{X} \overset{\Psi_\vartheta}{=} \mathscr{I}_2(\mathcal{X}). \tag{2.35}$$

Occasionally, we abbreviate (2.35) by omitting the subscript Ψ_ϑ if no confusion arises.

Definition 2.27. We define $\mathcal{E} \subset \mathcal{X} \otimes \mathcal{X}$ by

$$\mathcal{E} = \Psi_{\vartheta}^{-1}(\mathscr{I}_+(\mathcal{X})). \tag{2.36}$$

Proposition 2.28. *$\mathcal{E}$ is a Hilbert cone in $\mathcal{X} \otimes \mathcal{X}$.*

Proof. By Proposition 2.21, $\mathscr{I}_+(\mathcal{X})$ is a Hilbert cone. From Lemma 2.26, $\mathcal{E}$ is a Hilbert cone in $\mathcal{X} \otimes \mathcal{X}$. □

By (2.35), we can conclude the following lemma:

Lemma 2.29. *Let $\{e_j\}_j$ be a CONS of $\mathcal{X}$. We have*

$$\mathcal{E} = \left\{ \sum_{j,k} C_{j,k} e_j \otimes \vartheta e_k \,\middle|\, (C_{j,k})_{j,k} \geq 0, \sum_{j,k} |C_{j,k}|^2 < \infty \right\}, \tag{2.37}$$

where $(C_{j,k})_{j,k} \geq 0$ means that the matrix $(C_{j,k})_{j,k}$ is positive semidefinite.

Proof. Let $C \in \mathscr{I}_+(\mathcal{X})$. Then C can be expressed as

$$C = \sum_i \lambda_i |x_i\rangle\langle x_i|, \tag{2.38}$$

where λ_i are nonnegative numbers satisfying $\sum_i |\lambda_i|^2 < \infty$ and $\{x_i\}_i \subset \mathcal{X}$ is a CONS. Set $x_{i,j} = \langle e_j, x_i \rangle$. Then $x_i = \sum_j x_{i,j} e_j$ and

$$C = \sum_{i,j,k} \lambda_i x_{i,j} \overline{x_{i,k}} |e_j\rangle\langle e_k| \tag{2.39}$$

holds. Define $C_{j,k} = \sum_i \lambda_i x_{i,j} \overline{x_{i,k}}$. Since $(C_{j,k})_{j,k}$ is positive semidefinite and $\sum_{j,k} |C_{j,k}|^2 < \infty$, we have $\Psi_{\vartheta}(\mathcal{E}) = \mathscr{I}_+(\mathcal{X})$. □

Lemma 2.30. *Let $\{e_j\}_j$ be a CONS of $\mathcal{X}$. Let $\varphi \in \mathcal{E}$. Assume that $\langle e_j \otimes \vartheta e_j, \varphi \rangle = 0$ for any j. Then we have $\varphi = 0$.*

Proof. Since $\langle e_j \otimes \vartheta e_j, \varphi \rangle = 0$, we have

$$\langle e_j, \Psi_{\vartheta}(\varphi) e_j \rangle = \mathrm{Tr}[|e_j\rangle\langle e_j| \Psi_{\vartheta}(\varphi)] = \langle e_j \otimes \vartheta e_j, \varphi \rangle = 0 \tag{2.40}$$

for any j. Hence, we conclude $\varphi = 0$. □

Lemma 2.31. *Let $A \in \mathscr{B}(\mathcal{X})$. Under the identification (2.35), we have*

$$A \otimes 1 = \mathcal{L}(A), \quad 1 \otimes A = \mathcal{R}(\vartheta^* A^* \vartheta). \tag{2.41}$$

Proof. For any $\varphi, \psi \in \mathcal{X}$, we see that

$$A \otimes 1(\varphi \otimes \vartheta \psi) = (A\varphi) \otimes \vartheta \psi = |A\varphi\rangle\langle \psi| = \mathcal{L}(A)|\varphi\rangle\langle \psi|, \tag{2.42}$$

$$1 \otimes A(\varphi \otimes \vartheta \psi) = \varphi \otimes (A\vartheta \psi) = |\varphi\rangle\langle \vartheta^* A \vartheta \psi| = \mathcal{R}(\vartheta^* A^* \vartheta)|\varphi\rangle\langle \psi| \tag{2.43}$$

hold. □

Due to the identification (2.35), the following proposition holds.

Proposition 2.32. *Let $A \in \mathscr{B}(\mathcal{X})$. We have $A \otimes \vartheta A \vartheta^* \trianglerighteq 0$ w.r.t. $\mathcal{E}$.*

Proof. By Proposition 2.25, we have

$$A \otimes \vartheta A \vartheta^* = \mathcal{L}(A)\mathcal{R}(\vartheta^* \vartheta A^* \vartheta^* \vartheta) = \mathcal{L}(A)\mathcal{R}(A^*) \trianglerighteq 0 \text{ w.r.t. } \mathcal{E}. \quad \square \tag{2.44}$$

Corollary 2.33. *Let $A \in \mathscr{B}(\mathcal{X})$. Then $\exp[-\beta(A \otimes 1 + 1 \otimes \vartheta A \vartheta^*)] \trianglerighteq 0$ w.r.t. $\mathcal{E}$ holds.*

Proof. By Proposition 2.32, we have

$$e^{-\beta(A \otimes 1 + 1 \otimes \vartheta A \vartheta^*)} = e^{-\beta A} \otimes \vartheta e^{-\beta A} \vartheta^* \trianglerighteq 0 \text{ w.r.t. } \mathcal{E}. \tag{2.45}$$

□

2.2.3 A Hilbert cone in $Q_0(\mathcal{X} \otimes \mathcal{X})$

Let $Q_i \in \mathscr{B}(\mathcal{X}), i = 1, \ldots, n$ be projections. Set

$$Q_0 = \sum_{i=1}^{n} Q_i \otimes \vartheta Q_i \vartheta^*. \tag{2.46}$$

Proposition 2.34. *$Q_0\mathcal{E}$ is a Hilbert cone in $Q_0\mathcal{X} \otimes \mathcal{X}$*

Proof. Since $Q_0 \trianglerighteq 0$ w.r.t. $\mathcal{E}$ and Lemma 2.14, $Q_0\mathcal{E}$ is a Hilbert cone. □

$Q_0\mathcal{E}$ is an important Hilbert cone when we study the Kondo lattice model. The following lemma corresponds to Proposition 2.25.

Lemma 2.35. *Let $A \in \mathscr{B}(\mathcal{X} \otimes \mathcal{X})$. Assume the following:*

(i) *A commutes with Q_0.*

(ii) *$A \trianglerighteq 0$ w.r.t. $\mathcal{E}$.*

Then we have $A \restriction Q_0\mathcal{X} \otimes \mathcal{X} \trianglerighteq 0$ w.r.t. $Q_0\mathcal{E}$, where $A \restriction Q_0\mathcal{X} \otimes \mathcal{X}$ is the restriction of A to $Q_0\mathcal{X} \otimes \mathcal{X}$.

Proof. Since $Q_0 \trianglerighteq 0$ w.r.t. $\mathcal{E}$, we see $Q_0AQ_0 \trianglerighteq 0$ w.r.t. $\mathcal{E}$. Hence, for any $\phi, \psi \in \mathcal{E}$,

$$\langle \phi, Q_0AQ_0\psi\rangle = \langle Q_0\phi, AQ_0\psi\rangle \geq 0 \tag{2.47}$$

holds. Thus, we have $A \trianglerighteq 0$ w.r.t. $Q_0\mathcal{E}$. □

2.2.4 A Hilbert cone in $L^2(\mathbb{R}^d)$

Definition 2.36. $\mathcal{P} \subset L^2(\mathbb{R}^d)$ is given by

$$\mathcal{P} = \{f \in L^2(\mathbb{R}^d) \,|\, f(\boldsymbol{q}) \geq 0 \text{ a.e. } \boldsymbol{q}\}. \tag{2.48}$$

Lemma 2.37. *$\mathcal{P}$ is a Hilbert cone in $L^2(\mathbb{R}^d)$.*

Proof. For $f \in L^2(\mathbb{R}^d)$, let f_{r} be the real part of f and f_{i} be the imaginary part of f:

$$f_{\mathrm{r}}(x) = \frac{f(x) + \overline{f(x)}}{2}, \quad f_{\mathrm{i}}(x) = \frac{f(x) - \overline{f(x)}}{2i}, \quad x \in \mathbb{R}^d. \tag{2.49}$$

Set

$$f_{\mathrm{r}}^{\pm}(x) = \frac{|f_{\mathrm{r}}(x)| \pm f_{\mathrm{r}}(x)}{2}, \quad f_{\mathrm{i}}^{\pm}(x) = \frac{|f_{\mathrm{i}}(x)| \pm f_{\mathrm{i}}(x)}{2}, \tag{2.50}$$

then we see that $f_{\mathrm{r}}^{\pm}(x), f_{\mathrm{i}}^{\pm}(x) \geq 0$ and $f = f_{\mathrm{r}}^+ - f_{\mathrm{r}}^- + i(f_{\mathrm{i}}^+ - f_{\mathrm{i}}^-)$ hold. In addition, we have $\langle f_{\mathrm{r}}^+, f_{\mathrm{r}}^-\rangle = \langle f_{\mathrm{i}}^+, f_{\mathrm{i}}^-\rangle = 0$. Hence, $\mathcal{P}$ is a Hilbert cone. □

The following lemma is the well-known fact.

Lemma 2.38. *Let Δ be the d-dimensional Laplacian on $L^2(\mathbb{R}^d)$. Then we have*

$$e^{\beta\Delta} \rhd 0 \text{ w.r.t. } \mathcal{P} \tag{2.51}$$

for all $\beta > 0$.

Proof. Set

$$P_\beta(x,y) = (4\pi\beta)^{-\frac{d}{2}} e^{-\frac{|x-y|^2}{4\beta}}, \quad x,y \in \mathbb{R}^d. \tag{2.52}$$

For $f \in L^2(\mathbb{R}^d)$, $e^{\beta\Delta} f$ can be expressed as

$$(e^{\beta\Delta} f)(x) = \int_{\mathbb{R}^d} P_\beta(x,y) f(y)\, dy, \tag{2.53}$$

see [24]. Since $P_\beta(x,y) > 0$ for all $x, y \in \mathbb{R}^d$, we have

$$\langle f, e^{\beta\Delta} g\rangle = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} P_\beta(x,y) f(x) f(y)\, dxdy > 0 \tag{2.54}$$

for $f, g \in \mathcal{P} \setminus \{0\}$. Hence $e^{\beta\Delta} \rhd 0$ w.r.t. $\mathcal{P}$ holds for all $\beta > 0$. □

Note that the number operator N_p can be identified with

$$N_\mathrm{p} = -\frac{1}{2}\Delta + \frac{1}{2}\sum_{x\in\Lambda} q_x^2 - \frac{|\Lambda|}{2} \tag{2.55}$$

As is well-known, it holds that

$$e^{-\beta N_\mathrm{p}} \rhd 0 \text{ w.r.t. } \mathcal{P} \tag{2.56}$$

for all $\beta > 0$, see [19].

Lemma 2.39. *Let $\beta \ge 0$. It holds that*

$$|(e^{\beta\Delta} f)(x)| \le (e^{\beta\Delta}|f|)(x), \quad a.e.\ x \in \mathbb{R}^d \tag{2.57}$$

for all $f \in L^2(\mathbb{R}^d)$.

Proof. By (2.53), we have

$$\begin{aligned} |(e^{\beta\Delta} f)(x)| &= \Big| \int_{\mathbb{R}^d} P_\beta(x,y) f(y)\, dy \Big| \\ &\le \int_{\mathbb{R}^d} P_\beta(x,y) |f(y)|\, dy \\ &= (e^{\beta\Delta}|f|)(x) \end{aligned} \tag{2.58}$$

for a.e. $x \in \mathbb{R}^d$. □

By Lemma 2.39 and the Trotter product formula, we obtain the following lemma:

Lemma 2.40. *It holds that*

$$|(e^{-\beta N_\mathrm{p}} f)(x)| \le (e^{-\beta N_\mathrm{p}}|f|)(x), \quad a.e. x \in \mathbb{R}^d \tag{2.59}$$

for all $f \in L^2(\mathbb{R}^d)$ and $\beta \ge 0$.

Proof. Set

$$V = \frac{1}{2}\sum_{x\in\Lambda} q_x^2 - \frac{|\Lambda|}{2}. \tag{2.60}$$

By (2.55) and the Trotter product formula, we have

$$e^{-\beta N_{\rm P}} f = \lim_{n\to\infty} \left(e^{\frac{\beta\Delta}{2n}} e^{\frac{V}{n}} \right)^n f \tag{2.61}$$

for each $f \in L^2(\mathbb{R}^d)$ and $\beta \ge 0$. Because $e^{\frac{V}{n}} \trianglerighteq 0$ w.r.t. $\mathcal{P}$ and $e^{\frac{V}{n}}$ is a multiplication operator, we see that

$$|e^{\frac{V}{n}} f| \le e^{\frac{V}{n}} |f| \tag{2.62}$$

for all $f \in L^2(\mathbb{R}^d)$ and $\beta \ge 0$. By repeatedly applying Lemma 2.39 and (2.62), we have

$$\begin{aligned} |e^{-\beta N_{\rm P}} f| &= \lim_{n\to\infty} \left| \left(e^{\frac{\beta\Delta}{2n}} e^{\frac{V}{n}} \right)^n f \right| \\ &\le \lim_{n\to\infty} \left(e^{\frac{\beta\Delta}{2n}} e^{\frac{V}{n}} \right)^n |f| \\ &= e^{-\beta N_{\rm P}} |f| \end{aligned} \tag{2.63}$$

for all $f \in L^2(\mathbb{R}^d)$ and $\beta \ge 0$. □

This lemma will play an important role in Section 4.

2.2.5 A Hilbert cone in $\mathcal{X} \otimes L^2(\mathbb{R}^d)$

The Hilbert cone defined in this section is important when we investigate the KLM with the electron-phonon interaction. Let $\mathcal{C}$ be a Hilbert cone in a Hilbert space $\mathcal{X}$.

We can identify $\mathcal{X} \otimes L^2(\mathbb{R}^d)$ with $L^2(\mathbb{R}^d, d\mu; \mathcal{X})$ which is the set of all $\mathcal{X}$-valued square integrable functions on $\mathbb{R}^d$. By considering $\psi \in L^2(\mathbb{R}^d, d\mu; \mathcal{X})$ as $\psi = (\psi(x))_{x\in\mathbb{R}^d}$, we can think of $L^2(\mathbb{R}^d, d\mu; \mathcal{X})$ as a direct sum of $\mathcal{X}$. With this in mind, we write

$$L^2(\mathbb{R}^d, d\mu; \mathcal{X}) = \int_{\mathbb{R}^d}^{\oplus} \mathcal{X}\, d\mu \tag{2.64}$$

and call it the *constant fiber direct integral.*

Definition 2.41. We define $\mathcal{Q} \subset \mathcal{X} \otimes L^2(\mathbb{R}^d)$ by

$$\mathcal{Q} = \int_{\mathbb{R}^d}^{\oplus} \mathcal{C}\, d\boldsymbol{q}, \tag{2.65}$$

where the direct integral $\mathcal{C}$ over $\mathbb{R}^d$ is given by

$$\int_{\mathbb{R}^d}^{\oplus} \mathcal{C}\, d\boldsymbol{q} = \{\Phi \in \mathcal{X} \otimes L^2(\mathbb{R}^d) \,|\, \Phi(\boldsymbol{q}) \in \mathcal{C} \text{ a.e. } \boldsymbol{q}\} \tag{2.66}$$

Lemma 2.42. *$\mathcal{Q}$ is a Hilbert cone in $\mathcal{X} \otimes L^2(\mathbb{R}^d)$.*

Proof. We readily confirm that $\mathcal{Q}$ is a closed set. For any $\Phi, \Phi' \in \mathcal{Q}$, we have $\Phi(\boldsymbol{q}), \Phi'(\boldsymbol{q}) \in \mathcal{C}$ a.e. $\boldsymbol{q}$, which implies that

$$\langle \Phi, \Phi' \rangle = \int_{\mathbb{R}^d} \langle \Phi(\boldsymbol{q}), \Phi'(\boldsymbol{q}) \rangle \, d\boldsymbol{q} \geq 0. \tag{2.67}$$

For all $\Phi \in \mathcal{X} \otimes L^2(\mathbb{R}^d)$, there are $\Phi_i(\boldsymbol{q}) \in \mathcal{C}, i = 1, \dots, 4$ satisfying

$$\Phi(\boldsymbol{q}) = \Phi_1(\boldsymbol{q}) - \Phi_2(\boldsymbol{q}) + i(\Phi_3(\boldsymbol{q}) - \Phi_4(\boldsymbol{q})), \tag{2.68}$$
$$\langle \Phi_1(\boldsymbol{q}), \Phi_2(\boldsymbol{q}) \rangle = \langle \Phi_3(\boldsymbol{q}), \Phi_4(\boldsymbol{q}) \rangle = 0. \tag{2.69}$$

Thus we have $\Phi_i \in \mathcal{Q}, \Phi = \Phi_1 - \Phi_2 + i(\Phi_3 - \Phi_4)$ and $\langle \Phi_1, \Phi_2 \rangle = \langle \Phi_3, \Phi_4 \rangle = 0$. Therefore, $\mathcal{Q}$ is a Hilbert cone. □

The Hilbert cone $\mathcal{Q}$ can be expressed as follows.

Proposition 2.43. *Set*

$$\mathcal{Q}_0 = \text{coni}\{\psi \otimes f \in \mathcal{X} \otimes L^2(\mathbb{R}^d) \,|\, \psi \in \mathcal{C}, f \in \mathcal{P}\}. \tag{2.70}$$

One obtains that $\mathcal{Q} = \overline{\mathcal{Q}_0}$.

Proof. See Appendix D. □

The following proposition is useful in proving the Theorem 1.6.

Proposition 2.44. *Let* $A \in \mathscr{B}(\mathcal{X} \otimes L^2(\mathbb{R}^d))$. *If* $\langle \varphi \otimes f, A\psi \otimes g \rangle \geq 0$ *for all* $\varphi, \psi \in \mathcal{C}, f, g \in \mathcal{P}$, *then we have* $A \trianglerighteq 0$ *w.r.t.* $\mathcal{Q}$.

Proof. From Proposition 2.43, for any $u, v \in \mathcal{Q}$, there exist $u_i, v_i \in \mathcal{Q}_0$ such that $u = \lim_{i\to\infty} u_i$ and $v = \lim_{i\to\infty} v_i$. By the definition of $\mathcal{Q}_0$, there exist $\varphi_n^{(i)}, \psi_n^{(i)} \in \mathcal{C}$ and $f_n^{(i)}, g_n^{(i)} \in \mathcal{P}$ such that

$$u_i = \sum_{n\geq 1} \varphi_n^{(i)} \otimes f_n^{(i)}, \quad v_i = \sum_{n\geq 1} \psi_n^{(i)} \otimes g_n^{(i)}. \tag{2.71}$$

Then we obtain

$$\langle u, Av \rangle = \lim_{i\to\infty} \langle u_i, Av_i \rangle = \sum_{m,n\geq 1} \langle \varphi_m^{(i)} \otimes f_m^{(i)}, A\psi_n^{(i)} \otimes g_n^{(i)} \rangle \geq 0. \tag{2.72}$$

Hence, we have $A \trianglerighteq 0$ w.r.t. $\mathcal{Q}$. □

Lemma 2.45. *Let* $A \in \mathscr{B}(\mathcal{X} \otimes L^2(\mathbb{R}^d))$ *be a decomposable operator:*

$$A = \int_{\mathbb{R}^d}^{\oplus} A(\boldsymbol{q}) \, d\boldsymbol{q}. \tag{2.73}$$

If $A(\boldsymbol{q}) \trianglerighteq 0$ *w.r.t.* $\mathcal{C}$ *a.e.*$\boldsymbol{q}$, *then we have* $A \trianglerighteq 0$ *w.r.t.* $\mathcal{Q}$.

Proof. Let $\varphi, \psi \in \mathcal{C}, f, g \in \mathcal{P}$. Then we have

$$\langle \varphi \otimes f, A\psi \otimes g \rangle = \int_{\mathbb{R}^d} f(\boldsymbol{q}) g(\boldsymbol{q}) \langle \varphi, A(\boldsymbol{q})\psi \rangle \, d\boldsymbol{q}. \tag{2.74}$$

Since $A(\boldsymbol{q}) \trianglerighteq 0$ w.r.t. $\mathcal{C}$ a.e. $\boldsymbol{q}$, we see $\langle \varphi, A(\boldsymbol{q})\psi \rangle \geq 0$ a.e. $\boldsymbol{q}$, which implies $\langle \varphi \otimes f, A\psi \otimes g \rangle \geq 0$. By Proposition 2.44, $A \trianglerighteq 0$ w.r.t. $\mathcal{Q}$ holds. □

Remark 2.46. In Section 4, this proposition plays an important role when we show that semigroup generated by the Hamiltonian H is positivity preserving.

3 The Kondo lattice model

3.1 Main result in Section 3

The aim of this section is to prove Theorem 1.4. The proof is achieved by showing the following two theorems.

The first theorem is a claim about the uniqueness of the ground states and the spin structure of the ground states.

Theorem 3.1. *Assume* $(\mathbf{C_0})$.

(i) *The ground state of* $H_{\rm KL}$ *is unique.*

(ii) *We denote by* ψ *the ground state of* $H_{\rm KL}$. *Then* ψ *satisfy the following:*

$$\gamma_x\gamma_y\langle\psi, s_x^+s_y^-\psi\rangle > 0, \quad \gamma_u\gamma_v {\rm sgn} J_{x,u}{\rm sgn}J_{y,v}\langle\psi, S_u^+S_v^-\psi\rangle > 0 \tag{3.1}$$

for every $x, y\in\Lambda$ *and* $u, v\in\Omega$.

The proof of Theorem 3.1 will be provided in Section 3.5.3. The second theorem is a claim about the total spin of the ground state.

Theorem 3.2. *Assume* $(\mathbf{C_0})$. *Let* ψ *be the ground state of* $H_{\rm KL}$.

(i) *If* **(C.6)** *holds, then* ψ *has total spin* $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$.

(ii) *If* **(C.7)** *holds, then* ψ *has total spin* $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_2| - |\Lambda_2| - |\Omega_1|\big|$.

The proof of Theorem 3.2 will be given in Section 3.6.

3.2 Preliminary I: A Hilbert cone

In this section, we will define the Hilbert cone, which is necessary to analyze the Kondo lattice model. For this purpose, we introduce some symbols.

Let $\mathsf{c}_x, \mathsf{f}_u$ be the annihilation operators on $\mathscr{F}_{\rm F}(\ell^2(\Lambda)\oplus\ell^2(\Omega))$ satisfying

$$\{\mathsf{c}_x^*, \mathsf{c}_y\} = \delta_{x,y} \quad x, y\in\Lambda, \quad \{\mathsf{f}_u^*, \mathsf{f}_v\} = \delta_{u,v} \quad u, v\in\Omega \tag{3.2}$$

and

$$\{\mathsf{c}_x^*, \mathsf{f}_u\} = \{\mathsf{c}_x, \mathsf{f}_u\} = 0. \tag{3.3}$$

Note that $c_{x\sigma}$ and $f_{u\sigma}$ can be rewritten as

$$c_{x\uparrow} = \mathsf{c}_x\otimes 1, \quad f_{u\uparrow} = \mathsf{f}_u\otimes 1, \quad c_{x\downarrow} = (-1)^{\mathsf{N}}\otimes\mathsf{c}_x, \quad f_{u\downarrow} = (-1)^{\mathsf{N}}\otimes\mathsf{f}_u, \tag{3.4}$$

where N is the number operator given by

$$\mathsf{N} = \sum_{x\in\Lambda}\mathsf{n}_x^c + \sum_{u\in\Omega}\mathsf{n}_u^f \tag{3.5}$$

with $\mathsf{n}_x^c = \mathsf{c}_x^*\mathsf{c}_x$ and $\mathsf{n}_u^f = \mathsf{f}_u^*\mathsf{f}_u$. Using (2.41), we obtain the fundamental identifications:

$$c_{x\uparrow} = \mathcal{L}(\mathsf{c}_x), \quad c_{x\downarrow} = \mathcal{L}\big((-1)^{\mathsf{N}}\big)\mathcal{R}(\mathsf{c}_x^*), \quad f_{u\uparrow} = \mathcal{L}(\mathsf{f}_u), \quad f_{u\downarrow} = \mathcal{L}\big((-1)^{\mathsf{N}}\big)\mathcal{R}(\mathsf{f}_u^*). \tag{3.6}$$

From these formulas, we can freely produce useful formulas. For instance,

$$n^c_{x\uparrow} = \mathcal{L}(\mathsf{n}^c_x), \quad n^c_{x\downarrow} = \mathcal{R}(\mathsf{n}^c_x), \quad n^f_{u\uparrow} = \mathcal{L}(\mathsf{n}^f_u), \quad n^f_{u\downarrow} = \mathcal{R}(\mathsf{n}^f_u). \tag{3.7}$$

Set $E_\Lambda = \{0,1\}^\Lambda$ and $E_\Omega = \{0,1\}^\Omega$. For $\boldsymbol{\sigma}_c = (\sigma_{c,x})_{x\in\Lambda} \in E_\Lambda, \boldsymbol{\sigma}_f = (\sigma_{f,u})_{u\in\Omega} \in E_\Omega$, define

$$|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f\rangle = \prod_{x\in\Lambda}{}' (\mathsf{c}^*_x)^{\sigma_{c,x}} \prod_{u\in\Omega}{}' (\mathsf{f}^*_u)^{\sigma_{f,u}} |0\rangle_c \otimes |0\rangle_f, \tag{3.8}$$

where $|0\rangle_c \in \mathscr{F}_{\mathrm{F}}(\ell^2(\Lambda))$ and $|0\rangle_f \in \mathscr{F}_{\mathrm{F}}(\ell^2(\Omega))$ are the Fock vacuums, and $\prod'_{x\in\Lambda}$ and $\prod'_{u\in\Omega}$ indicate ordered products according to arbitrarily fixed orders in Λ and Ω respectively. We see that $\{|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f\rangle\}_{\sigma_c\in E_\Lambda, \sigma_f\in E_\Omega}$ is a CONS of $\mathscr{F}_{\mathrm{F}}(\ell^2(\Lambda)\oplus\ell^2(\Omega))$.

