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Rigorous results concerning the Holstein–Hubbard model

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Abstract. The Holstein model has been widely accepted as a model comprising electrons interacting with phonons; analysis of this model’s ground states was accomplished two decades ago. However, the results were obtained without completely taking repulsive Coulomb interactions into account. Recent progress has made it possible to treat such interactions rigorously; in this paper, we study the Holstein–Hubbard model with repulsive Coulomb interactions. The ground state properties of the model are investigated; in particular, the ground state of the Hamiltonian is proven to be unique for an even number of electrons on a bipartite connected lattice. In addition, we provide a rigorous upper bound on charge susceptibility.

1. Introduction and results

1.1. Background

The subtle interplay of electrons and phonons induces various physical phenomena. For instance, when electrons interact with phonons, they have a tendency to pair. As a result, the ground state of such a system exhibits either superconducting or charge-density-wave order. Another example is high-temperature superconductivity. Since the discovery of coupled electron-phonon systems, such systems have become increasingly active. However, a unanimously accepted mechanism for the origin of high-temperature superconductivity has not been established. The above-mentioned examples suggest that coupled electron-phonon systems offer a rich field of study toward the identification of such a mechanism. In this paper, we rigorously investigate the ground state properties of the Holstein–Hubbard model, which is a standard model of electron-phonon interaction.

The importance of the uniqueness of ground states for models of single particle interacting with a Bose field was recognized through rigorous studies of the quantum field theory [5, 7, 10, 11, 29, 35]. Field-theoretical methods

have been successfully adopted in condensed matter physics. In particular, Löwen [20] applied Fröhlich's method [7] to a model of a single electron positioned on a discrete lattice system and that interacts with the phonons of lattice. Recently, this method was extended to a two-electron system interacting with phonons [21]¹.

The importance of the uniqueness of ground states has also been appreciated in the field of many-electron systems [17, 18, 37]. In addition, some relationships between the notion of correlations and the uniqueness of the ground states have been revealed in recent years [26]. To explain why the uniqueness is important, we recall the Hubbard model [13] as a background:

$$H_{\text{Hubbard}} = - \sum_{\substack{\{x,y\} \in E \\ \sigma \in \{\uparrow, \downarrow\}}} t_{xy} c_{x\sigma}^* c_{y\sigma} + \frac{1}{2} \sum_{x \in \Lambda} U_x (n_x - \mathbb{1})^2, \quad U_x > 0. \quad (1)$$

For definitions of symbols, see Section 1.2. In general, the Pauli exclusion principle and the Coulomb repulsion are essential factors in the study of many-electron systems. This model takes the two factors into consideration, and has been regarded as a basic model of the theory of ferromagnetism. In [19], Lieb proved the uniqueness of the ground state of the Hubbard model using the method of spin-reflection positivity². Ferromagnetism in the ground state immediately follows from this result.

Let us now discuss the problem of electron-phonon interaction. As mentioned above, the field-theoretical approach successfully proves the uniqueness of the ground states of single and two-electron systems interacting with phonons, however, it is difficult to apply this approach to the general many-electron systems involving interactions with phonons. Freericks and Lieb invented a crucial approach to show the uniqueness of the many-body ground state of an electron-phonon Hamiltonian [6]. Their method also relied on spin-reflection positivity. The Freericks–Lieb method is applicable to a general class of models. To clarify the point of the argument, let us consider the Holstein model [12] since it is a representative model of the Lieb–Freericks class. The Hamiltonian of the Holstein model is given by the following:

$$H_{\text{Holstein}} = - \sum_{\substack{\{x,y\} \in E \\ \sigma \in \{\uparrow, \downarrow\}}} t_{xy} c_{x\sigma}^* c_{y\sigma} + \sum_{x \in \Lambda} g_x n_x (b_x^* + b_x) + \sum_{x \in \Lambda} \omega_0 b_x^* b_x. \quad (2)$$

The uniqueness of the ground states of H_{Holstein} was successfully proved in [6]. As a corollary, it was shown that the ground state has a total spin $S = 0$.

The Holstein model considers the Pauli exclusion principle, but not Coulomb repulsion. It is logical as well as important to ask whether we can prove (or disprove) the uniqueness of the ground state even if Coulomb repulsion is considered. The motivation of this study is to answer this question.

¹The Coulomb repulsion is considered, while the Pauli exclusion principle is not taken into account in [21]

²The spin-reflection positivity originated from quantum field theory [30], and has various applications to strongly correlated electron systems [8, 32, 38].

To investigate this problem, we analyzed the Holstein–Hubbard model that contains effects of the Coulomb repulsion:

$$H_{\text{HH}} = H_{\text{Holstein}} + \frac{1}{2} \sum_{x \in \Lambda} U_x (n_x - \mathbb{1})^2, \quad U_x > 0. \quad (3)$$

It should be noted that the Lieb–Freericks approach is inapplicable to this model³. Our first achievement is that we prove the uniqueness of the ground states of the extended Holstein–Hubbard model defined by (5). As a corollary, we elucidate the magnetic properties of the ground state. To this end, we apply the