Definition 3.3. The antiunitary operator ϑ on $\mathscr{F}_{\mathrm{F}}(\ell^2(\Lambda)\oplus\ell^2(\Omega))$ is defined by

$$\vartheta\Bigg(\sum_{\sigma_c\in E_\Lambda, \sigma_f\in E_\Omega} c_{\sigma_c,\sigma_f} |\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f\rangle\Bigg) = \sum_{\sigma_c\in E_\Lambda, \sigma_f\in E_\Omega} \overline{c_{\sigma_c,\sigma_f}} |\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f\rangle \tag{3.9}$$

where $c_{\sigma_c,\sigma_f} \in \mathbb{C}$.

Lemma 3.4. *For each $x \in \Lambda$ and $u \in \Omega$, we have*

$$\vartheta \mathsf{c}_x \vartheta^* = \mathsf{c}_x, \quad \vartheta \mathsf{f}_u \vartheta^* = \mathsf{f}_u. \tag{3.10}$$

Proof. Let $\boldsymbol{\sigma}_c = (\sigma_{c,x})_{x\in\Lambda} \in E_\Lambda, \boldsymbol{\sigma}_f = (\sigma_{f,u})_{u\in\Omega} \in E_\Omega$. By the definition of ϑ, we have

$$\vartheta \mathsf{c}_x \vartheta^* |\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f\rangle = \vartheta \mathsf{c}_x |\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f\rangle = \mathsf{c}_x |\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f\rangle. \tag{3.11}$$

Similarly, we obtain $\vartheta \mathsf{f}_u \vartheta^* = \mathsf{f}_u$. □

Define $\mathcal{F}_N = \wedge^{N/2}(\ell^2(\Lambda)\oplus\ell^2(\Omega))$ and

$$Q_0 = \prod_{u\in\Omega}\Big[n^f_{u,\uparrow} n^f_{u,\downarrow} + (1 - n^f_{u,\uparrow})(1 - n^f_{u,\downarrow})\Big]. \tag{3.12}$$

We are ready to introduce the Hilbert cone which is necessary for our analysis.

Definition 3.5. Set $\mathcal{E}_{\mathrm{KL}} = \Psi_\vartheta^{-1}(\mathscr{I}_+(\mathcal{F}_N))$. Define

$$\mathcal{Q}_{\mathrm{KL}} = Q_0 \mathcal{E}_{\mathrm{KL}}. \tag{3.13}$$

By the Proposition 2.34, $\mathcal{Q}_{\mathrm{KL}}$ is a Hilbert cone.

3.3 Preliminary II: The hole-particle transformation

In order to properly apply the theory given in Section 2, we introduce the hole-particle transformation in this subsection. Furthermore, we investigate in detail how the Hamiltonian H_{KL} is transformed by the hole-particle transformation.

Lemma 3.6. *There exists a unitary operator U such that*

$$U^* c_{x,\uparrow} U = c_{x,\uparrow}, \quad U^* f_{u,\uparrow} U = f_{u,\uparrow}, \quad U^* c_{x,\downarrow} U = \gamma_x c_{x,\downarrow}^*, \quad U^* f_{u,\downarrow} U = \gamma_u \mathrm{sgn} J_{x,u} f_{u,\downarrow}^*, \tag{3.14}$$

where

$$\gamma_z = \begin{cases} -1 & (z \in \Lambda_1 \text{ or } z \in \Omega_1) \\ 1 & (z \in \Lambda_2 \text{ or } z \in \Omega_2), \end{cases} \tag{3.15}$$

and $\mathrm{sgn} J_{x,u}$ *is defined in the assumption* **(C.2)**.

Proof. Let U_1 be the unitary operator on $\mathcal{H}_{\mathrm{c}}$ such that

$$U_1^* c_{x\uparrow} U_1 = c_{x\uparrow}, \quad U_1^* c_{x\downarrow} U_1 = \gamma_x c_{x\downarrow}^*. \tag{3.16}$$

Note that U_1 is the standard hole-particle transformation on $\mathcal{H}_{\mathrm{c}}$.

By **(C.2)**, for any $u \in \Omega$, there exists an $x_u \in \Lambda$ satisfying $J_{x_u,u} \neq 0$. Note that $\mathrm{sgn} J_{x_u,u}$ is independent of the choice of x_u. Let U_2 be the unitary operator on $\mathcal{H}_{\mathrm{f}}$ such that

$$U_2^* f_{u\uparrow} U_2 = f_{u\uparrow}, \quad U_2^* f_{u\downarrow} U_2 = \gamma_u \mathrm{sgn} J_{x_u,u} f_{u\downarrow}^*. \tag{3.17}$$

Choosing $U = U_1 \otimes U_2$, we readily confirm that U satisfies the desired properties in (3.14). □

By the definition of P_0, we have $U^* P_0 U = Q_0$.

Lemma 3.7.

$$U^* H_{\mathrm{KL}} U = \mathbb{T} - \mathbb{J} + \frac{1}{4} \sum_{x\in\Lambda, u\in\Omega} J_{x,u} (n_x^c - 1)(n_u^f - 1) \tag{3.18}$$

where

$$\mathbb{J} = \frac{1}{2} \sum_{x\in\Lambda, u\in\Omega} |J_{x,u}| \big(c_{x,\uparrow}^* f_{u,\uparrow} c_{x,\downarrow}^* f_{u,\downarrow} + f_{u,\uparrow}^* c_{x,\uparrow} f_{u,\downarrow}^* c_{x,\downarrow} \big). \tag{3.19}$$

Proof. By **(C.1)** and the definition of U, we have

$$U^* \mathbb{T} U = \mathbb{T}. \tag{3.20}$$

From **(C.2)** and **(C.4)**, it holds that

$$\begin{aligned} & U^* \sum_{x\in\Lambda, u\in\Omega} J_{x,u} \boldsymbol{s}_x \cdot \boldsymbol{S}_u U \\ &= \sum_{x\in\Lambda, u\in\Omega} J_{x,u} U^* \Big(\frac{1}{2} s_x^+ S_u^- + \frac{1}{2} s_x^- S_u^+ + s_x^{(3)} S_u^{(3)} \Big) U \\ &= \sum_{x\in\Lambda, u\in\Omega} J_{x,u} U^* \Big(\frac{1}{2} c_{x,\uparrow}^* c_{x,\downarrow} f_{u,\downarrow}^* f_{u,\uparrow} + \frac{1}{2} c_{x,\downarrow}^* c_{x,\uparrow} f_{u,\uparrow}^* f_{u,\downarrow} + \frac{1}{4} (n_{x,\uparrow}^c - n_{x,\downarrow}^c)(n_{u,\uparrow}^f - n_{u,\downarrow}^f) \Big) U \\ &= -\frac{1}{2} \sum_{x\in\Lambda, u\in\Omega} |J_{x,u}| \big(c_{x,\uparrow}^* f_{u,\uparrow} c_{x,\downarrow}^* f_{u,\downarrow} + f_{u,\uparrow}^* c_{x,\uparrow} f_{u,\downarrow}^* c_{x,\downarrow} \big) + \frac{1}{4} \sum_{x\in\Lambda, u\in\Omega} J_{x,u} (n_x^c - 1)(n_u^f - 1). \end{aligned} \tag{3.21}$$

□

3.4 Positivity preservingness of the semigroup

In this subsection, we show that the heat semigroup generated by the hole-particle transformed Hamiltonian $U^* H_{\mathrm{KL}} U$ is positivity preserving with respect to $\mathcal{Q}_{\mathrm{KL}}$.

First, we prove the following useful lemmas.

Lemma 3.8. *Let $A, B \in \mathscr{B}(\mathcal{F}_N)$. Assume that $A \otimes 1 + 1 \otimes \vartheta A \vartheta$ and $B \otimes \vartheta B \vartheta$ commute with Q_0. Then we have*

$$\exp\{(A \otimes 1 + 1 \otimes \vartheta A \vartheta) \restriction Q_0 \mathcal{L}_N\} \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}}, \tag{3.22}$$

$$B \otimes \vartheta B \vartheta \restriction Q_0 \mathcal{L}_N \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}}. \tag{3.23}$$

Proof. Using Proposition 2.32, we have

$$e^{A \otimes 1 + 1 \otimes \vartheta A \vartheta} = e^A \otimes \vartheta e^A \vartheta \trianglerighteq 0 \text{ w.r.t. } \mathcal{E}_{\mathrm{KL}}, \tag{3.24}$$

$$B \otimes \vartheta B \vartheta \trianglerighteq 0 \text{ w.r.t. } \mathcal{E}_{\mathrm{KL}}. \tag{3.25}$$

Thus, applying Lemma 2.35, we obtain the desired results. □

Proposition 3.9. *Set $H'_{\mathrm{KL}} = U^* H_{\mathrm{KL}} U$. We have*

$$e^{-\beta H'_{\mathrm{KL}}} \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}} \tag{3.26}$$

for all $\beta \geq 0$.

Proof. Set

$$X = \mathbb{T} + \frac{1}{4} \sum_{x \in \Lambda, u \in \Omega} J_{x,u} (n_x^c - 1)(n_u^f - 1) \tag{3.27}$$

and

$$\mathsf{T} = -\sum_{x,y \in \Lambda} t_{x,y} \mathsf{c}_x^* \mathsf{c}_y + \sum_{x \in \Lambda, u \in \Omega} J_{x,u} (2\mathsf{n}_x^c \mathsf{n}_u^f - \mathsf{n}_x^c - \mathsf{n}_u^f + 1/2). \tag{3.28}$$

Since $n_{u,\uparrow}^f = n_{u,\downarrow}^f$ on $\mathrm{ran}(Q_0)$, the range of Q_0, we have

$$e^{-\beta X} = e^{-\beta \mathsf{T}} \otimes \vartheta e^{-\beta \mathsf{T}} \vartheta^* \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}} \tag{3.29}$$

by Lemma 2.35. Similarly, we can show that $\mathbb{J} \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$. By using the Duhamel formula, we obtain

$$\begin{aligned} & e^{-\beta H'_{\mathrm{KL}}} \\ &= e^{-\beta X} + \sum_{n \geq 1} \beta^n \int_{0 < s_1 < \cdots < s_n < 1} e^{-s_1 \beta X} \mathbb{J} \cdots \mathbb{J} e^{-(1-s_n)\beta X} \, ds_n \cdots ds_1 \\ &\trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}}. \end{aligned} \tag{3.30}$$

□

A role of Proposition 3.9 is as follows: We wish to employ Theorem 2.17 (the Perron–Frobenius–Faris theorem) to prove the the uniqueness of the ground state of the Hamiltonian. Proposition 3.9 is a basic input in order to apply Theorem 2.17.

3.5 The uniqueness of ground states

In this section, we will prove the uniqueness of the ground states by using Theorem 2.17.

3.5.1 Some operator inequalities

For later use, we will prove some operator inequalities here.

Let

$$F = \{(x,u) \in \Lambda \times \Omega \,|\, J_{x,u} \neq 0\}, \tag{3.31}$$
$$F_x = \{u \in \Omega \,|\, J_{x,u} = 0\}. \tag{3.32}$$

Lemma 3.10. *We have the following equalities:*

(i)

$$\begin{aligned} N = 2\sum_{u\in\Omega} n_{u\uparrow}^f n_{u\downarrow}^f + \sum_{x\in\Lambda}\sum_{u\in F_x} |F_x|^{-1}(n_{x\uparrow}^c + n_{x\downarrow}^c) n_{u\uparrow}^f n_{u\downarrow}^f \\ + \sum_{x\in\Lambda}\sum_{u\in F_x} |F_x|^{-1}(n_{x\uparrow}^c + n_{x\downarrow}^c)(1-n_{u\uparrow}^f)(1-n_{u\downarrow}^f). \end{aligned} \tag{3.33}$$

(ii)

$$\begin{aligned} &n_{x\uparrow}^c(1-n_{u\uparrow}^f)n_{x\downarrow}^c(1-n_{u\downarrow}^f) + (1-n_{x\uparrow}^c)n_{u\uparrow}^f(1-n_{x\downarrow}^c)n_{u\downarrow}^f + (n_{x\uparrow}^c + n_{x\downarrow}^c)n_{u\uparrow}^f n_{u\downarrow}^f \\ &= n_{x\uparrow}^c n_{x\downarrow}^c + n_{u\uparrow}^f n_{u\downarrow}^f. \end{aligned} \tag{3.34}$$

(iii)

$$\begin{aligned} &n_{x\uparrow}^c(1-n_{u\uparrow}^f)n_{x\downarrow}^c(1-n_{u\downarrow}^f) + (1-n_{x\uparrow}^c)n_{u\uparrow}^f(1-n_{x\downarrow}^c)n_{u\downarrow}^f \\ &\quad + (n_{x\uparrow}^c + n_{x\downarrow}^c)(1-n_{u\uparrow}^f)(1-n_{u\downarrow}^f) + 1 \\ &= (1+n_{x\uparrow}^c)(1+n_{x\downarrow}^c)(1-n_{u\uparrow}^f)(1-n_{u\downarrow}^f) + n_{u\uparrow}^f n_{u\downarrow}^f + (1-n_{x\uparrow}^c)n_{u\uparrow}^f(1-n_{x\downarrow}^c)n_{u\downarrow}^f. \end{aligned} \tag{3.35}$$

Proof. By the definition of Q_0, i.e., (3.12), we have

$$n_{u\uparrow}^f = n_{u\downarrow}^f, \tag{3.36}$$
$$1 = n_{u\uparrow}^f n_{u\downarrow}^f + (1-n_{u\uparrow}^f)(1-n_{u\downarrow}^f) \tag{3.37}$$

on $Q_0\mathcal{L}_N$.

(i) Recalling that $N_e = N$ on $\mathcal{Q}_{KL}$, we obtain

$$\begin{aligned} N &= N_e \\ &= \sum_{x\in\Lambda}(n_{x\uparrow}^c + n_{x\downarrow}^c) + \sum_{u\in\Omega}(n_{u\uparrow}^f + n_{u\downarrow}^f) \\ &= \sum_{x\in\Lambda}\sum_{u\in F_x}|F_x|^{-1}(n_{x\uparrow}^c + n_{x\downarrow}^c)\{n_{u\uparrow}^f n_{u\downarrow}^f + (1-n_{u\uparrow}^f)(1-n_{u\downarrow}^f)\} + 2\sum_{u\in\Omega} n_{u\uparrow}^f n_{u\downarrow}^f \\ &= \text{the right hand side of (3.33)}. \end{aligned} \tag{3.38}$$

In the third equality, we have used (3.36) and (3.37).

(ii) We observe

$$
\begin{aligned}
&n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow})+(1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}+(n^c_{x\uparrow}+n^c_{x\downarrow})n^f_{u\uparrow}n^f_{u\downarrow}\\
&=n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow})+(1+n^c_{x\uparrow}n^c_{x\downarrow})n^f_{u\uparrow}n^f_{u\downarrow}\\
&\overset{(3.37)}{=} n^c_{x\uparrow}n^c_{x\downarrow}+n^f_{u\uparrow}n^f_{u\downarrow}.
\end{aligned}
\tag{3.39}
$$

(iii) We have

$$
\begin{aligned}
&n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow})+(1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}+(n^c_{x\uparrow}+n^c_{x\downarrow})(1-n^f_{u\uparrow})(1-n^f_{u\downarrow})+1\\
&\overset{(3.37)}{=}(1+n^c_{x\uparrow}+n^c_{x\downarrow}+n^c_{x\uparrow}n^c_{x\downarrow})(1-n^f_{u\uparrow})(1-n^f_{u\downarrow})+n^f_{u\uparrow}n^f_{u\downarrow}+(1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}\\
&=(1+n^c_{x\uparrow})(1+n^c_{x\downarrow})(1-n^f_{u\uparrow})(1-n^f_{u\downarrow})+n^f_{u\uparrow}n^f_{u\downarrow}+(1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}.
\end{aligned}
\tag{3.40}
$$

□

The following proposition is essential for the proof of Theorem 3.1 and Theorem 4.1:

Proposition 3.11. *One obtains*

$$
\frac{8}{J^2}\{JN+\mathbb{J}\}^2 \trianglerighteq \sum_{x\in\Lambda} n^c_{x\uparrow}n^c_{x\downarrow}+\sum_{u\in\Omega} n^f_{u\uparrow}n^f_{u\downarrow} \trianglerighteq 0 \ \textit{w.r.t.}\ \mathcal{Q}_{\mathrm{KL}},
\tag{3.41}
$$

where $J=\min_{(x,u)\in F}|J_{x,u}|$.

Proof. Let $V_{x,u}=c^*_{x\uparrow}f_{u\uparrow}c^*_{x\downarrow}f_{u\downarrow}$. Then we have

$$
V_{x,u}V^*_{x,u}+V^*_{x,u}V_{x,u}=n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow})+(1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}.
\tag{3.42}
$$

Because of Lemma 3.8, it holds that $V_{x,u}\trianglerighteq 0$ and $V^*_{x,u}\trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$. Hence, we find

$$
\begin{aligned}
\mathbb{J}^2 &\trianglerighteq \frac{1}{4}\sum_{x\in\Lambda,u\in\Omega}|J_{x,u}|^2\left(V_{x,u}+V^*_{x,u}\right)^2\\
&\trianglerighteq \frac{J^2}{4}\sum_{(x,u)\in F}\left(V_{x,u}V^*_{x,u}+V^*_{x,u}V_{x,u}\right)\\
&\overset{(3.42)}{=}\frac{J^2}{4}\sum_{(x,u)\in F}\left\{n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow})+(1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}\right\}\ \text{w.r.t.}\ \mathcal{Q}_{\mathrm{KL}}.
\end{aligned}
\tag{3.43}
$$

Using $\sum_{(x,u)\in F} = \sum_{x\in\Lambda}\sum_{u\in F_x}$ and recalling that $N = |\Lambda| + |\Omega|$, we obtain

$$
\begin{aligned}
&2\sum_{(x,u)\in F}\Big\{n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow}) + (1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}\Big\} + 2(|\Lambda|+|\Omega|)\\
&\overset{(3.33)}{=} 2\sum_{(x,u)\in F}\Big\{n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow}) + (1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}\Big\}\\
&\quad + |\Lambda| + |\Omega| + 2\sum_{u\in\Omega} n^f_{u\uparrow}n^f_{u\downarrow} + \sum_{x\in\Lambda}\sum_{u\in F_x}|F_x|^{-1}(n^c_{x\uparrow}+n^c_{x\downarrow})n^f_{u\uparrow}n^f_{u\downarrow}\\
&\quad + \sum_{x\in\Lambda}\sum_{u\in F_x}|F_x|^{-1}(n^c_{x\uparrow}+n^c_{x\downarrow})(1-n^f_{u\uparrow})(1-n^f_{u\downarrow})\\
&\overset{(3.34)}{\trianglerighteq} \sum_{x\in\Lambda}\sum_{u\in F_x}|F_x|^{-1}\left(n^c_{x\uparrow}n^c_{x\downarrow} + n^f_{u\uparrow}n^f_{u\downarrow}\right) + |\Lambda| + 2\sum_{u\in\Omega} n^f_{u\uparrow}n^f_{u\downarrow}\\
&\quad + \sum_{x\in\Lambda}\sum_{u\in F_x}|F_x|^{-1}(n^c_{x\uparrow}+n^c_{x\downarrow})(1-n^f_{u\uparrow})(1-n^f_{u\downarrow})\\
&\quad + \sum_{(x,u)\in F}\Big\{n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow}) + (1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}\Big\}\\
&\trianglerighteq \sum_{x\in\Lambda} n^c_{x\uparrow}n^c_{x\downarrow} + \sum_{u\in\Omega} n^f_{u\uparrow}n^f_{u\downarrow} + \sum_{x\in\Lambda}\sum_{u\in F_x}|F_x|^{-1}\Big\{(n^c_{x\uparrow}+n^c_{x\downarrow})(1-n^f_{u\uparrow})(1-n^f_{u\downarrow})\\
&\quad + n^c_{x\uparrow}(1-n^f_{u\uparrow})n^c_{x\downarrow}(1-n^f_{u\downarrow}) + (1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow} + 1\Big\}\\
&\overset{(3.35)}{=} \sum_{x\in\Lambda} n^c_{x\uparrow}n^c_{x\downarrow} + \sum_{u\in\Omega} n^f_{u\uparrow}n^f_{u\downarrow} +\\
&\quad + \sum_{x\in\Lambda}\sum_{u\in F_x}|F_x|^{-1}\Big\{(1+n^c_{x\uparrow})(1+n^c_{x\downarrow})(1-n^f_{u\uparrow})(1-n^f_{u\downarrow}) + n^f_{u\uparrow}n^f_{u\downarrow}\\
&\quad + (1-n^c_{x\uparrow})n^f_{u\uparrow}(1-n^c_{x\downarrow})n^f_{u\downarrow}\Big\}\\
&\trianglerighteq \sum_{x\in\Lambda} n^c_{x\uparrow}n^c_{x\downarrow} + \sum_{u\in\Omega} n^f_{u\uparrow}n^f_{u\downarrow} \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}}.
\end{aligned}
\tag{3.44}
$$

Hence, we get

$$
\frac{8}{J^2}\{JN + \mathbb{J}\}^2 \trianglerighteq \frac{8}{J^2}\mathbb{J}^2 + 2(|\Lambda|+|\Omega|) \trianglerighteq \sum_{x\in\Lambda} n^c_{x\uparrow}n^c_{x\downarrow} + \sum_{u\in\Omega} n^f_{u\uparrow}n^f_{u\downarrow} \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}}, \tag{3.45}
$$

where we have used the fact $\mathbb{J} \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$ in the first inequality. □

Remark 3.12. From Proposition 3.11, we can see that $\mathbb{J}$ contained in H'_{KL} has the same role as the Coulomb interaction in the Hubbard model in showing the uniqueness of the ground states. Compare Proposition 3.11 with Lemma C.9 in Appendix C.

3.5.2 The positivity improvingness of the semigroup

For later use, we introduce a useful complete orthonormal system(CONS) in $\mathcal{H}_{\mathrm{c}} \otimes \mathcal{H}_{\mathrm{f}}$ as follows: For $\boldsymbol{\sigma}_c \in E_\Lambda$, we define

$$
\boldsymbol{c}^*_\uparrow(\boldsymbol{\sigma}_c) = \prod_{x\in\Lambda}{}' (c^*_{x,\uparrow})^{\sigma_{c,x}}, \quad \boldsymbol{c}^*_\downarrow(\boldsymbol{\sigma}_c) = \prod_{x\in\Lambda}{}' (c^*_{x,\downarrow})^{\sigma_{c,x}}. \tag{3.46}
$$

$\prod'_{x\in\Lambda}$ indicates the ordered product according to an arbitrarily fixed order in Λ as in Subsection 3.2. Similarly, for $\boldsymbol{\sigma}_f \in E_\Omega$, we define $\boldsymbol{f}^*_\uparrow(\boldsymbol{\sigma}_f)$ and $\boldsymbol{f}^*_\downarrow(\boldsymbol{\sigma}_f)$. Given $\boldsymbol{\sigma}_c, \boldsymbol{\sigma}'_c \in E_\Lambda$ and $\boldsymbol{\sigma}_f, \boldsymbol{\sigma}'_f \in E_\Omega$, let

$$|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}'_f\rangle = \boldsymbol{c}^*_\uparrow(\boldsymbol{\sigma}_c)\boldsymbol{c}^*_\downarrow(\boldsymbol{\sigma}'_c)\boldsymbol{f}^*_\uparrow(\boldsymbol{\sigma}_f)\boldsymbol{f}^*_\downarrow(\boldsymbol{\sigma}'_f)|0\rangle \in \mathcal{H}_\mathrm{c}\otimes\mathcal{H}_\mathrm{f}. \tag{3.47}$$

We define $E_N \subset E_\Lambda \times E_\Omega$ by

$$E_N = \{(\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f) \in E_\Lambda \times E_\Omega \,|\, |\boldsymbol{\sigma}_c| + |\boldsymbol{\sigma}_f| = N/2\}, \tag{3.48}$$

where $|\boldsymbol{\sigma}_c| = \sum_{x\in\Lambda}\sigma_{c,x}$, $|\boldsymbol{\sigma}_f| = \sum_{u\in\Omega}\sigma_{f,u}$.

Lemma 3.13. *Let*

$$R = \mathbb{T} + \frac{1}{4}\sum_{x\in\Lambda, u\in\Omega} J_{x,u}(n^c_x - 1)(n^f_u - 1). \tag{3.49}$$

For each $(\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f), (\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f) \in E_N$*, we define*

$$S(t) = \left\langle \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f \middle| e^{-t(R-\frac{1}{2}\mathbb{J})} \middle| \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\right\rangle, \quad 0<t<1, \tag{3.50}$$

Assume either

(i) *there exist* $x, y \in \Lambda$ *such that* $t_{x,y} \neq 0$ *and*

$$|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f\rangle = c^*_{x,\uparrow}c_{y,\uparrow}c^*_{x,\downarrow}c_{y,\downarrow}|\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\rangle, \tag{3.51}$$

or

(ii) *there exist* $x \in \Lambda, u \in \Omega$ *such that* $J_{x,y} \neq 0$ *and*

$$|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f\rangle = (V_{x,u} + V^*_{x,u})|\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\rangle. \tag{3.52}$$

Then there exists a $\gamma > 0$ *such that if* $0<t<\gamma$*, then* $S(t) > 0$ *holds.*

Proof. Assume (i). By using the Duhamel formula, we have

$$\begin{aligned} &e^{-t(R-\frac{1}{2}\mathbb{J})}\\ &= e^{-tR} + \sum_{n\geq 1}\frac{t^n}{2^n}\int_{0\leq s_1\leq\cdots\leq s_n\leq 1} e^{-s_1 tR}\mathbb{J}\cdots\mathbb{J}e^{-(1-s_n)tR}\,ds_n\cdots ds_1\\ &\trianglerighteq e^{-tR} \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}} \end{aligned} \tag{3.53}$$

because $e^{-sR} \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$ for any $s \in \mathbb{R}$, and $\mathbb{J} \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$. Hence, we obtain

$$S(t) \geq \left\langle \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f \middle| e^{-tR} \middle| \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\right\rangle \tag{3.54}$$

By the assumption, we have

$$\langle \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f | \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\rangle = \langle \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f |R| \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\rangle = 0, \tag{3.55}$$

$$\langle \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f |R^2| \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\rangle = 2|t_{x,y}|^2. \tag{3.56}$$

Therefore,

$$\begin{aligned}
&S(t)\\
&\geq \sum_{n\geq 2}\frac{(-t)^n}{n!}\langle \boldsymbol{\sigma}_c,\boldsymbol{\sigma}_c,\boldsymbol{\sigma}_f,\boldsymbol{\sigma}_f|R^n|\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_f,\boldsymbol{\sigma}'_f\rangle\\
&=\frac{t^2}{2}\langle \boldsymbol{\sigma}_c,\boldsymbol{\sigma}_c,\boldsymbol{\sigma}_f,\boldsymbol{\sigma}_f|R^2|\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_f,\boldsymbol{\sigma}'_f\rangle+\sum_{n\geq 3}\frac{(-t)^n}{n!}\langle \boldsymbol{\sigma}_c,\boldsymbol{\sigma}_c,\boldsymbol{\sigma}_f,\boldsymbol{\sigma}_f|R^n|\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_f,\boldsymbol{\sigma}'_f\rangle\\
&\geq t^2|t_{x,y}|^2-\sum_{n\geq 3}\frac{t^n}{n!}\|R\|^n
\end{aligned}\tag{3.57}$$

holds. Set $\gamma=\min\{1,|t_{x,y}|^2e^{-\|R\|}\}$. Then for $0<t<\gamma$, we have

$$S(t)\geq t^2|t_{x,y}|^2-t^3e^{\|R\|}=t^2(|t_{x,y}|^2-te^{\|R\|})>0. \tag{3.58}$$

Assume (ii). By the assumption,

$$\begin{aligned}
\langle \boldsymbol{\sigma}_c,\boldsymbol{\sigma}_c,\boldsymbol{\sigma}_f,\boldsymbol{\sigma}_f|R^n|\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_f,\boldsymbol{\sigma}'_f\rangle&=0,\\
\langle \boldsymbol{\sigma}_c,\boldsymbol{\sigma}_c,\boldsymbol{\sigma}_f,\boldsymbol{\sigma}_f|\mathbb{J}|\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_f,\boldsymbol{\sigma}'_f\rangle&=\frac{|J_{x,u}|}{2}
\end{aligned}\tag{3.59}$$

holds for each $n\geq 0$. Therefore, we have

$$\begin{aligned}
S(t)&=\sum_{n\geq 1}\frac{t^n}{n!}\Big\langle \boldsymbol{\sigma}_c,\boldsymbol{\sigma}_c,\boldsymbol{\sigma}_f,\boldsymbol{\sigma}_f\Big|(\frac{1}{2}\mathbb{J}-R)^n\Big|\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_f,\boldsymbol{\sigma}'_f\Big\rangle\\
&=\frac{t|J_{x,u}|}{4}+\sum_{n\geq 2}\frac{t^n}{n!}\Big\langle \boldsymbol{\sigma}_c,\boldsymbol{\sigma}_c,\boldsymbol{\sigma}_f,\boldsymbol{\sigma}_f\Big|(\frac{1}{2}\mathbb{J}-R)^n\Big|\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_f,\boldsymbol{\sigma}'_f\Big\rangle\\
&\geq\frac{t|J_{x,u}|}{4}-\sum_{n\geq 2}\frac{t^n}{n!}(\frac{1}{2}\|\mathbb{J}\|+\|R\|)^n
\end{aligned}\tag{3.60}$$

Set $\gamma=\min\{1,e^{-\frac{1}{2}\|\mathbb{J}\|-\|R\|}|J_{x,u}|/4\}$. Then

$$S(t)\geq\frac{t|J_{x,u}|}{4}-t^2e^{\frac{1}{2}\|\mathbb{J}\|+\|R\|}>0 \tag{3.61}$$

holds. Thus, there is a $\gamma>0$ such that $S(t)>0$ for any $0<t<\gamma$. □

As we will see below, Lemma 3.13 plays an important role in the proof of Theorem 3.1. To properly use Lemma 3.13, the following lemma is needed.

Lemma 3.14. *For each* $(\boldsymbol{\sigma}_c,\boldsymbol{\sigma}_f),(\boldsymbol{\sigma}'_c,\boldsymbol{\sigma}'_f)\in E_N$*, there exist* $(\boldsymbol{\sigma}_{c,1},\boldsymbol{\sigma}_{f,1}),\ldots,(\boldsymbol{\sigma}_{c,n},\boldsymbol{\sigma}_{f,n})\in E_N, x_1,\ldots,x_{n+1},y_1,\ldots,y_{n+1}\in\Lambda, u_1,\ldots,u_{n+1}\in\Omega$ *such that any one of the following conditions holds for each* $j=0,1,\ldots,n$*:*

(i) $t_{x_{j+1},y_{j+1}}\neq 0$ *and*

$$\big|\boldsymbol{\sigma}_{c,j},\boldsymbol{\sigma}_{c,j},\boldsymbol{\sigma}_{f,j},\boldsymbol{\sigma}_{f,j}\big\rangle=c^*_{x_{j+1}\uparrow}c_{y_{j+1}\uparrow}c^*_{x_{j+1}\downarrow}c_{y_{j+1}\downarrow}\big|\boldsymbol{\sigma}_{c,j+1},\boldsymbol{\sigma}_{c,j+1},\boldsymbol{\sigma}_{f,j+1},\boldsymbol{\sigma}_{f,j+1}\big\rangle; \tag{3.62}$$

(ii) $J_{x_{j+1},u_{j+1}}\neq 0$ *and*

$$\big|\boldsymbol{\sigma}_{c,j},\boldsymbol{\sigma}_{c,j},\boldsymbol{\sigma}_{f,j},\boldsymbol{\sigma}_{f,j}\big\rangle=c^*_{x_{j+1}\uparrow}f_{u_{j+1}\uparrow}c^*_{x_{j+1}\downarrow}f_{u_{j+1}\downarrow}\big|\boldsymbol{\sigma}_{c,j+1},\boldsymbol{\sigma}_{c,j+1},\boldsymbol{\sigma}_{f,j+1},\boldsymbol{\sigma}_{f,j+1}\big\rangle; \tag{3.63}$$

(iii) $J_{x_{j+1},u_{j+1}} \neq 0$ *and*

$$\big|\boldsymbol{\sigma}_{c,j}, \boldsymbol{\sigma}_{c,j}, \boldsymbol{\sigma}_{f,j}, \boldsymbol{\sigma}_{f,j}\big\rangle = f^*_{u_{j+1}\uparrow} c_{x_{j+1}\uparrow} f^*_{u_{j+1}\downarrow} c_{x_{j+1}\downarrow} \big|\boldsymbol{\sigma}_{c,j+1}, \boldsymbol{\sigma}_{c,j+1}, \boldsymbol{\sigma}_{f,j+1}, \boldsymbol{\sigma}_{f,j+1}\big\rangle. \quad (3.64)$$

Proof. For readers' convenience, we provide a sketch of the proof. We divide the proof into two steps.

Step 1. Choose $\boldsymbol{\sigma}_c, \boldsymbol{\sigma}'_c \in \mathcal{S}_c$ with

$$\sum_{x\in\Lambda} \sigma_{c,x} = \sum_{x\in\Lambda} \sigma'_{c,x} = |\Lambda|/2. \quad (3.65)$$

Because the graph (Λ, E) is connected by the assumption **(C.1)**, we can prove the following: There exist $\boldsymbol{\sigma}_{c,1}, \dots, \boldsymbol{\sigma}_{c,n} \in \mathcal{S}_c, x_1 \dots, x_{n+1}, y_1, \dots, y_{n+1} \in \Lambda$ such that following (a) and (b) hold for each $j = 0, \dots, n$:

(a) $t_{x_{j+1},y_{j+1}} \neq 0$;

(b) $\big|\boldsymbol{\sigma}_{c,j}, \boldsymbol{\sigma}_{c,j}\big\rangle = c^*_{x_{j+1}\uparrow} c_{y_{j+1}\uparrow} c^*_{x_{j+1}\downarrow} c_{y_{j+1}\downarrow} \big|\boldsymbol{\sigma}_{c,j+1}, \boldsymbol{\sigma}_{c,j+1}\big\rangle$.

As for the proof, see, e.g., [6, 11, 25].

Step 2. Let $\Xi = \Lambda \cup \Omega$ and let

$$E' = \{\{x, y\} \subset \Xi \,|\, t_{x,y} \neq 0\} \cup \{\{x, u\} \subset \Xi \,|\, J_{x,u} \neq 0\}. \quad (3.66)$$

By using the assumptions **(C.1)** and **(C.4)**, the extended graph (Ξ, E') is connected. Thus, the assertion in Lemma 3.14 follows from the property stated in **Step 1**. □

In Appendix C, we prove that the heat semigroup generated by the Hamiltonian of the Hubbard model is positivity improving. The following theorem can be proved by applying the ideas of the proof of Theorem C.12 to the Kondo lattice model.

Theorem 3.15. *$e^{-\beta H'_{\mathrm{KL}}} \rhd 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$ for all $\beta > 0$.*

Proof. By applying Lemma 3.7, we have the following expression:

$$H'_{\mathrm{KL}} = U^* H_{\mathrm{KL}} U = \mathbb{T} - \mathbb{J} + \frac{1}{4} \sum_{x\in\Lambda, u\in\Omega} J_{x,u}(n^c_x - 1)(n^f_u - 1) \quad (3.67)$$

Choose $\psi, \phi \in \mathcal{Q}_{\mathrm{KL}} \setminus \{0\}$, arbitrarily. Because $\mathrm{Tr}[\Psi_\vartheta(\psi)] > 0$ and $\mathrm{Tr}[\Psi_\vartheta(\phi)] > 0$, we see that there exist $(\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f), (\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f) \in E_N$ satisfying

$$\langle \psi | \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f\rangle \neq 0, \quad \langle \phi | \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\rangle \neq 0. \quad (3.68)$$

With this in mind, we set $\psi_{\boldsymbol{\sigma}} = \langle \psi | \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f\rangle$ and $\phi_{\boldsymbol{\sigma}'} = \langle \phi | \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\rangle$. Since $\psi, \phi \in \mathcal{Q}_{\mathrm{KL}}$, it holds that $\psi_{\boldsymbol{\sigma}} > 0$ and $\phi_{\boldsymbol{\sigma}'} > 0$. By the Duhamel formula, we have

$$\begin{aligned}&\left\langle \psi, e^{-\beta H'_{\mathrm{KL}}} \phi \right\rangle \\ &= \sum_{m\geq 0} 2^{-m} \int_{0\leq s_1 \leq \cdots \leq s_m \leq \beta} \langle \psi, e^{-s_1 Y} X \cdots X e^{-(\beta - s_m)Y} \phi\rangle \, ds_m \cdots ds_1,\end{aligned} \quad (3.69)$$

where

$$X = JN + \mathbb{J}, \tag{3.70}$$

$$Y = \mathbb{T} - \frac{1}{2}\mathbb{J} + \frac{1}{4}\sum_{x\in\Lambda, u\in\Omega} J_{x,u}(n_x^c - 1)(n_u^f - 1) - \frac{1}{2}JN. \tag{3.71}$$

Since $\mathbb{J} \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\rm KL}$, we have $X \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\rm KL}$. In addition, by using arguments similar to those of the proof of Proposition 3.9, we can show that $e^{-sY} \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\rm KL}$ for each $s \ge 0$. Therefore, we obtain that

$$\langle \psi, e^{-s_1 Y} X \cdots X e^{-(\beta - s_n)Y} \phi \rangle \ge 0, \tag{3.72}$$

provided that $0 \le s_1 \le \cdots \le s_n \le \beta$. Hence, we obtain the following lower bound:

$$\begin{aligned} &\left\langle \psi, e^{-\beta H'_{\rm KL}} \phi \right\rangle \\ &\ge 2^{-m} \int_{0\le s_1 \le \cdots \le s_m \le \beta} \langle \psi, e^{-s_1 Y} X \cdots X e^{-(\beta - s_m)Y} \phi \rangle \, ds_m \cdots ds_1. \end{aligned} \tag{3.73}$$

Because the integrand of the right hand side of (3.73) is continuous in $s_1, \dots, s_m$ with $0 \le s_1 \le \cdots \le \beta$, it suffices to prove that there exist $m \in \mathbb{N}$ and $s_1, \dots, s_m \in \mathbb{R}$ with $0 \le s_1 \le \cdots \le s_m \le \beta$ satisfying

$$\langle \psi, e^{-s_1 Y} X \cdots X e^{-(\beta - s_m)Y} \phi \rangle > 0. \tag{3.74}$$

To prove (3.74), we first derive a useful operator inequality: By applying Proposition 3.11, we see that, for each $(\boldsymbol{\sigma}, \boldsymbol{\sigma}') \in E_N$,

$$\begin{aligned} \left(\frac{8}{J^2}\right)^{\frac{N}{2}} X^N &\trianglerighteq \left(\sum_{x\in\Lambda} n_{x\uparrow}^c n_{x\downarrow}^c + \sum_{u\in\Omega} n_{u\uparrow}^f n_{u\downarrow}^f\right)^{\frac{N}{2}} \\ &\trianglerighteq \left(\sum_{x\in\Lambda} n_{x\uparrow}^c n_{x\downarrow}^c\right)^{\frac{|\Lambda|}{2}} \left(\sum_{u\in\Omega} n_{u\uparrow} n_{u\downarrow}\right)^{\frac{|\Omega|}{2}} \\ &\trianglerighteq \prod_{x\in\Lambda} (n_{x\uparrow}^c n_{x\downarrow}^c)^{\sigma_x} \prod_{u\in\Omega} (n_{u\uparrow}^f n_{u\downarrow}^f)^{\sigma'_u} \\ &= |\boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle \langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'| \text{ w.r.t. } \mathcal{Q}_{\rm KL}. \end{aligned} \tag{3.75}$$

The inequality (3.75) is essential for the proof as we will see below.

Fix $k \in \mathbb{N}$, arbitrarily. Set $m = N(n + 2 + k)$ and define the function F by

$$F(s_1, \dots, s_m) = \left(\frac{8}{J^2}\right)^{\frac{m}{2}} \langle \psi, e^{-s_1 Y} X \cdots X e^{-(\beta - s_m)Y} \phi \rangle. \tag{3.76}$$

Let $\{(\boldsymbol{\sigma}_{c,1}, \boldsymbol{\sigma}_{f,1}), \dots, (\boldsymbol{\sigma}_{c,1}, \boldsymbol{\sigma}_{f,n})\} \subseteq E_N$ be the sequence given in Lemma 3.14. Recall that this sequence "connects" $(\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f)$ and $(\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f)$ as stated in Lemma 3.14. For notational simplicity, we set

$$|\boldsymbol{\sigma}_0\rangle = |\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f\rangle, \tag{3.77}$$

$$|\boldsymbol{\sigma}_j\rangle = |\boldsymbol{\sigma}_{c,j}, \boldsymbol{\sigma}_{c,j}, \boldsymbol{\sigma}_{f,j}, \boldsymbol{\sigma}_{f,j}\rangle, \ j = 1, \dots, n, \tag{3.78}$$

and

$$|\boldsymbol{\sigma}_{n+1}\rangle = |\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f\rangle. \tag{3.79}$$

Choose strictly positive numbers $t_1, \dots, t_{n+1}$ such that $0 < \varepsilon < \beta$, where $\varepsilon = \sum_{j=1}^{n+1} t_j$. Then we have

$$\begin{aligned}
&F\Bigg(\underbrace{0,\dots,0}_{N}, \underbrace{t_1,\dots,t_1}_{N}, \underbrace{t_1+t_2,\dots,t_1+t_2}_{N}, \dots, \varepsilon + \frac{\beta-\varepsilon}{k}, \dots, \varepsilon + \frac{\beta-\varepsilon}{k}, \dots, \beta, \dots, \beta\Bigg) \\
&= \left\langle \psi, \left(\frac{8}{J^2}\right)^{\frac{N}{2}} X^N e^{-t_1 Y} \cdots e^{-t_{n+1} Y} \left(\frac{8}{J^2}\right)^{\frac{N}{2}} X^N \phi \right\rangle \\
&\overset{(3.75)}{\geq} \left\langle \psi, \prod_{j=0}^{n} \left(|\boldsymbol{\sigma}_j\rangle\langle\boldsymbol{\sigma}_j| e^{-t_{j+1}Y}\right) \left(|\boldsymbol{\sigma}_{n+1}\rangle\langle\boldsymbol{\sigma}_{n+1}| e^{-\frac{\beta-\varepsilon}{k}Y}\right)^k |\boldsymbol{\sigma}_{n+1}\rangle\langle\boldsymbol{\sigma}_{n+1}|\phi \right\rangle \\
&= \psi_{\boldsymbol{\sigma}}\phi_{\boldsymbol{\sigma}'} \left\langle \boldsymbol{\sigma}_0 \left| \prod_{j=0}^{n} \left(|\boldsymbol{\sigma}_j\rangle\langle\boldsymbol{\sigma}_j| e^{-t_{j+1}Y}\right) \left(|\boldsymbol{\sigma}_{n+1}\rangle\langle\boldsymbol{\sigma}_{n+1}| e^{-\frac{\beta-\varepsilon}{k}Y}\right)^k |\boldsymbol{\sigma}_{n+1}\rangle\langle\boldsymbol{\sigma}_{n+1}| \right| \boldsymbol{\sigma}_{n+1} \right\rangle \\
&= \psi_{\boldsymbol{\sigma}}\phi_{\boldsymbol{\sigma}'} \prod_{j=0}^{n} \langle\boldsymbol{\sigma}_j| e^{-t_{j+1}Y} |\boldsymbol{\sigma}_{j+1}\rangle \langle\boldsymbol{\sigma}_{n+1}| e^{-\frac{\beta-\varepsilon}{k}Y} |\boldsymbol{\sigma}_{n+1}\rangle^k,
\end{aligned} \tag{3.80}$$

where in the first inequality, we used the inequality (3.75); in additon, we have used the fact that each $|\boldsymbol{\sigma}_j\rangle$ is positive w.r.t. $\mathcal{Q}_{\mathrm{KL}}$. By Lemma 3.13, there exist $t_1, \dots, t_{n+1} > 0$ such that $\langle\boldsymbol{\sigma}_j|e^{-t_{j+1}Y}|\boldsymbol{\sigma}_{j+1}\rangle > 0,\ j = 0, \dots, n+1$ hold. In addition, $\langle\boldsymbol{\sigma}_{n+1}|e^{-\frac{\beta-\varepsilon}{k}Y}|\boldsymbol{\sigma}_{n+1}\rangle^k > 0$ holds because $e^{-\frac{\beta-\varepsilon}{k}Y}$ is positive definite. Thus, we have

$$F\Bigg(\underbrace{0,\dots,0}_{N}, \underbrace{t_1,\dots,t_1}_{N}, \dots, \varepsilon + \frac{\beta-\varepsilon}{k}, \dots, \varepsilon + \frac{\beta-\varepsilon}{k}, \dots, \beta, \dots, \beta\Bigg) > 0, \tag{3.81}$$

which implies that

$$\left\langle \psi, e^{-\beta H'_{\mathrm{KL}}}\phi \right\rangle > 0 \tag{3.82}$$

for any $\psi, \phi \in \mathcal{Q}_{\mathrm{KL}}$ and $\beta > 0$. Therefore $e^{-\beta H'_{\mathrm{KL}}}$ is positivity improving w.r.t.$\mathcal{Q}_{\mathrm{KL}}$ for all $\beta > 0$. □

3.5.3 Proof of Theorem 3.1

Applying Theorems 2.17 and 3.15, we immediately obtain (i). In addition, the ground state, ψ, can be chosen such that $\psi > 0$ w.r.t. $U\mathcal{Q}_{\mathrm{KL}}$. Put $\phi = U^*\psi$. Trivially, $\phi > 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$ holds. By the definition of U, i.e, Lemma 3.6, we find that

$$\gamma_x\gamma_y U^* s_x^+ s_y^- U = \gamma_x\gamma_y U^* s_x^+ s_y^- U = c_{x\uparrow}^* c_{y\uparrow} c_{x\downarrow}^* c_{y\downarrow} \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}}, \tag{3.83}$$

$$\begin{aligned}
\gamma_u\gamma_v \mathrm{sgn}J_{x,u}\mathrm{sgn}J_{y,v} U^* S_u^+ S_v^- U &= \gamma_u\gamma_v \mathrm{sgn}J_{x,u}\mathrm{sgn}J_{y,v} U^* S_u^+ S_v^- U \\
&= f_{u\uparrow}^* f_{v\uparrow} f_{u\downarrow}^* f_{v\downarrow} \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}_{\mathrm{KL}}.
\end{aligned} \tag{3.84}$$

Due to lemma 2.13, $c_{x\uparrow}^* c_{y\uparrow} c_{x\downarrow}^* c_{y\downarrow} \phi \neq 0$ and $f_{u\uparrow}^* f_{v\uparrow} f_{u\downarrow}^* f_{v\downarrow} \phi \neq 0$ hold. Thus, we have

$$\begin{aligned}\gamma_x \gamma_y \langle \psi, s_x^+ s_y^- \psi \rangle &= \gamma_x \gamma_y \langle \phi, U^* s_x^+ s_y^- U \phi \rangle \\ &= \langle \phi, c_{x\uparrow}^* c_{y\uparrow} c_{x\downarrow}^* c_{y\downarrow} \phi \rangle > 0, \end{aligned} \tag{3.85}$$

$$\begin{aligned}\gamma_u \gamma_v \mathrm{sgn} J_{x,u} \mathrm{sgn} J_{y,v} \langle \psi, S_u^+ S_v^- \psi \rangle &= \gamma_u \gamma_v \mathrm{sgn} J_{x,u} \mathrm{sgn} J_{y,v} \langle \phi, U^* S_u^+ S_v^- U \phi \rangle \\ &= \langle \phi, f_{u\uparrow}^* f_{v\uparrow} f_{u\downarrow}^* f_{v\downarrow} \phi \rangle > 0. \end{aligned} \tag{3.86}$$

This completes the proof of Theorem 3.1. □

3.6 The total spin of the ground state

In this section, we determine the total spin of the ground state of H_{KL}, when the coupling is ferromagnetic and antiferromagnetic, respectively.

3.6.1 The main result in Section 3.6

Here we recall our target theorem.

Theorem 3.2. *Assume* **(C$_0$)**.

(i) *If* **(C.6)** *holds, then the ground state of H_{KL} has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$*

(ii) *If* **(C.7)** *holds, then the ground state of H_{KL} has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_2| - |\Lambda_2| - |\Omega_1|\big|$*

In this subsection, we prove Theorem 3.2.

3.6.2 Strategy

Here, we briefly explain our strategy of the proof of (i) of Theorem 4.18. As for (ii) of Theorem 4.18, we will provide a proof in Subsection 4.5.3.

Recall the definition of P_0, i.e., (1.11). The following proposition plays a key role in the remainder of this section.

Proposition 3.16. *Let $\mathcal{X}$ be any one of $P_0\mathcal{L}_N, \mathcal{L}_N, P_0\mathcal{L}_N \otimes \mathcal{H}_{\mathrm{ph}}$. Let $\mathcal{C} \subset \mathcal{X}$ be a Hilbert cone. Consider positive self-adjoint operators A and B acting on $\mathcal{X}$. Assume the following:*

(i) *A and B commutes with the total spin operators $S_{\mathrm{tot}}^{(3)}, S_{\mathrm{tot}}^{(+)}$ and $S_{\mathrm{tot}}^{(-)}$.*

(ii) *$\inf \mathrm{spec}(A)$ (resp. $\inf \mathrm{spec}(B)$) is an eigenvalue of A (resp. B).*

(iii) *$\{e^{-\beta A}\}_{\beta \geq 0}$ and $\{e^{-\beta B}\}_{\beta \geq 0}$ are ergodic w.r.t. $\mathcal{C}$. Hence, the ground state of each of A and B is unique and strictly positive w.r.t. $\mathcal{C}$ due to Theorem 2.17.*

We denote by S_1 (resp. S_2) the total spin of the ground state of A (resp. B). Then we have $S_1 = S_2$.

Proof. Let ψ_1 (resp. ψ_2) be the unique ground state of A (resp. B). By the assumption (iii), ψ_1 and ψ_2 are strictly positive w.r.t. $\mathcal{C}$. Because $\boldsymbol{S}_{\mathrm{tot}}^2$ is self-adjoint, we have

$$S_1(S_1+1)\langle \psi_1, \psi_2 \rangle = \langle \boldsymbol{S}_{\mathrm{tot}}^2 \psi_1, \psi_2 \rangle = \langle \psi_1, \boldsymbol{S}_{\mathrm{tot}}^2 \psi_2 \rangle = S_2(S_2+1)\langle \psi_1, \psi_2 \rangle. \tag{3.87}$$

Because $\langle \psi_1, \psi_2 \rangle > 0$, we conclude that $S_1 = S_2$. □

Note that the method of nonzero overlap between ground states has been extensively used in many-electron systems, see, e.g., [22, 26, 27, 28]. In [13], this method is further extended and applied to electron-phonon interacting systems. Proposition 3.16 is a mathematically abstracted form of the method, which is essentially proved in [13].

We divide the proof of Theorem 4.18 into two steps:

Step 1:

Definition 3.17. Define a self-adjoint operator on $\mathcal{L}_N$ by

$$\begin{aligned} K_1 =& \frac{1}{2}\sum_{x,y\in\Lambda}|t_{x,y}|^2(\boldsymbol{s}_x^+\cdot\boldsymbol{s}_y^-+\boldsymbol{s}_x^-\cdot\boldsymbol{s}_y^+)+\sum_{x\in\Lambda,u\in\Omega}|J_{x,u}|^2(\boldsymbol{s}_x^+\cdot\boldsymbol{S}_u^-+\boldsymbol{s}_x^-\cdot\boldsymbol{S}_u^+)\\ &+\sum_{x\in\Lambda}\left(n_{x\uparrow}^c-\frac{1}{2}\right)\left(n_{x\downarrow}^c-\frac{1}{2}\right)+\sum_{u\in\Omega}\left(n_{u\uparrow}^f-\frac{1}{2}\right)\left(n_{u\downarrow}^f-\frac{1}{2}\right), \end{aligned} \tag{3.88}$$

$$\begin{aligned} K_1' =& \frac{1}{2}\sum_{x,y\in\Lambda}|t_{x,y}|^2(\boldsymbol{s}_x^+\cdot\boldsymbol{s}_y^-+\boldsymbol{s}_x^-\cdot\boldsymbol{s}_y^+)+\sum_{x\in\Lambda_1,u\in\Omega_1}(\boldsymbol{s}_x^+\cdot\boldsymbol{S}_u^-+\boldsymbol{s}_x^-\cdot\boldsymbol{S}_u^+)\\ &+\sum_{x\in\Lambda_2,u\in\Omega_2}(\boldsymbol{s}_x^+\cdot\boldsymbol{S}_u^-+\boldsymbol{s}_x^-\cdot\boldsymbol{S}_u^+)+\sum_{x\in\Lambda}\left(n_{x\uparrow}^c-\frac{1}{2}\right)\left(n_{x\downarrow}^c-\frac{1}{2}\right)\\ &+\sum_{u\in\Omega}\left(n_{u\uparrow}^f-\frac{1}{2}\right)\left(n_{u\downarrow}^f-\frac{1}{2}\right). \end{aligned} \tag{3.89}$$

First, we examine the ground state properties of the restricted Hamiltonian:

$$\boldsymbol{K}_1 = K_1 \restriction P_0\mathcal{L}_N, \quad \boldsymbol{K}_1' = K_1' \restriction P_0\mathcal{L}_N \tag{3.90}$$

Note that

$$U^*\boldsymbol{K}_1U = U^*K_1U \restriction Q_0\mathcal{L}_N, \quad U^*\boldsymbol{K}_1'U = U^*K_1'U \restriction Q_0\mathcal{L}_N \tag{3.91}$$

where U is given by Lemma 3.6. We will prove following propositions in

Proposition 3.18. *Assume* **(C$_0$)** *and* **(C.6)**. *We have*

$$e^{-\beta U^*\boldsymbol{K}_1U} \rhd 0 \ \textit{w.r.t.}\ \mathcal{Q}_{\rm KL} \tag{3.92}$$

for every $\beta > 0$. Hence, the ground state of $\boldsymbol{K}_1$ is unique. Furthermore, the ground state of $\boldsymbol{K}_1$ has total spin $S = \frac{1}{2}\big||\Lambda_1|+|\Omega_1|-|\Lambda_2|-|\Omega_2|\big|$.

Proposition 3.19. *Assume* **(C$_0$)** *and* **(C.7)**. *We have*

$$e^{-\beta U^*\boldsymbol{K}_1'U} \rhd 0 \ \textit{w.r.t.}\ \mathcal{Q}_{\rm KL} \tag{3.93}$$

for every $\beta > 0$. Hence, the ground state of $\boldsymbol{K}_1'$ is unique. Furthermore, the ground state of $\boldsymbol{K}_1'$ has total spin $S = \frac{1}{2}\big||\Lambda_1|+|\Omega_2|-|\Lambda_2|-|\Omega_1|\big|$.

Remark 3.20. The readers would guess that since the form of $\boldsymbol{K}_1$ is similar to that of the Heisenberg Hamiltonian, $H_{\rm Heis}$, magnetic properties of the ground state of $\boldsymbol{K}_1$ are readily confirmed by the Marshall-Lieb-Mattis theorem [8, 9]. On the contrary, because the Hilbert space on which $\boldsymbol{K}_1$ acts is different from the one on which $H_{\rm Heis}$ acts, we cannot directly apply the Marshall-Lieb-Mattis theorem to $\boldsymbol{K}_1$. In Subsection 3.6.3, we will explain how to overcome this difficulty.

Step 2:

In Subsection 3.6.3, we will prove (i) of Theorem 3.6.1 and Proposition 3.18. In Subsection 3.6.4, we will prove (ii) of Theorem 3.6.1 and Proposition 3.19. As we will see, a variant of Proposition 3.16 is essential for the proof.

3.6.3 The case of antiferromagnetic coupling

Recall the definition of $\mathcal{E}_{\rm KL}$ given by Definiton 3.5. As a first step, we prepare an abstract lemma:

Lemma 3.21. *For $A_1, \dots, A_n \in \mathscr{B}(\mathcal{F}_N)$ and $c_n \in \mathbb{C}$, we have*

$$\exp\left[\sum_{k=1}^{n}(1+|c_k|^2 A_k \otimes \vartheta A_k \vartheta^*)\right] \trianglerighteq \exp\left[\sum_{k=1}^{n}(c_k A_k \otimes 1 + c_k^* 1 \otimes \vartheta A_k \vartheta^*)\right] \ \textit{w.r.t. } \mathcal{E}_{\rm KL} \tag{3.94}$$

Proof. For each $m \in \mathbb{N}$, one obtains, by applying Proposition 2.32,

$$\left(\frac{1}{\sqrt{m}} - \frac{c_k}{\sqrt{m}} A_k\right) \otimes \vartheta \left(\frac{1}{\sqrt{m}} - \frac{c_k^*}{\sqrt{m}} A_k\right) \vartheta^* \trianglerighteq 0 \text{ w.r.t. } \mathcal{E}_{\rm KL}, \tag{3.95}$$

which implies

$$\exp\left[\left(\frac{1}{\sqrt{m}} - \frac{c_k}{\sqrt{m}} A_k\right) \otimes \vartheta \left(\frac{1}{\sqrt{m}} - \frac{c_k^*}{\sqrt{m}} A_k\right) \vartheta^*\right] \trianglerighteq 1 \text{ w.r.t. } \mathcal{E}_{\rm KL}. \tag{3.96}$$

In addition, by using Proposition 2.25 again, we have

$$\exp\left[\frac{c_k}{m} A_k \otimes 1 + \frac{c_k^*}{m} 1 \otimes \vartheta A_k \vartheta^*\right] = \exp\left[\frac{c_k}{m} A_k\right] \otimes \vartheta^* \exp\left[\frac{c_k}{m} A_k\right] \vartheta^* \trianglerighteq 0 \text{ w.r.t. } \mathcal{E}_{\rm KL}. \tag{3.97}$$

Hence,

$$\begin{aligned}
&\exp\left[\frac{1}{m} + \frac{|c_k|^2}{m} A_k \otimes \vartheta A_k \vartheta^*\right] \\
&= \exp\left[\left(\frac{1}{\sqrt{m}} - \frac{c_k}{\sqrt{m}} A_k\right) \otimes \vartheta \left(\frac{1}{\sqrt{m}} - \frac{c_k^*}{\sqrt{m}} A_k\right) \vartheta^*\right] \exp\left[\frac{c_k}{m} A_k \otimes 1 + \frac{c_k^*}{m} 1 \otimes \vartheta A_k \vartheta^*\right] \\
&\trianglerighteq \exp\left[\frac{c_k}{m} A_k \otimes 1 + \frac{c_k^*}{m} 1 \otimes \vartheta A_k \vartheta^*\right] \text{ w.r.t. } \mathcal{E}_{\rm KL}.
\end{aligned} \tag{3.98}$$

Therefore, by applying the Trotter product formula, one finds

$$\begin{aligned}
\exp\left[\sum_{k=1}^{n}(c_k A_k \otimes 1 + c_k^* 1 \otimes \vartheta A_k \vartheta^*)\right] &= \lim_{m\to\infty}\left(\prod_{k=1}^{n} e^{\frac{1}{m}(c_k A_k \otimes 1 + c_k^* 1 \otimes \vartheta A_k \vartheta^*)}\right)^m \\
&\trianglelefteq \lim_{m\to\infty}\left(\prod_{k=1}^{n}\exp\left[\frac{1}{m} + \frac{|c_k|^2}{m} A_k \otimes \vartheta A_k \vartheta^*\right]\right)^m \\
&= \exp\left[\sum_{k=1}^{n}(1+|c_k|^2 A_k \otimes \vartheta A_k \vartheta^*)\right] \text{ w.r.t. } \mathcal{E}_{\rm KL}.
\end{aligned} \tag{3.99}$$

□

As an application of Lemma 3.21, we obtain:

Lemma 3.22. *Assume* **(C_0)** *and* (C.6)*. Define*

$$H_{\mathrm{H}} = -\sum_{x,y\in\Lambda} t_{x,y}(c_{x\uparrow}^* c_{y\uparrow} + c_{x\downarrow}^* c_{y\downarrow}) - \sum_{x\in\Lambda, u\in\Omega} J_{x,u}\left(c_{x\uparrow}^* f_{u\uparrow} + c_{x\downarrow}^* f_{u\downarrow} + f_{u\uparrow}^* c_{x\uparrow} + f_{u\downarrow}^* c_{x\downarrow}\right)$$
$$+\sum_{x\in\Lambda}\left(n_{x\uparrow}^c - \frac{1}{2}\right)\left(n_{x\downarrow}^c - \frac{1}{2}\right) + \sum_{u\in\Omega}\left(n_{u\uparrow}^f - \frac{1}{2}\right)\left(n_{u\downarrow}^f - \frac{1}{2}\right). \tag{3.100}$$

Then we have

$$e^{-\beta U^* K_1 U} e^{|\Lambda|^2 + |\Lambda||\Omega|} \trianglerighteq e^{-\beta U^* H_{\mathrm{H}} U} \rhd 0 \text{ w.r.t. } \mathcal{E}_{\mathrm{KL}} \tag{3.101}$$

for all $\beta > 0$. Hence, the ground state of K_1 is unique. Furthermore, the ground state of K_1 has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$.

Proof. First, we observe

$$U^* H_{\mathrm{H}} U = -\sum_{x,y\in\Lambda} t_{x,y}(c_{x\uparrow}^* c_{y\uparrow} + c_{x\downarrow}^* c_{y\downarrow}) - \sum_{x\in\Lambda, u\in\Omega} J_{x,u}\left(c_{x\uparrow}^* f_{u\uparrow} + f_{u\downarrow}^* c_{x\downarrow} + f_{u\uparrow}^* c_{x\uparrow} + c_{x\downarrow}^* f_{u\downarrow}\right)$$
$$-\sum_{x\in\Lambda}\left(n_{x\uparrow}^c - \frac{1}{2}\right)\left(n_{x\downarrow}^c - \frac{1}{2}\right) - \sum_{u\in\Omega}\left(n_{u\uparrow}^f - \frac{1}{2}\right)\left(n_{u\downarrow}^f - \frac{1}{2}\right) \tag{3.102}$$

and

$$U^* K_1 U = -\sum_{x,y\in\Lambda} |t_{x,y}|^2 c_{x\uparrow}^* c_{y\uparrow} c_{x\downarrow}^* c_{y\downarrow} - \sum |J_{x,u}|^2 (c_{x\uparrow}^* f_{u\uparrow} c_{x\downarrow}^* f_{u\downarrow} + f_{u\uparrow}^* c_{x\uparrow} f_{u\downarrow}^* c_{x\downarrow})$$
$$-\sum_{x\in\Lambda}\left(n_{x\uparrow}^c - \frac{1}{2}\right)\left(n_{x\downarrow}^c - \frac{1}{2}\right) - \sum_{u\in\Omega}\left(n_{u\uparrow}^f - \frac{1}{2}\right)\left(n_{u\downarrow}^f - \frac{1}{2}\right). \tag{3.103}$$

Without loss of generality, we may assume $\beta = 1$. Using (3.4) and (3.102), we can apply Lemma 3.21 to $U^* H_{\mathrm{H}} U$ and obtain

$$\begin{aligned}
&\exp\left[-U^* H_{\mathrm{H}} U\right] \\
&= \exp\Bigg[\sum_{x,y\in\Lambda} t_{x,y}(c_{x\uparrow}^* c_{y\uparrow} + c_{x\downarrow}^* c_{y\downarrow}) + \sum_{x\in\Lambda, u\in\Omega} J_{x,u}\left(c_{x\uparrow}^* f_{u\uparrow} + f_{u\downarrow}^* c_{x\downarrow} + f_{u\uparrow}^* c_{x\uparrow} + c_{x\downarrow}^* f_{u\downarrow}\right) \\
&\quad + \sum_{x\in\Lambda}\left(n_{x\uparrow}^c - \frac{1}{2}\right)\left(n_{x\downarrow}^c - \frac{1}{2}\right) + \sum_{u\in\Omega}\left(n_{u\uparrow}^f - \frac{1}{2}\right)\left(n_{u\downarrow}^f - \frac{1}{2}\right)\Bigg] \\
&\trianglelefteq \exp\Bigg[\sum_{x,y\in\Lambda} (1 + |t_{x,y}|^2 c_{x\uparrow}^* c_{y\uparrow} c_{x\downarrow}^* c_{y\downarrow}) + \sum_{x\in\Lambda, u\in\Omega} \left\{1 + |J_{x,u}|^2\left(c_{x\uparrow}^* f_{u\uparrow} c_{x\downarrow}^* f_{u\downarrow} + f_{u\uparrow}^* c_{x\uparrow} f_{u\downarrow}^* c_{x\downarrow}\right)\right\} \\
&\quad + \sum_{x\in\Lambda}\left(n_{x\uparrow}^c - \frac{1}{2}\right)\left(n_{x\downarrow}^c - \frac{1}{2}\right) + \sum_{u\in\Omega}\left(n_{u\uparrow}^f - \frac{1}{2}\right)\left(n_{u\downarrow}^f - \frac{1}{2}\right)\Bigg] \\
&= \exp\left[-U^* K_1 U\right] e^{|\Lambda|^2 + |\Lambda||\Omega|} \text{ w.r.t. } \mathcal{E}_{\mathrm{KL}},
\end{aligned} \tag{3.104}$$

where in the second equality, we have used (3.103). Because H_{H} is a Hubbard Hamiltonian on the connected bipartite lattice $\Lambda \sqcup \Omega$, we can apply a generalized version of Lieb's theorem presented in [11, 13] to $H_{\rm H}$. Thus, we find that $e^{-\beta U^* H_{\rm H} U} \rhd 0$ w.r.t. $\mathcal{E}_{\rm KL}$ for all $\beta > 0$. Combining this fact with (3.113), we obtain the inequality (3.101).

In order to specify the value of the total spin of the ground state, we recall Lieb's theorem for readers' convenience: Lieb's theorem claims that with a bipartite lattice and a half-filled band, the ground state of the repulsive Hubbard model has total spin

$$S = \frac{1}{2}\big||A| - |B|\big|, \tag{3.105}$$

where $|A|$ (resp. $|B|$) is the number of sites in the A-sublattice (resp. B-sublattice), see [7] for details. Because $H_{\rm H}$ is a Hubbard Hamiltonian on the bipartite lattice with $A = \Lambda_1 \cup \Omega_1$ and $B = \Lambda_2 \cup \Omega_2$, the ground state of $H_{\rm H}$ has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$. Hence, due to Proposition 3.16, the ground state of K_1 has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$ as well. □

To complete the proof of Propositions 3.18 and 3.19, the following lemma is useful:

Lemma 3.23. *Let H_0 be a self-adjoint operator acting in $\mathcal{L}_N$. Assume that*

(i) $e^{-\beta H_0} \rhd 0$ *w.r.t.* $\mathcal{E}_{\rm KL}$ *for all* $\beta > 0$*;*

(ii) H_0 *commutes with* Q_0*.*

Then we obtain $\exp(-\beta H_0 \restriction Q_0\mathcal{L}_N) \rhd 0$ *w.r.t.* $Q_0\mathcal{E}_{\rm KL}$ *for all* $\beta > 0$*.*

Proof. Take $Q_0\varphi_1, Q_0\varphi_2 \in Q_0\mathcal{E}_{\rm KL} \setminus \{0\}$, arbitrarily. Because $Q_0 \unrhd 0$ w.r.t. $\mathcal{E}_{\rm KL}$, we have $Q_0\varphi_1 \geq 0$ and $Q_0\varphi_2 \geq 0$ w.r.t. $\mathcal{E}_{\rm KL}$ as vectors in $\mathcal{L}_N$. Using this, we have

$$\big\langle Q_0\varphi_1, e^{-\beta H_0 \restriction Q_0\mathcal{L}_N} Q_0\varphi_2\big\rangle_{Q_0\mathcal{L}_N} = \big\langle Q_0\varphi_1, e^{-\beta H_0} Q_0\varphi_2\big\rangle_{\mathcal{L}_N} > 0, \tag{3.106}$$

where in the first equality, we have used the assumption (ii), and in the first inequality, we have used the assumption (i). This completes the proof. □

Proof of Proposition 3.18

Taking (3.91) into consideration, we can apply Lemma 3.23 with $H_0 = U^* K_1 U$ and obtain (3.92). Hence, the ground state, $\varphi_{\rm g}$, of $\boldsymbol{K}_1$ is unique and strictly positive w.r.t. $UQ_0\mathcal{E}_{\rm KL}$. Let ψ be the ground state of K_1. By Lemma 3.22, ψ has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$. Because K_1 commutes with P_0, $P_0\psi$ is the ground state of $\boldsymbol{K}_1$. Hence, due to the uniqueness, $\varphi_{\rm g}$ and $P_0\psi$ are identical. In addition, since $\boldsymbol{S}_{\rm tot}^2$ commutes with P_0, the total spin of $P_0\psi$ coincides with that of ψ. □

Proof of (i) of Theorem 3.6.1

From Theorem 3.15 and Theorem 2.17, $H_{\rm KL}$ has the unique ground state $\psi_{KL} > 0$ w.r.t. $P_0\mathcal{E}_{\rm KL}$. By Proposition 3.18, the ground state ψ_1 of $\boldsymbol{K}_1$ is unique and strictly positive w.r.t. $P_0\mathcal{E}_{\rm KL}$. Since $\boldsymbol{S}_{\rm tot}^2$ commutes with $H_{\rm KL}$ and $\boldsymbol{K}_1$, ψ_{KL} and ψ_1 are eigenvectors of $\boldsymbol{S}_{\rm tot}^2$. We see $\langle \psi_{KL}, \psi_1\rangle > 0$ because ψ_{KL} and ψ_1 are strictly positive w.r.t. $P_0\mathcal{E}_{\rm KL}$. Since ψ_1 has total spin $\frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$ from Proposition 3.18, ψ_{KL} has total spin $\frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$. □

3.6.4 The case of ferromagnetic coupling

The following lemma corresponds to Lemma 3.22:

Lemma 3.24. *Assume* $(\mathbf{C_0})$ *and* (C.7)*. Define*

$$\begin{aligned} H'_{\mathrm{H}} = &-\sum_{x,y\in\Lambda} t_{x,y}(c^*_{x\uparrow}c_{y\uparrow} + c^*_{x\downarrow}c_{y\downarrow}) + \sum_{x\in\Lambda_1,u\in\Omega_1} (c^*_{x\uparrow}f_{u\uparrow} + c^*_{x\downarrow}f_{u\downarrow} + f^*_{u\uparrow}c_{x\uparrow} + f^*_{u\downarrow}c_{x\downarrow}) \\ &+ \sum_{x\in\Lambda_2,u\in\Omega_2} (c^*_{x\uparrow}f_{u\uparrow} + c^*_{x\downarrow}f_{u\downarrow} + f^*_{u\uparrow}c_{x\uparrow} + f^*_{u\downarrow}c_{x\downarrow}) + \sum_{x\in\Lambda}\left(n^c_{x\uparrow}-\frac{1}{2}\right)\left(n^c_{x\downarrow}-\frac{1}{2}\right) \\ &+\sum_{u\in\Omega}\left(n^f_{u\uparrow}-\frac{1}{2}\right)\left(n^f_{u\downarrow}-\frac{1}{2}\right). \end{aligned} \tag{3.107}$$

Then we have

$$e^{-\beta U^*K'_1U}e^{|\Lambda|^2+2|\Lambda_1||\Omega_1|+2|\Lambda_2||\Omega_2|} \unrhd e^{-\beta U^*H'_{\mathrm{H}}U} \rhd 0 \ \textit{w.r.t.}\ \mathcal{E}_{\mathrm{KL}} \tag{3.108}$$

for all $\beta > 0$*. Hence, the ground state of* K'_1 *is unique. Furthermore the ground state of* K'_1 *has total spin* $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_2| - |\Lambda_2| - |\Omega_1|\big|$.

Proof. First, we observe

$$\begin{aligned} U^*H'_{\mathrm{H}}U = &-\sum_{x,y\in\Lambda} t_{x,y}(c^*_{x\uparrow}c_{y\uparrow} + c^*_{x\downarrow}c_{y\downarrow}) + \sum_{x\in\Lambda_1,u\in\Omega_1} (c^*_{x\uparrow}f_{u\uparrow} + c^*_{x\downarrow}f_{u\downarrow} + f^*_{u\uparrow}c_{x\uparrow} + f^*_{u\downarrow}c_{x\downarrow}) \\ &+ \sum_{x\in\Lambda_2,u\in\Omega_2} (c^*_{x\uparrow}f_{u\uparrow} + c^*_{x\downarrow}f_{u\downarrow} + f^*_{u\uparrow}c_{x\uparrow} + f^*_{u\downarrow}c_{x\downarrow}) - \sum_{x\in\Lambda}\left(n^c_{x\uparrow}-\frac{1}{2}\right)\left(n^c_{x\downarrow}-\frac{1}{2}\right) \\ &-\sum_{u\in\Omega}\left(n^f_{u\uparrow}-\frac{1}{2}\right)\left(n^f_{u\downarrow}-\frac{1}{2}\right). \end{aligned} \tag{3.109}$$

and

$$\begin{aligned} U^*K'_1U = &-\sum_{x,y\in\Lambda} |t_{x,y}|^2 c^*_{x\uparrow}c_{y\uparrow}c^*_{x\downarrow}c_{y\downarrow} + \sum_{x\in\Lambda_1,u\in\Omega_1} (c^*_{x\uparrow}f_{u\uparrow}c^*_{x\downarrow}f_{u\downarrow} + f^*_{u\uparrow}c_{x\uparrow}f^*_{u\downarrow}c_{x\downarrow}) \\ &+ \sum_{x\in\Lambda_2,u\in\Omega_2} (c^*_{x\uparrow}f_{u\uparrow}c^*_{x\downarrow}f_{u\downarrow} + f^*_{u\uparrow}c_{x\uparrow}f^*_{u\downarrow}c_{x\downarrow}) - \sum_{x\in\Lambda}\left(n^c_{x\uparrow}-\frac{1}{2}\right)\left(n^c_{x\downarrow}-\frac{1}{2}\right) \\ &-\sum_{u\in\Omega}\left(n^f_{u\uparrow}-\frac{1}{2}\right)\left(n^f_{u\downarrow}-\frac{1}{2}\right) \end{aligned} \tag{3.110}$$

Without loss of generality, we may assume $\beta = 1$. Set

$$A_{x,u} = c^*_{x\uparrow}f_{u\uparrow} + f^*_{u\downarrow}c_{x\downarrow} + f^*_{u\uparrow}c_{x\uparrow} + c^*_{x\downarrow}f_{u\downarrow}, \tag{3.111}$$

$$B_{x,u} = c^*_{x\uparrow}f_{u\uparrow}c^*_{x\downarrow}f_{u\downarrow} + f^*_{u\uparrow}c_{x\uparrow}f^*_{u\downarrow}c_{x\downarrow}. \tag{3.112}$$

Using (3.4) and (3.109), we can apply Lemma 3.21 to $U^*H'_{\rm H}U$ and obtain

$$\begin{aligned}
&\exp\left[-U^*H'_{\rm H}U\right]\\
&=\exp\Bigg[\sum_{x,y\in\Lambda}t_{x,y}(c^*_{x\uparrow}c_{y\uparrow}+c^*_{x\downarrow}c_{y\downarrow})+\sum_{x\in\Lambda,u\in\Omega}J_{x,u}A_{x,u}\\
&\quad+\sum_{x\in\Lambda}\left(n^c_{x\uparrow}-\frac{1}{2}\right)\left(n^c_{x\downarrow}-\frac{1}{2}\right)+\sum_{u\in\Omega}\left(n^f_{u\uparrow}-\frac{1}{2}\right)\left(n^f_{u\downarrow}-\frac{1}{2}\right)\Bigg]\\
&\trianglelefteq\exp\Bigg[\sum_{x,y\in\Lambda}\left(1+|t_{x,y}|^2c^*_{x\uparrow}c_{y\uparrow}c^*_{x\downarrow}c_{y\downarrow}\right)+\sum_{x\in\Lambda,u\in\Omega}\left(1+|J_{x,u}|^2B_{x,u}\right)\\
&\quad+\sum_{x\in\Lambda}\left(n^c_{x\uparrow}-\frac{1}{2}\right)\left(n^c_{x\downarrow}-\frac{1}{2}\right)+\sum_{u\in\Omega}\left(n^f_{u\uparrow}-\frac{1}{2}\right)\left(n^f_{u\downarrow}-\frac{1}{2}\right)\Bigg]\\
&=\exp\left[-U^*K'_1U\right]e^{|\Lambda|^2+|\Lambda_1||\Omega_1|+|\Lambda_2||\Omega_2|}\ \text{w.r.t. }\mathcal{E}_{\rm KL},
\end{aligned}\tag{3.113}$$

where in the second equality, we have used (3.103). Because $H_{\rm H}$ is a Hubbard Hamiltonian on the connected bipartite lattice $\Lambda\sqcup\Omega$, we can apply a generalized version of Lieb's theorem presented in [11, 13] to $H_{\rm H}$. Thus, we find that $e^{-\beta U^*H_{\rm H}U}\rhd 0$ w.r.t. $\mathcal{E}_{\rm KL}$ for all $\beta>0$. Combining this fact with (3.113), we obtain the inequality (3.101).

Because $H_{\rm H}$ is a Hubbard Hamiltonian on the bipartite lattice with $A=\Lambda_1\sqcup\Omega_1$ and $B=\Lambda_2\sqcup\Omega_2$, Lieb's theorem tells us that the ground state of $H_{\rm H}$ has total spin $S=\frac{1}{2}\big||\Lambda_1|+|\Omega_1|-|\Lambda_2|-|\Omega_2|\big|$. Hence, due to Proposition 3.16, the ground state of K_1 has total spin $S=\frac{1}{2}\big||\Lambda_1|+|\Omega_1|-|\Lambda_2|-|\Omega_2|\big|$ as well. □

Proof of Proposition 3.19

Taking (3.91) into consideration, we can apply Lemma 3.23 with $H_0=U^*K'_1U$ and obtain (3.93). Hence, the ground state, $\varphi_{\rm g}$, of $\boldsymbol{K}'_1$ is unique and strictly positive w.r.t. $UQ_0\mathcal{E}_{\rm KL}$. Let ψ be the ground state of K'_1. By Lemma 3.24, ψ has total spin $S=\frac{1}{2}\big||\Lambda_1|+|\Omega_2|-|\Lambda_2|-|\Omega_1|\big|$. Because K'_1 commutes with P_0, $P_0\psi$ is the ground state of $\boldsymbol{K}'_1$. Hence, due to the uniqueness, $\varphi_{\rm g}$ and $P_0\psi$ are identical. In addition, since $\boldsymbol{S}^2_{\rm tot}$ commutes with P_0, the total spin of $P_0\psi$ coincides with that of ψ. □

Proof of (ii) of Theorem 3.6.1

From Theorem 3.15 and Theorem 2.17, $H_{\rm KL}$ has the unique ground state $\psi_{KL}>0$ w.r.t. $P_0\mathcal{E}_{\rm KL}$. By Proposition 3.19, the ground state ψ_1 of $\boldsymbol{K}'_1$ is unique and strictly positive w.r.t. $P_0\mathcal{E}_{\rm KL}$. Since $\boldsymbol{S}^2_{\rm tot}$ commutes with $H_{\rm KL}$ and $\boldsymbol{K}'_1$, ψ_{KL} and ψ_1 are eigenvectors of $\boldsymbol{S}^2_{\rm tot}$. We see $\langle\psi_{KL},\psi_1\rangle>0$ because ψ_{KL} and ψ_1 are strictly positive w.r.t. $P_0\mathcal{E}_{\rm KL}$. Since ψ_1 has total spin $\frac{1}{2}\big||\Lambda_1|+|\Omega_1|-|\Lambda_2|-|\Omega_2|\big|$ from Proposition 3.19, ψ_{KL} has total spin $\frac{1}{2}\big||\Lambda_1|+|\Omega_1|-|\Lambda_2|-|\Omega_2|\big|$. □

4 The Kondo lattice model with electron-phonon interaction

4.1 Main results in Section 4

The purpose of this section is to prove Theorem 1.6. As with the proof of Theorem 1.4, the proof is accomplished by showing two theorems; The first theorem is a claim about the uniqueness of the ground state and the spin structure of the ground state. The second theorem is a claim about the total spin of the ground state.

Theorem 4.1. *Assume* **(C)**. *We have the following (i) and (ii):*

(i) $\{e^{-\beta H}\}_{\beta \geq 0}$ *is ergodic w.r.t.* $\mathcal{Q}$.

(ii) *We denote by* ψ *the ground state of* H. *Then* ψ *satisfy the following:*

$$\gamma_x \gamma_y \langle \psi, s_x^+ s_y^- \psi \rangle > 0, \quad \gamma_u \gamma_v \mathrm{sgn} J_{x,u} \mathrm{sgn} J_{y,v} \langle \psi, S_u^+ S_v^- \psi \rangle > 0 \tag{4.1}$$

for every $x, y \in \Lambda$ *and* $u, v \in \Omega$.

We will prove Theorem 4.1 in Subsection 4.4.

Theorem 4.2. *Assume* **(C)**. *Let* ψ *be the ground state of* H.

(i) *If* **(C.6)** *holds, then* ψ *has total spin* $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$.

(ii) *If* **(C.7)** *holds, then* ψ *has total spin* $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_2| - |\Lambda_2| - |\Omega_1|\big|$.

Theorem 4.2 will be shown in Subsection 4.5.

The claims in Theorem 4.1 and Theorem 4.2 are the same as the corresponding theorems in Section 3, so the readers may think that the proofs of the theorems are the same. Considering the electron-phonon interaction, the unitary transformation required to apply the theory given in Section 2 is more complicated than the hole-particle transformation. Therefore, the proof of these theorems requires a more technically sophisticated analysis.

4.2 Preliminary I: A Hilbert cone

To properly handle the electron-phonon interaction, we consider the tensor product of $\mathcal{Q}_{\mathrm{KL}}$ and a Hilbert cone in the Hilbert space which describes phonons.

Definition 4.3. We define $\mathcal{Q} \subset Q_0(\mathcal{F}_N \otimes \mathcal{F}_N) \otimes L^2(\mathbb{R}^{|\Lambda|})$ by

$$\mathcal{Q} = \int_{\mathbb{R}^{|\Lambda|}}^{\oplus} \mathcal{Q}_{\mathrm{KL}}\, d\boldsymbol{q}, \tag{4.2}$$

where $\mathcal{Q}_{\mathrm{KL}}$ is given by (3.13). As shown in Lemma 2.42, $\mathcal{Q}$ is a Hilbert cone.

In what follows, we use the following identification:

$$Q_0 \mathcal{L}_N \otimes \mathcal{H}_{\mathrm{ph}} = \int_{\mathbb{R}^{|\Lambda|}}^{\oplus} Q_0 \mathcal{L}_N d\boldsymbol{q}, \tag{4.3}$$

where the right hand side of (4.3) is the constant fiber direct integral, see (2.64).

The following lemma is often used in this section.

Lemma 4.4. *Let $A \in \mathscr{B}(Q_0\mathcal{L}_N \otimes \mathcal{H}_{\rm ph})$ be a decomposable operator*[3]*:*

$$A = \int_{\mathbb{R}^{|\Lambda|}}^{\oplus} A(\boldsymbol{q})\, d\boldsymbol{q}. \tag{4.4}$$

If $A(\boldsymbol{q}) \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\rm KL}$ for a.e. $\boldsymbol{q}$, then we have $A \trianglerighteq 0$ w.r.t. $\mathcal{Q}$.

Proof. Take $\varphi, \psi \in \mathcal{Q}_{\rm KL}$ and $f, g \in \mathcal{P}$, arbitrarily. Since $A(\boldsymbol{q}) \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\rm KL}$ and $f(\boldsymbol{q}), g(\boldsymbol{q}) \geq 0$ a.e., we have

$$\langle \varphi \otimes f, A\psi \otimes g\rangle = \int_{\mathbb{R}^{|\Lambda|}} f(\boldsymbol{q})g(\boldsymbol{q})\, \langle \varphi, A(\boldsymbol{q})\psi\rangle\ d\boldsymbol{q} \geq 0. \tag{4.5}$$

By Proposition 2.44, we conclude that $A \trianglerighteq 0$ w.r.t. $\mathcal{Q}$. □

Lemma 4.5. *Let $A \in \mathscr{B}(Q_0\mathcal{L}_N)$. Assume that $A \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\rm KL}$. Then we have $A \otimes 1 \trianglerighteq 0$ w.r.t. $\mathcal{Q}$,*

Proof. For any $\varphi, \psi \in \mathcal{Q}_{\rm KL}$ and $f, g \in \mathcal{P}$, we observe that

$$\langle \varphi \otimes f, A \otimes 1\psi \otimes g\rangle = \langle \varphi, A\psi\rangle\langle f, g\rangle \geq 0. \tag{4.6}$$

Hence, by applying Proposition 2.44, we conclude that $A \otimes 1 \trianglerighteq 0$ w.r.t. $\mathcal{Q}$. □

Lemma 4.6. *Let $A \in \mathscr{B}(Q_0\mathcal{L}_N \otimes \mathcal{H}_{\rm ph})$. Assume $A \trianglerighteq 0$ w.r.t. $\mathcal{Q}$. Then we have $e^A \trianglerighteq 0$ w.r.t. $\mathcal{Q}$.*

Proof. By the assumption, we obtain $A^n \trianglerighteq 0$ w.r.t. $\mathcal{Q}$ for each $n = 0, 1, \ldots$. Thus, we find

$$e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}. \tag{4.7}$$

□

4.3 Preliminary II: Unitary transformations

As seen in Section 3, the hole-particle transformation played an essential role when analyzing the KLM. However, when considering the Kondo lattice model with the electron-phonon interaction, the hole-particle transformation is not sufficient to analyze this model. To overcome this difficulty, in the following lemma, we introduce the key transformation called the *Lang–Firsov transformation.*

For each $x \in \Lambda$, define self-ajoint operators, p_x and q_x, by

$$p_x = \frac{i}{\sqrt{2}}(\overline{b_x^* - b_x}), \quad q_x = \frac{1}{\sqrt{2}}(\overline{b_x^* + b_x}), \tag{4.8}$$

where $\overline{A}$ indicates the closure of A. As is well-known, these operators satisfy the standard commutation relation: $[q_x, p_y] = i\delta_{x,y}$.

[3] As for the definition of the decomposable operators, see, e.g., [19, Section XIII.16].

Lemma 4.7. *We set*

$$L_c = -i\frac{\sqrt{2}}{\omega_0}\sum_{x,y\in\Lambda} g_{x,y} n_x^c p_y. \tag{4.9}$$

Let $N_{\rm p}$ *be the phonon number operator:* $N_{\rm p} = \sum_{x\in\Lambda} b_x^* b_x$*. Then*

$$\begin{aligned} & e^{i\frac{\pi}{2}N_{\rm p}} e^{L_c} H e^{-L_c} e^{-i\frac{\pi}{2}N_{\rm p}} \\ &= -T_\uparrow^+ - T_\downarrow^+ + \sum_{x\in\Lambda, u\in\Omega} J_{x,u} \boldsymbol{s}_x \cdot \boldsymbol{S}_u + \mathbb{U}_{\rm eff} + \omega_0 N_{\rm p} - \omega_0^{-1} g^2 |\Lambda| \end{aligned} \tag{4.10}$$

holds, where $T_\sigma^\pm, \mathbb{U}_{\rm eff}$ *and* g *are defined respectively by*

- $T_\sigma^\pm = \displaystyle\sum_{x,y\in\Lambda} t_{x,y} c_{x\sigma}^* c_{y\sigma} \exp\left(\pm i\Phi_{x,y}\right)$ *with* $\Phi_{x,y} = \frac{\sqrt{2}}{\omega_0}\sum_{z\in\Lambda}(g_{xz} - g_{yz}) q_z$*;*
- $\mathbb{U}_{\rm eff} = \displaystyle\sum_{x,y\in\Lambda} U_{{\rm eff},xy}(n_x^c - 1)(n_y^c - 1)$ *with* $U_{{\rm eff},xy}$ *given by (1.25);*
- $g = \sum_{x\in\Lambda} g_{x,y}$*. Note that* g *is independent of* y *due to* **(C.5)**.

Proof. Let $\mathbb{T} = \displaystyle\sum_{x,y\in\Lambda}\sum_{\sigma=\uparrow,\downarrow} t_{x,y} c_{x\sigma} c_{y\sigma}$. Applying properties of basic operators in Appendix A, we have

$$e^{i\frac{\pi}{2}N_{\rm p}} e^{L_c} \mathbb{T} e^{-L_c} e^{-i\frac{\pi}{2}N_{\rm p}} = -T_\uparrow^+ - T_\downarrow^+, \tag{4.11}$$

$$e^{i\frac{\pi}{2}N_{\rm p}} e^{L_c} \left(\sum_{x\in\Lambda, u\in\Omega} J_{x,u} \boldsymbol{s}_x \cdot \boldsymbol{S}_u\right) e^{-L_c} e^{-i\frac{\pi}{2}N_{\rm p}} = \sum_{x\in\Lambda, u\in\Omega} J_{x,u} \boldsymbol{s}_x \cdot \boldsymbol{S}_u, \tag{4.12}$$

$$e^{i\frac{\pi}{2}N_{\rm p}} e^{L_c} \left\{\sum_{x,y\in\Lambda} U_{x,y}(n_x^c - 1)(n_y^c - 1)\right\} e^{-L_c} e^{-i\frac{\pi}{2}N_{\rm p}} = \sum_{x,y\in\Lambda} U_{x,y}(n_x^c - 1)(n_y^c - 1), \tag{4.13}$$

$$e^{L_c}\left\{\sum_{x,y\in\Lambda} g_{x,y} n_x^c (b_y^* + b_y)\right\} e^{-L_c} = \sum_{x,y\in\Lambda} g_{x,y} n_x^c (b_y^* + b_y) - \frac{2}{\omega_0}\sum_{x,y,z\in\Lambda} g_{x,z} g_{y,z} n_x^c n_y^c, \tag{4.14}$$

$$e^{L_c} N_{\rm p} e^{-L_c} = N_{\rm p} - \frac{1}{\omega_0}\sum_{x,y\in\Lambda} g_{x,y} n_x^c (b_y^* + b_y) + \omega_0^{-2}\sum_{x,y,z\in\Lambda} g_{x,z} g_{y,z} n_x^c n_y^c. \tag{4.15}$$

Combining (4.14) and (4.15), we find

$$\begin{aligned}
&e^{i\frac{\pi}{2}N_{\rm p}}e^{L_c}\left\{\sum_{x,y\in\Lambda}g_{x,y}n_x^c(b_y^*+b_y)+\omega_0N_{\rm p}\right\}e^{-L_c}e^{-i\frac{\pi}{2}N_{\rm p}}\\
&=\omega_0N_{\rm p}-\sum_{x,y\in\Lambda}V_{x,y}n_x^cn_y^c\\
&=\omega_0N_{\rm p}-\sum_{x,y\in\Lambda}V_{x,y}(n_x^c-1)(n_y^c-1)-\sum_{x,y\in\Lambda}V_{x,y}(n_x^c+n_y^c)+\sum_{x,y\in\Lambda}V_{x,y}\\
&=\omega_0N_{\rm p}-\sum_{x,y\in\Lambda}V_{x,y}(n_x^c-1)(n_y^c-1)-\omega_0^{-1}\sum_{x,y,z\in\Lambda}g_{x,z}g_{y,z}(n_x^c+n_y^c)+\omega_0^{-1}\sum_{x,y,z\in\Lambda}g_{x,z}g_{y,z}\\
&=\omega_0N_{\rm p}-\sum_{x,y\in\Lambda}V_{x,y}(n_x^c-1)(n_y^c-1)-\omega_0^{-1}g\sum_{x,z\in\Lambda}g_{x,z}n_x^c-\omega_0^{-1}g\sum_{y,z\in\Lambda}g_{y,z}n_y^c+\omega_0^{-1}g^2|\Lambda|\\
&=\omega_0N_{\rm p}-\sum_{x,y\in\Lambda}V_{x,y}(n_x^c-1)(n_y^c-1)-2\omega_0^{-1}g^2\sum_{x\in\Lambda}n_x^c+\omega_0^{-1}g^2|\Lambda|\\
&=\omega_0N_{\rm p}-\sum_{x,y\in\Lambda}V_{x,y}(n_x^c-1)(n_y^c-1)-\omega_0^{-1}g^2|\Lambda|, \qquad (4.16)
\end{aligned}$$

where $V_{x,y}=\omega_0^{-1}\sum_{z\in\Lambda}g_{x,z}g_{y,z}$. Therefore, we finally obtain

$$\begin{aligned}
&e^{i\frac{\pi}{2}N_{\rm p}}e^{L_c}He^{-L_c}e^{-i\frac{\pi}{2}N_{\rm p}}\\
&=-T_\uparrow^+-T_\downarrow^++\sum_{x\in\Lambda,u\in\Omega}J_{x,u}\boldsymbol{s}_x\cdot\boldsymbol{S}_u+\mathbb{U}_{\rm eff}+\omega_0N_{\rm p}-\omega_0^{-1}g^2|\Lambda|. \qquad (4.17)
\end{aligned}$$

□

Remark 4.8. With the Lang–Firsov transformation, we can see from Lemma 4.7 that the effect of the electron-phonon interaction appears only in the hopping matrix. At first glance, this may seem complicated, but as we will see below, spin reflection positivity can be applied to this model in this representation.

Lemma 4.9. *Let H' be the Lang–Firsov transformed Hamiltonian:*

$$H'=-T_\uparrow^+-T_\downarrow^++\sum_{x\in\Lambda,u\in\Omega}J_{x,u}\boldsymbol{s}_x\cdot\boldsymbol{S}_u+\mathbb{U}_{\rm eff}. \qquad (4.18)$$

Let U be the hole-particle transformation given by (3.14). Then we have

$$U^*H'U=R-\frac{1}{2}\sum_{x\in\Lambda,u\in\Omega}|J_{x,u}|\left(c_{x\uparrow}^*f_{u\uparrow}c_{x\downarrow}^*f_{u\downarrow}+f_{u\uparrow}^*c_{x\uparrow}f_{u\downarrow}^*c_{x\downarrow}\right)-\tilde{\mathbb{U}}, \qquad (4.19)$$

where

$$R=-T_\uparrow^+-T_\downarrow^-+\frac{1}{4}\sum_{x\in\Lambda,u\in\Omega}J_{x,u}(n_x^c-1)(n_u^f-1)+\sum_{x,y\in\Lambda}U_{{\rm eff},x,y}(n_{x\uparrow}^cn_{y\uparrow}^c+n_{x\downarrow}^cn_{y\downarrow}^c), \qquad (4.20)$$

$$\tilde{\mathbb{U}}=2\sum_{x,y\in\Lambda}U_{{\rm eff},x,y}n_{x\uparrow}^cn_{y\downarrow}^c. \qquad (4.21)$$

Proof. By using (C.1) and (C.3), we have

$$
\begin{aligned}
U^*(T_\uparrow^+ + T_\downarrow^+)U &= T_\uparrow^+ + \sum_{x,y\in\Lambda} t_{x,y}\gamma_x\gamma_y c_{x\downarrow}c_{y\downarrow}^* \exp(i\Phi_{x,y}) \\
&= T_\uparrow^+ - \sum_{x,y\in\Lambda} t_{x,y} c_{x\downarrow}c_{y\downarrow}^* \exp(i\Phi_{x,y}) \\
&= T_\uparrow^+ + \sum_{x,y\in\Lambda} t_{x,y} c_{y\downarrow}^* c_{x\downarrow} \exp(-i\Phi_{y,x}) \\
&= T_\uparrow^+ + T_\downarrow^-, \qquad (4.22)\\
U^*\mathbb{U}U &= \sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}(n_{x\uparrow}^c - n_{x\downarrow}^c)(n_{y\uparrow}^c - n_{y\downarrow}^c) \\
&= \sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}(n_{x\uparrow}^c n_{y\uparrow}^c + n_{x\downarrow}^c n_{y\downarrow}^c) - 2\sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y} n_{x\uparrow}^c n_{y\downarrow}^c, \qquad (4.23)
\end{aligned}
$$

and

$$
\begin{aligned}
&U^* \sum_{x\in\Lambda,u\in\Omega} J_{x,u}\boldsymbol{s}_x\cdot\boldsymbol{S}_u U \\
&= \sum_{x\in\Lambda,u\in\Omega} J_{x,u}U^*\Big(\frac{1}{2}s_x^+S_u^- + \frac{1}{2}s_x^-S_u^+ + s_x^{(3)}S_u^{(3)}\Big)U \\
&= \sum_{x\in\Lambda,u\in\Omega} J_{x,u}U^*\Big\{\frac{1}{2}c_{x\uparrow}^*c_{x\downarrow}f_{u\downarrow}^*f_{u\uparrow} + \frac{1}{2}c_{x\downarrow}^*c_{x\uparrow}f_{u\uparrow}^*f_{u\downarrow} + \frac{1}{4}(n_{x\uparrow}^c - n_{x\downarrow}^c)(n_{u\uparrow}^f - n_{u\downarrow}^f)\Big\}U \\
&= -\frac{1}{2}\sum_{x\in\Lambda,u\in\Omega} |J_{x,u}|\left(c_{x\uparrow}^*f_{u\uparrow}c_{x\downarrow}^*f_{u\downarrow} + f_{u\uparrow}^*c_{x\uparrow}f_{u\downarrow}^*c_{x\downarrow}\right) + \frac{1}{4}\sum_{x\in\Lambda,u\in\Omega} J_{x,u}(n_x^c-1)(n_u^f-1).
\end{aligned} \tag{4.24}
$$

Combining (4.22) and (4.24), we conclude (4.19). □

Corollary 4.10. *Define*

$$\mathcal{U} = e^{-L_c}e^{-i\frac{\pi}{2}N_{\mathrm{p}}}U. \tag{4.25}$$

Then we have

$$\mathcal{U}^*H\mathcal{U} = R - \mathbb{J} - \tilde{\mathbb{U}} + \omega_0 N_{\mathrm{p}} - \omega_0^{-1}g^2|\Lambda|. \tag{4.26}$$

4.4 The uniqueness of ground states

4.4.1 Positivity preservingness of the semigroup

Here, we show that the heat semigroup generated by the Hamiltonian is positivity preserving. Due to the effect of the electron-phonon interaction, the proof is more complicated than the corresponding Propositon 3.9 condering the Kondo lattice model.

Lemma 4.11. *For each $x, y \in \Lambda$ and $\boldsymbol{q} = (q_z)_{z\in\Lambda} \in \mathbb{R}^{|\Lambda|}$, define*

$$
\begin{aligned}
R(\boldsymbol{q}) = &-\sum_{x,y\in\Lambda} t_{x,y}c_{x\uparrow}^*c_{y\uparrow}\exp\left(i\Phi_{x,y}(\boldsymbol{q})\right) - \sum_{x,y\in\Lambda} t_{x,y}c_{x\downarrow}^*c_{y\downarrow}\exp\left(-i\Phi_{x,y}(\boldsymbol{q})\right) \\
&+\frac{1}{4}\sum_{x\in\Lambda,u\in\Omega} J_{x,u}(n_x^c-1)(n_u^f-1) + \sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}(n_{x\uparrow}^c n_{y\uparrow}^c + n_{x\downarrow}^c n_{y\downarrow}^c),
\end{aligned} \tag{4.27}
$$

where $\Phi_{x,y}(\boldsymbol{q}) = \frac{\sqrt{2}}{\omega_0}\sum_{z\in\Lambda}(g_{xz} - g_{yz})q_z$. *Then we have* $e^{-\beta R(\boldsymbol{q})} \trianglerighteq 0$ *w.r.t.* $\mathcal{Q}_{\mathrm{KL}}$ *for any* $\boldsymbol{q} \in \Lambda \in \mathbb{R}^{|\Lambda|}$ *and* $\beta \geq 0$.

Proof. By the definition of Q_0, $n^f_{u\uparrow} = n^f_{u\downarrow}$ holds on $Q_0\mathcal{L}_N$. Hence, by (3.7),

$$\begin{aligned}
&\sum_{x\in\Lambda,u\in\Omega} J_{x,u}(n^c_x - 1)(n^f_u - 1) + 4\sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}(n^c_{x\uparrow}n^c_{y\uparrow} + n^c_{x\downarrow}n^c_{y\downarrow}) \\
&= \sum_{x\in\Lambda,u\in\Omega} J_{x,u}\left(n^c_x n^f_u - n^c_x - n^f_u + 1\right) + 4\sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}(n^c_{x\uparrow}n^c_{y\uparrow} + n^c_{x\downarrow}n^c_{y\downarrow}) \\
&= \sum_{x\in\Lambda,u\in\Omega} J_{x,u}\left(2n^c_{x\uparrow}n^f_{u\uparrow} + 2n^c_{x\downarrow}n^f_{u\downarrow} - n^c_{x\uparrow} - n^f_{u\uparrow} - n^c_{x\downarrow} - n^f_{u\downarrow} + 1\right) \\
&\quad + 4\sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}(n^c_{x\uparrow}n^c_{y\uparrow} + n^c_{x\downarrow}n^c_{y\downarrow}) \\
&= \sum_{x\in\Lambda,u\in\Omega} J_{x,u}\left(2n^c_{x\uparrow}n^f_{u\uparrow} - n^c_{x\uparrow} - n^f_{u\uparrow} + \frac{1}{2}\right) + 4\sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}n^c_{x\uparrow}n^c_{y\uparrow} \\
&\quad + \sum_{x\in\Lambda,u\in\Omega} J_{x,u}\left(2n^c_{x\downarrow}n^f_{u\downarrow} - n^c_{x\downarrow} - n^f_{u\downarrow} + \frac{1}{2}\right) + 4\sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}n^c_{x\downarrow}n^c_{y\downarrow} \\
&= \mathcal{L}(\mathsf{J}_{\mathsf{n}}) + \mathcal{R}(\vartheta \mathsf{J}_{\mathsf{n}}\vartheta)
\end{aligned} \tag{4.28}$$

on $Q_0\mathcal{L}_N$, where

$$\mathsf{J}_{\mathsf{n}} = \sum_{x\in\Lambda,u\in\Omega} J_{x,u}\left(2\mathsf{n}^c_x\mathsf{n}^f_u - \mathsf{n}^c_x - \mathsf{n}^f_u + \frac{1}{2}\right) + 4\sum_{x,y\in\Lambda} U_{\mathrm{eff},x,y}\mathsf{n}^c_x\mathsf{n}^c_y. \tag{4.29}$$

We set

$$\mathsf{J}_{\mathsf{c}}(\boldsymbol{q}) = -\sum_{x,y\in\Lambda} t_{x,y}\mathsf{c}^*_x\mathsf{c}_y\exp(i\Phi_{x,y}(\boldsymbol{q})). \tag{4.30}$$

Then using (4.28), we find that

$$R(\boldsymbol{q}) = \mathcal{L}(\mathsf{J}_{\mathsf{c}}(\boldsymbol{q})) + \mathcal{R}(\vartheta\mathsf{J}_{\mathsf{c}}(\boldsymbol{q})\vartheta) + \frac{1}{4}\mathcal{L}(\mathsf{J}_{\mathsf{n}}) + \frac{1}{4}\mathcal{R}(\vartheta\mathsf{J}_{\mathsf{n}}\vartheta) \tag{4.31}$$

holds on $Q_0\mathcal{L}_N$. Thus, we can write $R(\boldsymbol{q})$ as $R(\boldsymbol{q}) = \mathsf{R}(\boldsymbol{q})\otimes 1 + 1\otimes\vartheta\mathsf{R}(\boldsymbol{q})\vartheta$ with

$$\mathsf{R}(\boldsymbol{q}) = \mathsf{J}_{\mathsf{c}}(\boldsymbol{q}) + \frac{1}{4}\mathsf{J}_{\mathsf{n}}. \tag{4.32}$$

Using this expression and Lemma 3.8, we can conclude that $e^{-\beta R(\boldsymbol{q})} \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$ for each $\boldsymbol{q} \in \Lambda \in \mathbb{R}^{|\Lambda|}$ and $\beta \geq 0$. □

Proposition 4.12. *Suppose that* U_{eff} *is positive semi-definite. For all* $\beta \geq 0$, *one has* $e^{-\beta\mathcal{U}^*H\mathcal{U}} \trianglerighteq 0$ *w.r.t.* $\mathcal{Q}$.

Proof. By Lemmas 4.4 and 4.11, we have

$$e^{-\beta R} = \int^{\oplus}_{\mathbb{R}^{|\Lambda|}} e^{-\beta R(\boldsymbol{q})}\,d\boldsymbol{q} \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}. \tag{4.33}$$

Next, we will show that

$$\tilde{\mathbb{U}} \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}. \tag{4.34}$$

Note that $\tilde{\mathbb{U}}$ commutes with Q_0. Hence, taking Lemmas 2.35 and 4.5 into account, it suffices to prove that $\tilde{\mathbb{U}} \trianglerighteq 0$ w.r.t. $\mathcal{E}_{\text{KL}}$. Using the identifications (3.4), we can express $\tilde{\mathbb{U}}$ as

$$\tilde{\mathbb{U}} = 2 \sum_{x,y\in\Lambda} U_{\text{eff},x,y} \mathsf{n}_x^c \otimes \vartheta \mathsf{n}_y^c \vartheta. \tag{4.35}$$

Hence, by Proposition 2.32, we conclude that $\tilde{\mathbb{U}} \trianglerighteq 0$ w.r.t. $\mathcal{Q}$.

Recall the definition of $\mathbb{J}$, i.e., (3.19). We already proved that

$$\mathbb{J} \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}. \tag{4.36}$$

in the proof of Proposition 3.9. Hence, by applying Lemma 4.6, we readily confirm that

$$\exp\left[\frac{\beta}{n}(\mathbb{J}+\tilde{\mathbb{U}})\right] \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q} \tag{4.37}$$

for all $\beta \ge 0$ and $n \in \mathbb{N}$. By the Trotter product formula [20, Theorem S.20], we have

$$\begin{aligned} \exp\left[-\beta \mathcal{U}^* H \mathcal{U}\right] &= \exp\left[-\beta R + \beta\mathbb{J} + \beta\tilde{\mathbb{U}} - \beta\omega_0 N_{\text{p}} + \beta\omega_0^{-1} g^2|\Lambda|\right] \\ &= e^{\beta\omega_0^{-1}g^2|\Lambda|} \text{s-}\lim_{n\to\infty}\left\{\exp\left[-\frac{\beta}{n}R\right]\exp\left[\frac{\beta}{n}(\mathbb{J}+\tilde{\mathbb{U}})\right]\exp\left[-\frac{\beta}{n}\omega_0 N_{\text{p}}\right]\right\}^n. \end{aligned} \tag{4.38}$$

Using (2.51), (4.33) and (4.37), we see that the right hand side of (4.38) is positivity preserving w.r.t. $\mathcal{Q}$ for all $\beta \ge 0$. □

4.4.2 The positivity improvingness of the semigroup

In order to show the uniqueness of the ground state of H, we prove that the heat semigroup generated by H is positivity improving. We will prepare some lemmas necessary for this purpose.

Lemma 4.13. *Let* $(\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f), (\boldsymbol{\sigma}_c', \boldsymbol{\sigma}_f') \in E_N$. *Let* $g, h \in \mathcal{P} \setminus \{0\}$. *Set*

$$S(t) = \left\langle \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f, g \left| e^{-t\left(R - \frac{1}{2}\mathbb{J} + \omega_0 N_{\text{p}}\right)} \right| \boldsymbol{\sigma}_c', \boldsymbol{\sigma}_c', \boldsymbol{\sigma}_f', \boldsymbol{\sigma}_f', h \right\rangle, \quad 0 < t < 1, \tag{4.39}$$

where $\left|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f, g\right\rangle = \left|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f\right\rangle \otimes g$.

Assume either

(i) *there exist* $x, y \in \Lambda$ *such that* $t_{x,y} \neq 0$ *and* $\left|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f\right\rangle = c_{x\uparrow}^* c_{y\uparrow} c_{x\downarrow}^* c_{y\downarrow} \left|\boldsymbol{\sigma}_c', \boldsymbol{\sigma}_c', \boldsymbol{\sigma}_f', \boldsymbol{\sigma}_f'\right\rangle$,

or

(ii) *there exist* $x \in \Lambda, u \in \Omega$ *such that* $J_{x,u} \neq 0$ *and* $\left|\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f\right\rangle = (c_{x\uparrow}^* f_{u\uparrow} c_{x\downarrow}^* f_{u\downarrow} + f_{u\uparrow}^* c_{x\uparrow} f_{u\downarrow}^* c_{x\downarrow}) \left|\boldsymbol{\sigma}_c', \boldsymbol{\sigma}_c', \boldsymbol{\sigma}_f', \boldsymbol{\sigma}_f'\right\rangle$.

Then there exists a $\gamma(g,h)>0$ depending on g and h such that if $0<t<\gamma(g,h)$, then $S(t)>0$ holds.

Proof. See [14, Appendix C] . □

Lemma 4.14. *Let $n\in\mathbb{N}$ and $\beta>0$. For each $j=1,\dots,n+1$, let $\{G_j(s)\}_{s\ge0}$ be a family of bounded self-adjoint operators on $L^2(\mathbb{R}^{|\Lambda|})$. Assume the following:*

(i) *$G_j(s)\trianglerighteq 0$ w.r.t. $\mathcal{P}$ for all $s\ge0$ and $j=1,\dots,n+1$.*

(ii) *For any given $g,h\in\mathcal{P}\setminus\{0\}$ and $j=1,\dots,n$, there exists a $\gamma_j(g,h)>0$ such that if $0<s<\gamma_j(g,h)$, then $\langle g,G_j(s)h\rangle>0$ holds.*

(iii) *For any given $g,h\in\mathcal{P}\setminus\{0\}$, there exists a $\gamma_{n+1}>0$, independent of g and h, such that if $0<s<\gamma_{n+1}$, then $\langle g,G_{n+1}(s)h\rangle>0$ holds.*

Then, for any given $g,h\in\mathcal{P}\setminus\{0\}$ and $\beta>0$, there exist positive numbers $s_1,\dots,s_n$ with $\sum_{j=1}^n s_j<\beta$ such that

$$\langle g,G_1(s_1)G_2(s_2)\cdots G_n(s_n)G_{n+1}(s)^k h\rangle>0. \tag{4.40}$$

holds for any $k\in\mathbb{N}$ and $0<s<\gamma_{n+1}$.

Proof. If $0<s_1<\min\{\gamma_1(g,h),\beta/n\}$, then

$$\langle g,G_1(s_1)h\rangle>0 \tag{4.41}$$

holds due to the condition (ii). Hence, using (i), we conclude that $G_1(s_1)g\in\mathcal{P}\setminus\{0\}$. For $j=2,\dots,n$, choose s_j such that

$$0<s_j<\min\Big\{\gamma_j\big(G_{j-1}(s_{j-1})\cdots G_1(s_1)g,h\big),\frac{\beta}{n}\Big\}. \tag{4.42}$$

Then $\langle g,G_1(s_1)\cdots G_j(s_j)h\rangle>0$ holds, which implies that $G_j(s_j)\cdots G_1(s_1)g\in\mathcal{P}\setminus\{0\}$. By induction on j, there are positive numbers $s_1,\dots,s_n$ with $\sum_{j=1}^n s_j<\beta$ such that $G_n(s_n)\cdots G_1(s_1)g\in\mathcal{P}\setminus\{0\}$ holds. Because of the condition (iii), it holds that

$$G_{n+1}(s)\rhd 0 \text{ w.r.t. } \mathcal{P}, \tag{4.43}$$

if $0<s<\gamma_{n+1}$. Hence, we have $G_{n+1}(s)^k\rhd0$ w.r.t. $\mathcal{P}$. Therefore, for any $k\in\mathbb{N}$,

$$\langle g,G_1(s_1)G_2(s_2)\cdots G_n(s_n)G_{n+1}(s)^k h\rangle>0 \tag{4.44}$$

holds, provided that $0<s<\gamma_{n+1}$. □

Lemma 4.15. *Let $\boldsymbol{\sigma}\in E_N$ and $g,h\in\mathcal{P}\setminus\{0\}$. Set*

$$\alpha=2\sum_{x,y\in\Lambda}|t_{x,y}|+\sum_{x\in\Lambda,u\in\Omega}|J_{x,u}|+2\sum_{x,y\in\Lambda}|U_{\mathrm{eff},x,y}|+\frac{1}{2}\|\mathbb{J}\|. \tag{4.45}$$

If $0<t<e^{-\alpha}$, then we have

$$\langle\boldsymbol{\sigma},\boldsymbol{\sigma},g|e^{-t(R-\frac12\mathbb{J}+\omega_0N_{\mathrm{p}})}|\boldsymbol{\sigma},\boldsymbol{\sigma},h\rangle>0. \tag{4.46}$$

Proof. Set $X = R - \frac{1}{2}\mathbb{J}$. By using the Duhamel formula, we have

$$
\begin{aligned}
&\langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, g | e^{-t(R-\frac{1}{2}\mathbb{J}+\omega_0 N_{\mathrm{p}})} | \boldsymbol{\sigma}, \boldsymbol{\sigma}, h\rangle \\
&= \left\langle g, e^{-t\omega_0 N_{\mathrm{p}}} h \right\rangle \\
&\quad + \sum_{n\geq 1} (-t)^n \int_{0\leq s_1 \leq \cdots \leq s_m \leq 1} \left\langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, g \middle| e^{-s_1 t\omega_0 N_{\mathrm{p}}} X \cdots X e^{-(1-s_n)t\omega_0 N_{\mathrm{p}}} \middle| \boldsymbol{\sigma}, \boldsymbol{\sigma}, h \right\rangle ds_n \cdots ds_1 \\
&\geq \left\langle g, e^{-t\omega_0 N_{\mathrm{p}}} h \right\rangle \\
&\quad - \sum_{n\geq 1} \frac{t^n}{n!} \left(2 \sum_{x,y\in\Lambda} |t_{x,y}| + \sum_{x\in\Lambda, u\in\Omega} |J_{x,u}| + 2 \sum_{x,y\in\Lambda} |U_{\mathrm{eff},x,y}| + \frac{1}{2}\|\mathbb{J}\| \right)^n \left\langle g, e^{-t\omega_0 N_{\mathrm{p}}} h \right\rangle \\
&\geq \left\langle g, e^{-t\omega_0 N_{\mathrm{p}}} h \right\rangle - t \sum_{n\geq 1} \frac{\alpha^n}{n!} \left\langle g, e^{-t\omega_0 N_{\mathrm{p}}} h \right\rangle \\
&\geq (1 - te^{\alpha}) \left\langle g, e^{-t\omega_0 N_{\mathrm{p}}} h \right\rangle, \qquad (4.47)
\end{aligned}
$$

where in the first inequality, we have used Lemma 2.40. Because $e^{-t\omega_0 N_{\mathrm{p}}} \rhd 0$ w.r.t. $\mathcal{P}$, we have $\langle g, e^{-t\omega_0 N_{\mathrm{p}}} h\rangle > 0$. Hence, the right hand side of (4.47) is strictly positive. □

Proposition 4.16. *Set*

$$\mathcal{I} = \{ |\boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle \otimes f \,|\, (\boldsymbol{\sigma}, \boldsymbol{\sigma}') \in E_N,\ f \in \mathcal{P} \setminus \{0\} \}. \qquad (4.48)$$

For any $u \in \mathcal{Q} \setminus \{0\}$, there exists a $\varphi \in \mathcal{I}$ such that

$$(JN + \mathbb{J})^N u \geq \varphi \ \text{w.r.t. } \mathcal{Q}. \qquad (4.49)$$

Proof. Recall (3.75), that is, for each $(\boldsymbol{\sigma}, \boldsymbol{\sigma}') \in E_N$,

$$\left(\frac{8}{J^2}\right)^{\frac{N}{2}} (JN + \mathbb{J})^N \unrhd |\boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle\langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'| \text{ w.r.t. } \mathcal{Q}. \qquad (4.50)$$

Define $u_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \in \mathcal{P}$ by $u_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}(\boldsymbol{q}) = \langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}' | u(\boldsymbol{q})\rangle$. Then we obtain

$$
\begin{aligned}
|\boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle\langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'| u &= \int_{\mathbb{R}^{|\Lambda|}}^{\oplus} \langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}' | u(\boldsymbol{q})\rangle |\boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle \, d\boldsymbol{q} \\
&= |\boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle \otimes u_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}. \qquad (4.51)
\end{aligned}
$$

Suppose that $u_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} = 0$ for any $(\boldsymbol{\sigma}, \boldsymbol{\sigma}') \in E_N$. Let μ be the Lebesgue measure on $\mathbb{R}^{|\Lambda|}$ and set

$$D_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} = \{ \boldsymbol{q} \in \mathbb{R}^{|\Lambda|} \,|\, \langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}' | u(\boldsymbol{q})\rangle > 0 \}. \qquad (4.52)$$

Since $\langle \boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}' | u(\boldsymbol{q})\rangle = 0$ a.e. $\boldsymbol{q}$ for any $(\boldsymbol{\sigma}, \boldsymbol{\sigma}') \in E_N$, $\mu(D_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}) = 0$ holds. Therefore,

$$\mu\left(\bigcup_{(\boldsymbol{\sigma},\boldsymbol{\sigma}')\in E_N} D_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \right) = 0 \qquad (4.53)$$

holds because $\mathcal{H}_{\mathrm{KL}}$ is a finite dimensional linear space. Hence, by Lemma 2.30, we have $u(\boldsymbol{q}) = 0$ a.e. $\boldsymbol{q}$. This contradicts with $u \neq 0$. Thus, there exists a $(\boldsymbol{\sigma}, \boldsymbol{\sigma}') \in E_N$ with $u_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \neq 0$. Then $\alpha|\boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle \otimes u_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \in \mathcal{I}$ for any $\alpha > 0$ and we obtain

$$(JN + \mathbb{J})^N u \geq \left(\frac{J^2}{8}\right)^{\frac{N}{2}} |\boldsymbol{\sigma}, \boldsymbol{\sigma}, \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle \otimes u_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \text{ w.r.t. } \mathcal{Q}. \qquad (4.54)$$

□

Theorem 4.17. *Suppose that $U_{\rm eff}$ is positive semi-definite. Set $\widehat{H} = \mathcal{U}^* H \mathcal{U} + \omega_0^{-1} g^2 |\Lambda| - \frac{1}{2} JN$. Then we obtain $e^{-\beta \widehat{H}} \rhd 0$ w.r.t. $\mathcal{Q}$ for all $\beta > 0$.*

Proof. By applying Corollary 4.10, we have the following expression:

$$\widehat{H} = R - \mathbb{J} - \tilde{\mathbb{U}} + \omega_0 N_{\rm p} - \frac{1}{2} JN. \tag{4.55}$$

From Propositions 2.19 and 4.16, it suffices to prove that

$$\big\langle \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f, g \big| e^{-\beta \widehat{H}} \big| \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f, h \big\rangle > 0 \tag{4.56}$$

for any $\beta > 0$, $(\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f), (\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f) \in E_N$ and $g, h \in \mathcal{P} \setminus \{0\}$. Define

$$|\boldsymbol{\sigma}, g\rangle = |\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f, \boldsymbol{\sigma}_f, g\rangle, \tag{4.57}$$
$$|\boldsymbol{\sigma}', h\rangle = |\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f, \boldsymbol{\sigma}'_f, h\rangle. \tag{4.58}$$

By the Duhamel formula, we have

$$\begin{aligned} &\big\langle \boldsymbol{\sigma}, g \big| e^{-\beta \widehat{H}} \big| \boldsymbol{\sigma}', h \big\rangle \\ &= \sum_{m \ge 0} 2^{-m} \int_{0 \le s_1 \le \cdots \le s_m \le \beta} \big\langle \boldsymbol{\sigma}, g \big| e^{-s_1 Y} X' \cdots X' e^{-(\beta - s_m) Y} \big| \boldsymbol{\sigma}', h \big\rangle \, ds_m \cdots ds_1, \end{aligned} \tag{4.59}$$

where $X = JN + \mathbb{J}$, $X' = X + 2\tilde{\mathbb{U}}$ and $Y = R - \frac{1}{2}\mathbb{J} + \omega_0 N_{\rm p}$. In the proof of Proposition 4.12, we have already proved that $\tilde{\mathbb{U}} \unrhd 0$ and $X \unrhd 0$ w.r.t. $\mathcal{Q}$. In addition, by using arguments similar to those of the proof of Proposition 4.12, we can show that $e^{-sY} \unrhd 0$ w.r.t. $\mathcal{Q}$ for each $s \ge 0$. Therefore, we obtain that

$$\big\langle \boldsymbol{\sigma}, g | e^{-s_1 Y} X_1 \cdots X_{n-1} e^{-(\beta - s_n) Y} | \boldsymbol{\sigma}', h \big\rangle \ge 0 \tag{4.60}$$

holds, provided that $0 \le s_1 \le \cdots \le s_n \le \beta$, where $X_i = X$ or $2\tilde{\mathbb{U}}$. Hence, we obtain the following lower bound:

$$\begin{aligned} &\big\langle \boldsymbol{\sigma}, g \big| e^{-\beta \widehat{H}} \big| \boldsymbol{\sigma}', h \big\rangle \\ &\ge 2^{-m} \int_{0 \le s_1 \le \cdots \le s_m \le \beta} \big\langle \boldsymbol{\sigma}, g \big| e^{-s_1 Y} X \cdots X e^{-(\beta - s_m) Y} \big| \boldsymbol{\sigma}', h \big\rangle \, ds_m \cdots ds_1. \end{aligned} \tag{4.61}$$

Because the integrand of the right hand side of (4.61) is continuous in $s_1, \dots, s_m$ with $0 \le s_1 \le \cdots \le \beta$, it suffices to prove that there exist $m \in \mathbb{N}$ and $s_1, \dots, s_m \in \mathbb{R}$ with $0 \le s_1 \le \cdots \le s_m \le \beta$ satisfying

$$\big\langle \boldsymbol{\sigma}, g \big| e^{-s_1 Y} X \cdots X e^{-(\beta - s_m) Y} \big| \boldsymbol{\sigma}', h \big\rangle > 0. \tag{4.62}$$

For each $(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2) \in E_N$,

$$\left(\frac{8}{J^2} \right)^{\frac{N}{2}} X^N \unrhd |\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_2\rangle \langle \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_2| \text{ w.r.t. } \mathcal{Q}. \tag{4.63}$$

Fix $k \in \mathbb{N}$, arbitrarily. Set $m = N(n + 2 + k)$ and define the function F by

$$F(s_1, \dots, s_m) = \left(\frac{8}{J^2} \right)^{\frac{m}{2}} \big\langle \boldsymbol{\sigma}, g \big| e^{-s_1 Y} X \cdots X e^{-(\beta - s_m) Y} \big| \boldsymbol{\sigma}', h \big\rangle. \tag{4.64}$$

Let $\{(\boldsymbol{\sigma}_{c,1}, \boldsymbol{\sigma}_{f,1}), \dots, (\boldsymbol{\sigma}_{c,n}, \boldsymbol{\sigma}_{f,n})\} \subseteq E_N$ be the sequence given in Lemma 3.14. Choose strictly positive numbers $t_1, \dots, t_{n+1}$ such that $0 < \varepsilon < \beta$, where $\varepsilon = \sum_{j=1}^{n+1} t_j$. We have

$$
\begin{aligned}
&F\left(\underbrace{0,\dots,0}_{N},\underbrace{t_1,\dots,t_1}_{N},\dots,\varepsilon,\dots,\varepsilon,\varepsilon+\frac{\beta-\varepsilon}{k},\dots,\varepsilon+\frac{\beta-\varepsilon}{k},\dots,\beta,\dots,\beta\right)\\
&=\left\langle \boldsymbol{\sigma}, g\middle| \left(\frac{8}{J^2}\right)^{\frac{N}{2}} X^N e^{-t_1 Y}\cdots e^{-t_{n+1}Y}\left(\frac{8}{J^2}\right)^{\frac{N}{2}} X^N \middle| \boldsymbol{\sigma}', h\right\rangle\\
&\overset{(4.63)}{\geq} \left\langle \boldsymbol{\sigma}, g\middle| \prod_{j=0}^{n}\left(|\boldsymbol{\sigma}_j\rangle\langle\boldsymbol{\sigma}_j|e^{-t_{j+1}Y}\right)\left(|\boldsymbol{\sigma}_{n+1}\rangle\langle\boldsymbol{\sigma}_{n+1}|e^{-\frac{\beta-\varepsilon}{k}Y}\right)^k |\boldsymbol{\sigma}_{n+1}\rangle\langle\boldsymbol{\sigma}_{n+1}|\middle|\boldsymbol{\sigma}', h\right\rangle\\
&=\left\langle \boldsymbol{\sigma}_0, g\middle| \prod_{j=0}^{n}\left(|\boldsymbol{\sigma}_j\rangle\langle\boldsymbol{\sigma}_j|e^{-t_{j+1}Y}\right)\left(|\boldsymbol{\sigma}_{n+1}\rangle\langle\boldsymbol{\sigma}_{n+1}|e^{-\frac{\beta-\varepsilon}{k}Y}\right)^k |\boldsymbol{\sigma}_{n+1}\rangle\langle\boldsymbol{\sigma}_{n+1}|\middle|\boldsymbol{\sigma}_{n+1}, h\right\rangle, \qquad (4.65)
\end{aligned}
$$

where in the first inequality, we used the inequality (4.63); in additon, we have used the fact that each $|\boldsymbol{\sigma}_j\rangle$ is positive w.r.t. $\mathcal{Q}_{\mathrm{KL}}$.

By [14, Proposition B.4], there exists the kernel operator $K_t(\boldsymbol{q}, \boldsymbol{q}')$ of e^{-tY}. In terms of $K_t(\boldsymbol{q}, \boldsymbol{q}')$, we have the following expressions:

$$\langle \boldsymbol{\sigma}_{j-1}, g|e^{-tY}|\boldsymbol{\sigma}_j, h\rangle = \int g(\boldsymbol{q})h(\boldsymbol{q}')\langle\boldsymbol{\sigma}_{j-1}|K_t(\boldsymbol{q},\boldsymbol{q}')|\boldsymbol{\sigma}_j\rangle d\boldsymbol{q}d\boldsymbol{q}', \quad j=1,\dots,n+1, \qquad (4.66)$$

$$\langle \boldsymbol{\sigma}_{n+1}, g|e^{-tY}|\boldsymbol{\sigma}_{n+1}, h\rangle = \int g(\boldsymbol{q})h(\boldsymbol{q}')\langle\boldsymbol{\sigma}_{n+1}|K_t(\boldsymbol{q},\boldsymbol{q}')|\boldsymbol{\sigma}_{n+1}\rangle d\boldsymbol{q}d\boldsymbol{q}'. \qquad (4.67)$$

With this in mind, we define $K_j(t) \in \mathscr{B}(L^2(\mathbb{R}^{|\Lambda|}))$ by

$$\langle g, K_j(t)h\rangle = \text{the right hand side of (4.66)}, \quad j=1,\dots,n+1, \qquad (4.68)$$

$$\langle g, K_{n+2}(t)h\rangle = \text{the right hand side of (4.67)}. \qquad (4.69)$$

Note that $K_t(\boldsymbol{q}, \boldsymbol{q}') \trianglerighteq 0$ w.r.t. $\mathcal{Q}_{\mathrm{KL}}$ holds due to [14, Proposition B.4]. Hence, we have

$$\langle\boldsymbol{\sigma}_{j-1}|K_t(\boldsymbol{q},\boldsymbol{q}')|\boldsymbol{\sigma}_j\rangle \geq 0, \quad \langle\boldsymbol{\sigma}_{n+1}|K_t(\boldsymbol{q},\boldsymbol{q}')|\boldsymbol{\sigma}_{n+1}\rangle \geq 0 \qquad (4.70)$$

for a.e. $\boldsymbol{q}, \boldsymbol{q}'$, which imply that $K_j(t) \trianglerighteq 0$ w.r.t. $\mathcal{P}$ for all $t \geq 0$ and $j = 1, \dots, n+2$. Rewriting the right hand side of (4.65) by using $K_j(t)$, we get

$$
\begin{aligned}
&F\left(0,\dots,0,t_1,\dots,t_1,\dots,\varepsilon,\dots,\varepsilon,\varepsilon+\frac{\beta-\varepsilon}{k},\dots,\varepsilon+\frac{\beta-\varepsilon}{k},\dots,\beta,\dots,\beta\right)\\
&\geq \left\langle g, K_1(t_1)K_2(t_2)\cdots K_{n+1}(t_{n+1})K_{n+2}\left(\frac{\beta-\varepsilon}{k}\right)^k h\right\rangle. \qquad (4.71)
\end{aligned}
$$

By Lemmas 4.13 and 3.14, we see that for any $g, h \in \mathcal{P}\setminus\{0\}$, $\langle g, K_j(t)h\rangle > 0$ holds, provided that $0 < t < \gamma(g, h)$. Because $\varepsilon < \beta$, there exists a $k \in \mathbb{N}$ such that $\frac{\beta-\varepsilon}{k} < e^{-\alpha}$. In the remainder of the proof, we assume that k satisfies this inequality. We are aiming to apply Lemma 4.14 with the correspondence $G_j(t) = K_j(t)$. For this purpose, we have to check the assumptions (i)-(iii) of Lemma 4.14. We readily check (i) and (ii); by using

Lemma 4.15, we can confirm that the assumption (iii) is satisfied. Hence, from Lemma 4.14, there exist $t_1, \dots, t_{n+1} > 0$ with $\sum_{j=1}^{n+1} t_j < \beta$ such that

$$\left\langle g, K_1(t_1) \cdots K_{n+1}(t_{n+1}) K_{n+2} \left(\frac{\beta - \varepsilon}{k} \right)^k h \right\rangle > 0 \tag{4.72}$$

holds. Hence, by (4.71) , we have

$$F\left(0, \dots, 0, t_1, \dots, t_1, \dots, \varepsilon, \dots, \varepsilon, \varepsilon + \frac{\beta - \varepsilon}{k}, \dots, \varepsilon + \frac{\beta - \varepsilon}{k}, \dots, \beta, \dots, \beta\right) > 0. \tag{4.73}$$

Therefore, for any $(\boldsymbol{\sigma}_c, \boldsymbol{\sigma}_f), (\boldsymbol{\sigma}'_c, \boldsymbol{\sigma}'_f) \in E_N$ and $g, h \in \mathcal{P} \setminus \{0\}$,

$$\left\langle \boldsymbol{\sigma}, g \left| e^{-\beta \widehat{H}} \right| \boldsymbol{\sigma}', h \right\rangle > 0 \tag{4.74}$$

holds. Hence, we conclude that $e^{-\beta \widehat{H}} \rhd 0$ w.r.t. $\mathcal{Q}$ for all $\beta > 0$. □

4.5 The total spin of the ground state

4.5.1 The main result in Section 4.5

We already proved the uniqueness of the ground state of H in Theorem 4.1. Our goal in this section is to prove the following theorem.

Theorem 4.18. *Assume* **(C)**. *Assume that $U_{\rm eff}$ is positive semi-definite. Then we have the following* (i) *and* (ii)*:*

(i) *If* (C.6) *holds, then the ground state of H has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$.*

(ii) *If* (C.7) *holds, then the ground state of H has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_2| - |\Lambda_2| - |\Omega_1|\big|$.*

The basic strategy of the proof is the similar to that of Theorem 3.2 in Section 3. However, due to the effect of the electron-phonon interaction, some parts of the proof must be changed. In what follows, we clarify these changes and give the proof of Theorem 4.18.

4.5.2 The case of antiferromagnetic coupling

Set

$$L_2 = \boldsymbol{K}_1 + \omega_0 N_{\rm p}. \tag{4.75}$$

Trivially, L_2 is self-adjoint on $\mathrm{dom}(N_{\rm p})$ and bounded from below. Recall the definition of $\mathcal{Q}$, i.e, (4.2).

Lemma 4.19. *Assume* **(C)** *and* (C.6)*. Then we have*

$$\exp\left[-\beta U^* L_2 U\right] \rhd 0 \ \textit{w.r.t.}\ \mathcal{Q} \tag{4.76}$$

for any $\beta > 0$. Hence, the ground state of L_2 is unique. In addition, the ground state of L_2 has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$.

Proof. Since $\boldsymbol{K}$ commutes with $N_{\rm p}$ and $\exp(-\beta N_{\rm p}) \trianglerighteq 0$w.r.t. $\mathcal{P}$ for any $\beta > 0$, we have

$$\exp\left[-\beta U^* L_2 U\right] = \exp\left[-\beta U^* \boldsymbol{K} U\right] e^{-\beta\omega_0 N_{\rm p}} \trianglerighteq 0 \text{ w.r.t. } \mathcal{Q}, \tag{4.77}$$

where we have used (2.51) and (3.92). Let ψ be the ground state of $\boldsymbol{K}_1$ and let η_0 be the bosonic Fock vacuum in $\mathcal{H}_{\rm ph}$. Trivially, the vector $\psi \otimes \eta_0$ is the ground state of L_2. Since the vector ψ has total spin $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_1| - |\Lambda_2| - |\Omega_2|\big|$ due to Proposition 3.18, $\psi \otimes \eta_0$ has the same total spin. □

Due to the effect of the electron-phonon interaction, Proposition 3.16 cannot be applied directly. The following lemma is an extension of Proposition 3.16 that can be applied in the presence of the electron-phonon interaction.

Lemma 4.20. *Set $\mathcal{X} = Q_0\mathcal{L}_N \otimes \mathcal{H}_{\rm ph}$. Let A and B be self-adjoint operators on $\mathcal{H}$, bounded from below, where $\mathcal{H}$ is defined by (1.21). Let $V_1 \in \mathscr{B}(\mathcal{H})$ be unitary and let $V_2 \in \mathscr{B}(\mathcal{X}, \mathcal{H})$ be isometry. We assume the following:*

(i) *A and B commute with the total spin operators $S^{(3)}_{\rm tot}, S^+_{\rm tot}$ and $S^-_{\rm tot}$.*

(ii) *Let $V = V_1V_2$. $e^{-sV^*AV} \trianglerighteq 0$ and $e^{-tV_2^*BV_2} \trianglerighteq 0$ w.r.t. $\mathcal{Q}$ for some $s, t > 0$.*

(iii) *V_1 commutes with $\boldsymbol{S}^2_{\rm tot}$.*

(iv) *$\inf\operatorname{spec}(A)$ (resp. $\inf\operatorname{spec}(B)$) is an eigenvalue of A (resp. B).*

We denote by S_A (resp. S_B) the total spin of the ground state of A (resp. B). Then we have $S_A = S_B$.

Proof. We denote by ψ_A (resp. ψ_B) the ground state of V^*AV (resp. $V_2^*BV_2$). By the assumption (ii), ψ_A and ψ_B are strictly positive w.r.t. $\mathcal{Q}$. Because $V\psi_A$ (resp. $V_2\psi_B$) is the ground state of A (resp. B), we have

$$\boldsymbol{S}^2_{\rm tot} V\psi_A = S_A(S_A+1)V\psi_A, \tag{4.78}$$

$$\boldsymbol{S}^2_{\rm tot} V_2\psi_B = S_B(S_B+1)V_2\psi_B. \tag{4.79}$$

Applying the assumption (iii), we readily confirm that

$$\boldsymbol{S}^2_{\rm tot} V_2\psi_A = S_A(S_A+1)V_2\psi_A. \tag{4.80}$$

Using the strict positivity of ψ_A and ψ_B, we have

$$\langle V_2\psi_A, V_2\psi_B\rangle = \langle \psi_A, \psi_B\rangle > 0. \tag{4.81}$$

Therefore, by applying the method of nonzero overlap between the ground states, we have

$$\begin{aligned} S_A(S_A+1)\langle V_2\psi_A, V_2\psi_B\rangle &= \langle \boldsymbol{S}^2_{\rm tot} V_2\psi_A, V_2\psi_B\rangle \\ &= \langle V_2\psi_A, \boldsymbol{S}^2_{\rm tot} V_2\psi_B\rangle \\ &= S_B(S_B+1)\langle V_2\psi_A, V_2\psi_B\rangle, \end{aligned} \tag{4.82}$$

which implies that $S_A = S_B$. □

Proof of (i) of Theorem 4.18

Taking Theorem 4.17 and Lemma 4.19 into consideration, we can apply Lemma 4.20 with $V_1 = e^{-L_c}e^{-i\frac{\pi}{2}N_{\rm p}}$, $V_2 = U$, $V = V_1V_2 = \mathcal{U}$, $A = H$ and $B = L_2$. $\square$

4.5.3 The case of ferromagnetic coupling

The idea of proof of (ii) of Theorem 4.18 is parallel to that of the proof of (i). Therefore, we will provide a sketch only.

Using a method of proof similar to that applied to Lemma 4.19, we obtain the following:

Lemma 4.21. *Assume* **(C)** *and* **(C.7)**. *Set* $L_2' = \boldsymbol{K}_1' + \omega_0 N_{\rm p}$. *Then we have*

$$e^{-U^*L_2'U} \rhd 0 \ w.r.t.\ \mathcal{Q}. \tag{4.83}$$

Hence, the ground state of L_2' *is unique. In addition, the ground state of* L_2' *has total spin* $S = \frac{1}{2}\big||\Lambda_1| + |\Omega_2| - |\Lambda_2| - |\Omega_1|\big|$.

Proof of (ii) of Theorem 4.18

Taking Theorem 4.17 and Lemma 4.21 into consideration, we can apply Lemma 4.20 with $V_1 = e^{-L_c}e^{-i\frac{\pi}{2}N_{\rm p}}$, $V_2 = U$, $V = V_1V_2 = \mathcal{U}$, $A = H$ and $B = L_2'$. $\square$

A Basic properties of the Lang–Firsov transformation

In this appendix, we review some basic properties of the Lang–Firsov transformation.

For each $\theta \in \mathbb{R}$, we have

$$e^{i\theta N_{\rm p}} b_x e^{-i\theta N_{\rm p}} = e^{-i\theta} b_x. \tag{A.1}$$

Hence,

$$e^{i\frac{\pi}{2}N_{\rm p}} q_x e^{-i\frac{\pi}{2}N_{\rm p}} = p_x, \quad e^{i\frac{\pi}{2}N_{\rm p}} p_x e^{-i\frac{\pi}{2}N_{\rm p}} = -q_x, \tag{A.2}$$

where p_x and q_x are defined by (4.8).

Next, we set

$$L_c = -i\frac{\sqrt{2}}{\omega_0}\sum_{x,y\in\Lambda} g_{x,y} n_x^c p_y. \tag{A.3}$$

Then we readily confirm that

$$e^{L_c} c_{x\sigma} e^{-L_c} = \exp\left(i\frac{\sqrt{2}}{\omega_0}\sum_{y\in\Lambda} g_{x,y} p_y\right) c_{x\sigma}, \tag{A.4}$$

$$e^{L_c} f_{u\sigma} e^{-L_c} = f_{u\sigma}, \tag{A.5}$$

$$e^{L_c} b_x e^{-L_c} = b_x - \frac{1}{\omega_0}\sum_{y\in\Lambda} g_{y,x} n_y^c. \tag{A.6}$$

B Self-adjointness of the Hamiltonian of the Kondo lattice model with electron-phonon interaction

In this section, we prove the self-adjointness of the Hamiltonian H by applying the Kato–Rellich theorem.

B.1 The Kato–Rellich theorem

Definition B.1. Let A and B be densely defined linear operators on a Hilbert space $\mathcal{X}$. Assume that

(i) $\mathrm{dom}(A) \subset \mathrm{dom}(B)$,

(ii) For some $a, b \in \mathbb{R}$ and all $\varphi \in \mathrm{dom}(A)$,

$$\|B\varphi\| \le a\|A\varphi\| + b\|\varphi\|. \tag{B.1}$$

Then B is said to be A*-bounded*. The infimum of such a is called the *relative bound* of B with respect to A.

The following theorem is known as the Kato–Rellich theorem.

Theorem B.2 ([18]). *Let $\mathcal{X}$ be a Hilbert space. Let A and B be densely defined linear operators. Suppose that B is A-bounded with relative bound $a < 1$. Assume that A is self-adjoint and B is symmetric. Then $A + B$ is self-adjoint on* $\mathrm{dom}(A)$. *Further, if A is bounded from below, then $A + B$ is bounded from below.*

B.2 Proof of the self-adjointness of H

Lemma B.3. *We have following inequalities:*

$$\left\| b_x (N_\mathrm{p} + 1)^{-\frac{1}{2}} \right\| \le 1, \tag{B.2}$$

$$\left\| b_x^* (N_\mathrm{p} + 1)^{-\frac{1}{2}} \right\| \le 1. \tag{B.3}$$

Proof. Let $\mathcal{H}_{\mathrm{ph},0}$ be a finite-particle subspace in $\mathcal{H}_\mathrm{ph}$. For any $\varphi \in \mathcal{H}_{\mathrm{ph},0}$, we have

$$\left\| b_x (N_\mathrm{p} + 1)^{-\frac{1}{2}} \varphi \right\|^2 = \left\langle \varphi, (N_\mathrm{p} + 1)^{-\frac{1}{2}} b_x^* b_x (N_\mathrm{p} + 1)^{-\frac{1}{2}} \varphi \right\rangle \tag{B.4}$$

$$\le \left\langle \varphi, (N_\mathrm{p} + 1)^{-\frac{1}{2}} N_\mathrm{p} (N_\mathrm{p} + 1)^{-\frac{1}{2}} \varphi \right\rangle \tag{B.5}$$

$$\le \|\varphi\|^2. \tag{B.6}$$

Since $\mathcal{H}_{\mathrm{ph},0}$ is dense, we see that $b_x (N_\mathrm{p} + 1)^{-\frac{1}{2}}$ is a bounded operator. Therefore, (B.2) holds. Similarly, (B.3) holds. □

Lemma B.4. *For any $\varepsilon > 0$ and $\varphi \in \mathrm{dom}(N_\mathrm{p})$, we have*

$$\left\| (N_\mathrm{p} + 1)^{\frac{1}{2}} \varphi \right\| \le \varepsilon \|(N_\mathrm{p} + 1)\varphi\| + \frac{1}{4\varepsilon} \|\varphi\|. \tag{B.7}$$

Proof. Let $\varepsilon > 0$ and $\varphi \in \mathrm{dom}(N_\mathrm{p})$. By Schwarz's inequality and the elementary inequality $a^2 + b^2 \geq 2ab$ for each $a, b \geq 0$, we see that

$$\begin{aligned}\left\|(N_\mathrm{p}+1)^{\frac{1}{2}}\varphi\right\| &= \langle \varphi, (N_\mathrm{p}+1)\varphi\rangle^{\frac{1}{2}} \\ &\leq 2\sqrt{\varepsilon}\|(N_\mathrm{p}+1)\varphi\|^{\frac{1}{2}}\frac{1}{2\sqrt{\varepsilon}}\|\varphi\|^{\frac{1}{2}} \\ &\leq \varepsilon\|(N_\mathrm{p}+1)\varphi\| + \frac{1}{4\varepsilon}\|\varphi\|. \end{aligned} \tag{B.8}$$

□

Proposition B.5. *Let* $\mathbb{G} = \sum_{x,y\in\Lambda} g_{x,y} n_x^c (b_y^* + b_y)$*. Then* $\mathbb{G}$ *is* N_p*-bounded and the relative bound of* $\mathbb{G}$ *with respect to* N_p *is less than 1.*

Proof. Let $\varphi \in \mathcal{H}_{\mathrm{KL}} \otimes \mathrm{dom}(N_\mathrm{p})$. By Lemmas B.3 and B.4, for any $\varepsilon > 0$, we have

$$\begin{aligned}\|\mathbb{G}\varphi\| &= \left\|\sum_{x,y\in\Lambda} g_{x,y} n_x^c (b_y^* + b_y)(N_\mathrm{p}+1)^{-\frac{1}{2}}(N_\mathrm{p}+1)^{\frac{1}{2}}\varphi\right\| \\ &\leq 2\sum_{x,y\in\Lambda}|g_{x,y}|\left\|(b_y^* + b_y)(N_\mathrm{p}+1)^{-\frac{1}{2}}(N_\mathrm{p}+1)^{\frac{1}{2}}\varphi\right\| \\ &\leq 4\sum_{x,y\in\Lambda}|g_{x,y}|\left\|(N_\mathrm{p}+1)^{\frac{1}{2}}\varphi\right\| \\ &\leq 4\sum_{x,y\in\Lambda}|g_{x,y}|\left(\varepsilon\|(N_\mathrm{p}+1)\varphi\| + \frac{1}{4\varepsilon}\|\varphi\|\right). \end{aligned} \tag{B.9}$$

Hence, $\mathbb{G}$ is N_p-bounded. Since ε is arbitrary, we can take $\varepsilon > 0$ such that the relative bound $4\sum_{x,y\in\Lambda}|g_{x,y}|\varepsilon < 1$. □

Theorem B.6. H *is a self-adjoint operator on* $\mathcal{H}_{\mathrm{KL}} \otimes \mathrm{dom}(N_\mathrm{p})$ *which is bounded from below.*

Proof. From Theorem B.2 and Proposition B.5, we see that H is a self-adjoint operator. Furthermore, by Theorem B.2, H is bounded from below since N_p is bounded from below. □

C The Hubbard model

In this appendix, we prove Lieb's theorem concerning the Hubbard model for the convenience of readers. The idea of the proof given here is a basic guideline for analyzing the magnetic properties (Theorems 1.4 and 1.6) of the ground states of the KLM and the KLM with electron-phonon interaction in Sections 3 and 4. In contrast to Lieb's paper, our approach uses a new operator inequality to analyze the heat semigroup. This approach, first discovered by Miyao in [12], expresses the spin reflection positivity in terms of operator inequalities, and makes it possible to analyze models with more complex interactions such as the electron-phonon interactions.

The Hamiltonian of the Hubbard model is given by

$$H_{\mathrm{HM}} = \mathbb{T} + \mathbb{U}_0, \tag{C.1}$$

$$\mathbb{U}_0 = U_0\sum_{x\in\Lambda}\left(n_{x,\uparrow} - \frac{1}{2}\right)\left(n_{x,\downarrow} - \frac{1}{2}\right). \tag{C.2}$$

where $n_{x,\sigma} = c_{x,\sigma}^* c_{x,\sigma}$. H_{HM} acts on $\mathcal{H}_{\mathrm{c}}$, which is defined by (1.6). Let us consider the subspace $\mathcal{H}_{\mathrm{H}} = \wedge^{|\Lambda|/2}\ell^2(\Lambda) \otimes \wedge^{|\Lambda|/2}\ell^2(\Lambda)$. We are interested in the ground state properties of $H_{\mathrm{HM}} \restriction \mathcal{H}_{\mathrm{H}}$. In what follows, we assume that

- The graph $(\Lambda, \{\{x,y\} \,|\, t_{x,y} \neq 0\})$ is connected and bipartite.

Hence, Λ consists of two disjoint subsets Λ_1 and Λ_2 such that $t_{x,y} = 0$ if $x, y \in \Lambda_1$ or $x, y \in \Lambda_2$. The purpose of this section is to prove following theorem.

Theorem C.1. *Assume $U_0 > 0$.*

(i) *Ground states of H_{HM} are unique.*

(ii) *The ground state of H_{HM} has total spin $S = \frac{1}{2}||\Lambda_1| - |\Lambda_2||$.*

C.1 The hole-particle transformation

In order to apply the theory of operator inequality to the Hubbard model, we introduce the hole-particle transformation.

Definition C.2. We define $\mathcal{S}$ and $\mathcal{S}_\Lambda$ by

$$\mathcal{S} = \{0,1\}^{|\Lambda|}, \tag{C.3}$$

$$\mathcal{S}_\Lambda = \left\{ \boldsymbol{\sigma} = (\sigma_x)_{x\in\Lambda} \in \mathcal{S} \,\middle|\, \sum_{x\in\Lambda} \sigma_x = |\Lambda|/2 \right\}. \tag{C.4}$$

For $\boldsymbol{\sigma}, \boldsymbol{\sigma'} \in \mathcal{S}$, let

$$|\boldsymbol{\sigma}, \boldsymbol{\sigma'}\rangle = \prod_{x\in\Lambda} (c_{x,\uparrow}^*)^{\sigma_x} \prod_{y\in\Lambda} (c_{y,\downarrow}^*)^{\sigma_y} |0\rangle \tag{C.5}$$

where $|0\rangle$ is the Fock vacuum in $\mathcal{H}_{\mathrm{c}}$. Note that $\{|\boldsymbol{\sigma}, \boldsymbol{\sigma'}\rangle\}_{\boldsymbol{\sigma},\boldsymbol{\sigma'}\in\mathcal{S}_\Lambda}$ is a CONS of $\mathcal{H}_{\mathrm{H}}$.

Lemma C.3. *There exists a unitary operator U_{HM} on $\mathcal{H}_{\mathrm{c}}$ such that $U_{\mathrm{HM}}\mathcal{H}_{\mathrm{H}} = \mathcal{H}_{\mathrm{H}}$ and*

$$U_{\mathrm{HM}}^* c_{x,\uparrow} U_{\mathrm{HM}} = c_{x,\uparrow}, \quad U_{\mathrm{HM}}^* c_{x,\downarrow} U_{\mathrm{HM}} = \gamma_x c_{x,\downarrow}^* \tag{C.6}$$

where

$$\gamma_x = \begin{cases} -1 & (x \in \Lambda_1) \\ 1 & (x \in \Lambda_2). \end{cases} \tag{C.7}$$

Proof. Define $U_{\mathrm{HM}} \in \mathscr{B}(\mathcal{H}_{\mathrm{H}})$ as

$$U_{\mathrm{HM}}|\boldsymbol{\sigma}, \boldsymbol{\sigma'}\rangle = \prod_{z\in\Lambda_1} (-1)^{1-\sigma'_z} \prod_{x\in\Lambda} (c_{x,\uparrow}^*)^{\sigma_x} \prod_{y\in\Lambda} (c_{y,\downarrow}^*)^{1-\sigma'_y} |0\rangle \quad \boldsymbol{\sigma}, \boldsymbol{\sigma'} \in \mathcal{S}. \tag{C.8}$$

Then U_{HM}^* satisfies

$$U_{\mathrm{HM}}^*|\boldsymbol{\sigma}, \boldsymbol{\sigma'}\rangle = \prod_{z\in\Lambda_1} (-1)^{\sigma'_z} \prod_{x\in\Lambda} (c_{x,\uparrow}^*)^{\sigma_x} \prod_{y\in\Lambda} (c_{y,\downarrow}^*)^{1-\sigma'_y} |0\rangle \tag{C.9}$$

Thus, we see that U_{HM} is a unitary operator satisfying

$$U_{\mathrm{HM}}^* c_{x,\uparrow} U_{\mathrm{HM}} = c_{x,\uparrow}, \quad U_{\mathrm{HM}}^* c_{x,\downarrow} U_{\mathrm{HM}} = \gamma_x c_{x,\downarrow}^*. \tag{C.10}$$

on $\mathcal{H}_{\mathrm{c}}$. By the definition of U_{HM}, we have $U_{\mathrm{HM}}\mathcal{H}_{\mathrm{H}} = \mathcal{H}_{\mathrm{H}}$. □

Lemma C.4. *We have*

$$U_{\mathrm{HM}}^* H_{\mathrm{HM}} U_{\mathrm{HM}} = \mathbb{T} - \mathbb{U}_0. \tag{C.11}$$

Proof. Since $(\Lambda, \{\{x,y\} \mid t_{x,y} \neq 0\})$ is bipartite, we obtain

$$U_{\mathrm{HM}}^* \mathbb{T} U_{\mathrm{HM}} = \sum_{x,y\in\Lambda} t_{x,y}(c_{x,\uparrow}^* c_{y,\downarrow} + c_{x,\uparrow} c_{y,\downarrow}^*) = \mathbb{T}. \tag{C.12}$$

Since $U_{\mathrm{HM}}^* n_{x,\downarrow} U_{\mathrm{HM}} = 1 - n_{x,\downarrow}$, we have $U_{\mathrm{HM}}^* \mathbb{U} U_{\mathrm{HM}} = -\mathbb{U}$. □

C.2 Positivity preservingness of the semigroups

In this subsection, we show that the heat semigroup generated by the hole-particle transformed Hamiltonian is positivity preserving.

Definition C.5. Let ϑ be the antiunitary operator with $\vartheta|\boldsymbol{\sigma}, \boldsymbol{\sigma}'\rangle = |\boldsymbol{\sigma}, \boldsymbol{\sigma}'\rangle$. Define $\mathcal{E}_{\mathrm{HM}}$ as

$$\mathcal{E}_{\mathrm{HM}} = \Psi_\vartheta^{-1}\Big(\mathscr{I}_+\big(\wedge^{|\Lambda|/2}\, \ell^2(\Lambda)\big)\Big), \tag{C.13}$$

where Ψ_ϑ is defined by (2.33).

By Proposition 2.28, $\mathcal{E}_{\mathrm{HM}}$ is a Hilbert cone in $\mathcal{H}_{\mathrm{H}}$.

Lemma C.6. *Suppose $U_0 \geq 0$. Then we have $\mathbb{U}_0 \trianglerighteq 0$ w.r.t. $\mathcal{E}_{\mathrm{HM}}$.*

Proof. By the definition of ϑ, we see $\vartheta n_{x,\sigma} \vartheta^* = n_{x,\sigma}$, $\sigma = \uparrow, \downarrow$. From Proposition 2.32,

$$\left(n_{x,\uparrow} - \frac{1}{2}\right)\left(n_{x,\downarrow} - \frac{1}{2}\right) \trianglerighteq 0 \text{ w.r.t. } \mathcal{E}_{\mathrm{HM}} \tag{C.14}$$

holds for all $x \in \Lambda$. Since $U_0 \geq 0$, we have $\mathbb{U}_0 \trianglerighteq 0$ w.r.t. $\mathcal{E}_{\mathrm{HM}}$. □

Lemma C.7. *$e^{-\beta\mathbb{T}} \trianglerighteq 0$ w.r.t. $\mathcal{E}_{\mathrm{HM}}$ for all $\beta \geq 0$.*

Proof. Let $T_\sigma = \sum_{x,y\in\Lambda} t_{x,y} c_{x,\sigma}^* c_{y,\sigma}$. Then

$$T_\uparrow = \sum_{x,y\in\Lambda} t_{x,y} \hat{c}_x^* \hat{c}_y \otimes 1, \tag{C.15}$$

$$T_\downarrow = 1 \otimes \vartheta \sum_{x,y\in\Lambda} t_{x,y} \hat{c}_x^* \hat{c}_y \vartheta^* \tag{C.16}$$

holds. By Proposition 2.32, we have $e^{-\beta\mathbb{T}} = e^{-\beta T_\uparrow} e^{-\beta T_\downarrow} \trianglerighteq 0$ w.r.t. $\mathcal{E}_{\mathrm{HM}}$. □

Proposition C.8. *Suppose $U_0 \geq 0$. For all $\beta \geq 0$, we have $e^{-\beta U_{\mathrm{HM}}^* H_{\mathrm{HM}} U_{\mathrm{HM}}} \trianglerighteq 0$ w.r.t. $\mathcal{E}_{\mathrm{HM}}$.*

Proof. By Lemma C.4 and using the Duhamel formula, we have

$$\begin{aligned} & e^{-\beta U_{\mathrm{HM}}^* H_{\mathrm{HM}} U_{\mathrm{HM}}} \\ &= e^{-\beta(\mathbb{T} - \mathbb{U}_0)} \\ &= e^{-\beta\mathbb{T}} + \sum_{n\geq 1} \beta^n \int_{0<s_1<\cdots<s_n<1} e^{-\beta s_1 \mathbb{T}} \mathbb{U}_0 \cdots \mathbb{U}_0 e^{-\beta(1-s_n)\mathbb{T}}\, ds_n \ldots ds_1. \end{aligned} \tag{C.17}$$

From Lemmas C.6 and C.7, it follows that

$$\int_{0<s_1<\cdots<s_n<1} e^{-\beta s_1 \mathbb{T}} \mathbb{U}_0 \cdots \mathbb{U}_0 e^{-\beta(1-s_n)\mathbb{T}}\, ds_n \ldots ds_1 \trianglerighteq 0 \text{ w.r.t. } \mathcal{E}_{\mathrm{HM}}. \tag{C.18}$$

Thus, we see $e^{-\beta U_{\mathrm{HM}}^* H_{\mathrm{HM}} U_{\mathrm{HM}}} \trianglerighteq 0$ w.r.t. $\mathcal{E}_{\mathrm{HM}}$. □

C.3 The uniqueness of ground states

In this subsection, we prove the uniqueness of the ground states of $H_{\rm HM}$ by using Theorem 2.17.

The following proposition is essential for the proof of Theorem C.1.

Proposition C.9. *For each $\boldsymbol{\sigma} \in \mathcal{S}_\Lambda$, we have*

$$\left(\mathbb{U}_0 + \frac{|\Lambda|U_0}{4}\right)^{\frac{|\Lambda|}{2}} \trianglerighteq U_0^{\frac{|\Lambda|}{2}} |\boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle\langle \boldsymbol{\sigma}, \boldsymbol{\sigma}| \ \text{w.r.t. } \mathcal{E}_{\rm HM}. \tag{C.19}$$

Proof. Let $\boldsymbol{\sigma} \in \mathcal{S}_\Lambda$. By the assumption, $\sum_{x\in\Lambda}(n_{x,\uparrow} + n_{x,\downarrow}) = |\Lambda|$ holds. Hence we have

$$\begin{aligned}\mathbb{U}_0 + \frac{|\Lambda|U_0}{4} &= U_0 \sum_{x\in\Lambda} n_{x,\uparrow}n_{x,\downarrow} - \frac{U_0}{2}\sum_{x\in\Lambda}(n_{x,\uparrow} + n_{x,\downarrow}) + \frac{|\Lambda|U_0}{2} \\ &= U_0 \sum_{x\in\Lambda} n_{x,\uparrow}n_{x,\downarrow}.\end{aligned} \tag{C.20}$$

Since $n_{x,\uparrow}n_{x,\downarrow} \trianglerighteq 0$ w.r.t. $\mathcal{E}_{\rm HM}$, we see that

$$\begin{aligned}\left(\mathbb{U}_0 + \frac{|\Lambda|U_0}{4}\right)^{\frac{|\Lambda|}{2}} &= U_0^{\frac{|\Lambda|}{2}} \left(\sum_{x\in\Lambda} n_{x,\uparrow}n_{x,\downarrow}\right)^{\frac{|\Lambda|}{2}} \\ &\trianglerighteq U_0^{\frac{|\Lambda|}{2}} \prod_{x\in\Lambda}(n_{x,\uparrow}n_{x,\downarrow})^{\sigma_x} \text{ w.r.t. } \mathcal{E}_{\rm HM} \\ &= U_0^{\frac{|\Lambda|}{2}} |\boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle\langle\boldsymbol{\sigma}, \boldsymbol{\sigma}|\end{aligned} \tag{C.21}$$

holds. □

Lemma C.10. *Let $\boldsymbol{\sigma}, \boldsymbol{\sigma}' \in \mathcal{S}$ and $0 < t < 1$. Assume that there exist $x, y \in \Lambda$ such that $t_{x,y} \neq 0$ and, $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$ are related by*

$$|\boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle = c_{x,\uparrow}^* c_{y,\uparrow} c_{x,\downarrow}^* c_{y,\downarrow} |\boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle. \tag{C.22}$$

Set

$$S(t) = \left\langle \boldsymbol{\sigma}', \boldsymbol{\sigma}' | e^{-t\mathbb{T}} | \boldsymbol{\sigma}, \boldsymbol{\sigma}\right\rangle. \tag{C.23}$$

If $0 < t < \min\{1, |t_{x,y}|^2 e^{-\|\mathbb{T}\|}\}$, then we have $S(t) > 0$.

Proof. By (C.22), we obtain $\langle \boldsymbol{\sigma}', \boldsymbol{\sigma}' | \boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle = \langle \boldsymbol{\sigma}', \boldsymbol{\sigma}' |\mathbb{T}| \boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle = 0$ and $\langle \boldsymbol{\sigma}', \boldsymbol{\sigma}' |\mathbb{T}^2| \boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle = 2|t_{x,y}|^2$. Hence

$$\begin{aligned}S(t) &= \frac{t^2}{2}\langle \boldsymbol{\sigma}', \boldsymbol{\sigma}' |\mathbb{T}^2| \boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle + \sum_{n\geq 3}\frac{(-t)^n}{n!}\langle \boldsymbol{\sigma}', \boldsymbol{\sigma}' |\mathbb{T}^n| \boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle \\ &\geq t^2|t_{x,y}|^2 - \sum_{n\geq 3}\frac{t^n\|\mathbb{T}\|^n}{n!}\end{aligned} \tag{C.24}$$

holds. Since $0 < t < \min\{1, |t_{x,y}|^2 e^{-\|\mathbb{T}\|}\}$, we obtain

$$S(t) \geq t^2|t_{x,y}|^2 - t^3 e^{\|\mathbb{T}\|} = t^2(|t_{x,y}|^2 - te^{\|\mathbb{T}\|}) > 0. \tag{C.25}$$

□

As we will see below, Lemma C.10 plays an important role in the proof of Theorem C.1. To properly use Lemma C.10, the following lemma is needed.

Lemma C.11. *For any $\boldsymbol{\sigma}, \boldsymbol{\sigma}' \in \mathcal{S}_\Lambda$, there exist $\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n \in \mathcal{S}_\Lambda$ and $x_0, \dots, x_n, y_0, \dots, y_n \in \Lambda$ such that $t_{x_j,y_j} \neq 0$ and*

$$|\boldsymbol{\sigma}_{j+1}, \boldsymbol{\sigma}_{j+1}\rangle = c_{x_j,\uparrow}^* c_{y_j,\uparrow} c_{x_j,\downarrow}^* c_{y_j,\downarrow} |\boldsymbol{\sigma}_j, \boldsymbol{\sigma}_j\rangle, \quad j = 0, \dots, n \tag{C.26}$$

where $\boldsymbol{\sigma}_0 = \boldsymbol{\sigma}$, $\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}'$.

Proof. See, e.g., [6, 11, 25].

Theorem C.12. *Assume $U_0 > 0$. Then $e^{-\beta U_{\mathrm{HM}}^* H_{\mathrm{HM}} U_{\mathrm{HM}}}$ is positivity improving w.r.t. $\mathcal{E}_{\mathrm{HM}}$ for all $\beta > 0$.*

Proof. Choose $\psi, \varphi \in \mathcal{E}_{\mathrm{HM}} \setminus \{0\}$ arbitrarily. By Lemma 2.29, we can identify ψ, φ as positive semi-definite matrix. Therefore, there exist $\boldsymbol{\sigma}, \boldsymbol{\sigma}' \in \mathcal{S}_\Lambda$ such that $\langle \varphi | \boldsymbol{\sigma}, \boldsymbol{\sigma}\rangle > 0$ and $\langle \psi | \boldsymbol{\sigma}', \boldsymbol{\sigma}'\rangle > 0$. Applying Lemma C.11, there exist $\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_n \in \mathcal{S}_\Lambda$ and $x_0, \dots, x_n, y_0, \dots, y_n \in \Lambda$ such that $t_{x_j,y_j} \neq 0$ and

$$|\boldsymbol{\sigma}_{j+1}, \boldsymbol{\sigma}_{j+1}\rangle = c_{x_j,\uparrow}^* c_{y_j,\uparrow} c_{x_j,\downarrow}^* c_{y_j,\downarrow} |\boldsymbol{\sigma}_j, \boldsymbol{\sigma}_j\rangle, \quad j = 0, \dots, n \tag{C.27}$$

where $\boldsymbol{\sigma}_0 = \boldsymbol{\sigma}$, $\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}'$. By using the Duhamel formula, we obtain

$$\begin{aligned} &\left\langle \psi, e^{-\beta(\mathbb{T} - U_0 \sum_{x\in\Lambda} n_{x,\uparrow} n_{x,\downarrow})} \varphi \right\rangle \\ &= \langle \psi, e^{-\beta \mathbb{T}} \varphi \rangle + \sum_{m\geq 1} \beta^m U_0^m \int_{0\leq s_1 \leq \cdots \leq s_m \leq 1} F(s_1, \dots, s_m)\, ds_m \dots ds_1, \end{aligned} \tag{C.28}$$

where

$$F(s_1, \dots, s_m) = \left\langle \psi, e^{-\beta s_1 \mathbb{T}} \Big(\sum_{x\in\Lambda} n_{x,\uparrow} n_{x,\downarrow} \Big) \cdots \Big(\sum_{x\in\Lambda} n_{x,\uparrow} n_{x,\downarrow} \Big) e^{-\beta(1-s_m)\mathbb{T}} \varphi \right\rangle. \tag{C.29}$$

Since $\psi, \varphi \in \mathcal{E}_{\mathrm{HM}}$, we see that $F(s_1, \dots, s_m) \geq 0$. Let $l \in \mathbb{N}$. Set $m = (n + 2l + 2)|\Lambda|/2$ and $k = n + 2l + 2$. Let

$$G(\beta) = F\left(0, \dots, 0, \frac{1}{k}, \dots, \frac{1}{k}, \dots, \frac{k-1}{k}, \dots, \frac{k-1}{k}, 1, \dots, 1\right), \tag{C.30}$$

then we have

$$G(\beta) = \left\langle \psi, X^{\frac{|\Lambda|}{2}} e^{-\frac{\beta}{n}\mathbb{T}} \cdots e^{-\frac{\beta}{n}\mathbb{T}} X^{\frac{|\Lambda|}{2}} \varphi \right\rangle, \tag{C.31}$$

where $X = \sum_{x\in\Lambda} n_{x,\uparrow} n_{x,\downarrow}$. Define the projections P_j $(j = 0, \dots, n+1)$ by

$$P_j = |\boldsymbol{\sigma}_j, \boldsymbol{\sigma}_j\rangle\langle \boldsymbol{\sigma}_j, \boldsymbol{\sigma}_j|. \tag{C.32}$$

By Proposition C.9, we obtain

$$G(\beta) \geq \left\langle \psi, \left(P_{n+1} e^{-\frac{\beta}{k}\mathbb{T}}\right)^{l+1} P_n e^{-\frac{\beta}{k}\mathbb{T}} \cdots e^{-\frac{\beta}{k}\mathbb{T}} P_1 \left(e^{-\frac{\beta}{k}\mathbb{T}} P_0\right)^{l+1} \varphi \right\rangle. \tag{C.33}$$

Recalling the definition of $\boldsymbol{\sigma}, \boldsymbol{\sigma}'$, we see that

$$\psi_{\boldsymbol{\sigma}'} = \langle \psi | \boldsymbol{\sigma}', \boldsymbol{\sigma}' \rangle > 0, \quad \varphi_{\boldsymbol{\sigma}} = \langle \varphi | \boldsymbol{\sigma}, \boldsymbol{\sigma} \rangle > 0. \tag{C.34}$$

Therefore,

$$G(\beta) \ge \psi_{\boldsymbol{\sigma}'} \varphi_{\boldsymbol{\sigma}} \big\langle \boldsymbol{\sigma}', \boldsymbol{\sigma}' | e^{-\frac{\beta}{k}\mathbb{T}} | \boldsymbol{\sigma}', \boldsymbol{\sigma}' \big\rangle^l \prod_{j=0}^{n} \big\langle \boldsymbol{\sigma}_{j+1}, \boldsymbol{\sigma}_{j+1} | e^{-\frac{\beta}{k}\mathbb{T}} | \boldsymbol{\sigma}_j, \boldsymbol{\sigma}_j \big\rangle \big\langle \boldsymbol{\sigma}, \boldsymbol{\sigma} | e^{-\frac{\beta}{k}\mathbb{T}} | \boldsymbol{\sigma}, \boldsymbol{\sigma} \big\rangle^l \tag{C.35}$$

holds. Because $\exp(-\frac{\beta}{k}\mathbb{T})$ is positive definite, we have

$$\big\langle \boldsymbol{\sigma}', \boldsymbol{\sigma}' | e^{-\frac{\beta}{k}\mathbb{T}} | \boldsymbol{\sigma}', \boldsymbol{\sigma}' \big\rangle > 0 \ \text{ and } \ \big\langle \boldsymbol{\sigma}, \boldsymbol{\sigma} | e^{-\frac{\beta}{k}\mathbb{T}} | \boldsymbol{\sigma}, \boldsymbol{\sigma} \big\rangle > 0. \tag{C.36}$$

If l is sufficiently large, then $\frac{\beta}{k}$ is sufficiently small. Hence, Taking Lemma C.10 into consideration, we have

$$\big\langle \boldsymbol{\sigma}_{j+1}, \boldsymbol{\sigma}_{j+1} | e^{-\frac{\beta}{k}\mathbb{T}} | \boldsymbol{\sigma}_j, \boldsymbol{\sigma}_j \big\rangle > 0 \tag{C.37}$$

for each $j = 0, \dots, n$. Therefore, $G(\beta) > 0$ holds. Thus, we conclude that there exist $s_1, \dots, s_m$ with $F(s_1, \dots, s_m) > 0$. Since $F(s_1, \dots, s_m)$ is a continuous function, we have

$$\int_{0 \le s_1 \le \dots \le s_m \le 1} F(s_1, \dots, s_m)\, ds_m \dots ds_1 > 0. \tag{C.38}$$

Hence, for each $\psi, \varphi \in \mathcal{E}_{\mathrm{HM}} \setminus \{0\}$, we have

$$\big\langle \psi, e^{-\beta \mathbb{T} + \beta U_0 \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow}} \varphi \big\rangle > 0. \tag{C.39}$$

Since

$$U_{\mathrm{HM}}^* H_{\mathrm{HM}} U_{\mathrm{HM}} = \mathbb{T} - U_0 \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow} + \frac{|\Lambda| U_0}{4} \tag{C.40}$$

holds, we see that $e^{-\beta U_{\mathrm{HM}}^* H_{\mathrm{HM}} U_{\mathrm{HM}}}$ is positivity improving w.r.t. $\mathcal{E}_{\mathrm{HM}}$. □

Proof of Theorem C.1

(i) Applying Theorem 2.17 and Theorem C.12, we immediately obtain that ground states of H_{HM} are unique.

(ii) See [7]. □

D Proof of Proposition 2.43

In Appendix D, we will prove Proposition 2.43. For this purpose, let (M, Σ, μ) be a σ-finite measure space. We assume that $L^2(M)$ is separable.

Define

$$\mathcal{A} = \left\{ \int_M^{\oplus} F(x)\, d\mu(x) \in \mathcal{X} \otimes L^2(M) \,\middle|\, F(x) \in \mathcal{C} \ \mu\text{-a.e.} \right\}. \tag{D.1}$$

As is well-known, $\mathcal{A}$ is a Hilbert cone in $\mathcal{X} \otimes L^2(M)$, see, e.g., [2] and [12, Proof of Proposition 4.2].

Proposition D.1. *One obtains*

$$\mathcal{A} = \overline{\text{coni}}\{\phi \otimes f \in \mathcal{X} \otimes L^2(M) \,|\, \phi \in \mathcal{C}, f \in L^2_+(M)\}, \tag{D.2}$$

where $L^2_+(M)$ is a canonical Hilbert cone in $L^2(M)$:

$$L^2_+(M) = \{f \in L^2(M) \,|\, f(x) \geq 0 \ \mu\text{-a.e.}\}. \tag{D.3}$$

Proof. First, we recall a useful fact: Let $\mathcal{R}$ be a convex cone in $\mathcal{X}$. Then the *dual cone* of $\mathcal{R}$ is defined by

$$\mathcal{R}^\dagger = \{\phi \in \mathcal{X} \,|\, \langle \phi, \psi \rangle \geq 0 \ \forall \psi \in \mathcal{R}\}. \tag{D.4}$$

We say that $\mathcal{R}$ is *self-dual*, if $\mathcal{R} = \mathcal{R}^\dagger$. Note that $\mathcal{R}$ is a self-dual cone, if and only if, $\mathcal{R}$ is a Hilbert cone [2, 3].

We denote by $\mathcal{A}_0$ the right hand side of (D.2). Let $\phi \in \mathcal{C}$ and $f \in L^2_+(M)$. Trivially, $\phi \otimes f \in \mathcal{A}_0$. Because $f(x)\phi \in \mathcal{C}$ μ-a.e., we have

$$\phi \otimes f = \int_M^\oplus f(x)\phi \, d\mu(x) \in \mathcal{A}, \tag{D.5}$$

which implies $\mathcal{A}_0 \subseteq \mathcal{A}$. Therefore, $\mathcal{A}_0^\dagger \supseteq \mathcal{A}^\dagger = \mathcal{A}$ holds, where we have used the above fact.

It suffices to prove $\mathcal{A}_0^\dagger \subseteq \mathcal{A}$. Let $\psi \in \mathcal{A}_0^\dagger$. For any $\phi \in \mathcal{C}$ and $f \in L^2_+(M)$, we have

$$\langle \psi, \phi \otimes f \rangle = \int_M \langle \psi(x), \phi \rangle f(x) \, d\mu(x) \geq 0. \tag{D.6}$$

Since

$$\int_M \text{Im}\langle \psi(x), \phi \rangle f(x) \, d\mu(x) = 0 \tag{D.7}$$

for any $f \in L^2_+(M)$, we conclude $\text{Im}\langle \psi(x), \phi \rangle = 0$ μ-a.e.. Next, we claim that $\text{Re}\langle \psi(x), \phi \rangle \geq 0$. To this end, suppose

$$\mu(\{x \in M \,|\, \text{Re}\langle \psi(x), \phi \rangle < 0\}) > 0. \tag{D.8}$$

Because M is σ-finite, there exists a subset

$$D \subset \{x \in M \,|\, \text{Re}\langle \psi(x), \phi \rangle < 0\} \tag{D.9}$$

with $0 < \mu(D) < \infty$. Let χ_D be the indicator function of the set D. Because $\chi_D \in L^2_+(M)$, we have

$$\langle \psi, \phi \otimes \chi_D \rangle = \int_D \text{Re}\langle \psi(x), \phi \rangle \, d\mu(x) < 0. \tag{D.10}$$

This contradicts with the property $\langle \psi, \phi \otimes \chi_D \rangle \geq 0$, which follows from the fact that $\phi \otimes \chi_D \in \mathcal{A}_0$. Hence, $\text{Re}\langle \psi(x), \phi \rangle \geq 0$ holds for μ-a.e. x. Therefore, we finally conclude that $\psi(x) \in \mathcal{C}$ μ-a.e. and $\mathcal{A}_0^\dagger \subseteq \mathcal{A}$. □

Proof of Proposition 2.43

Apply Proposition D.1 with $M = \mathbb{R}^{|\Lambda|}$ and μ the Lebesgue measure on $\mathbb{R}^{|\Lambda|}$. $\square$

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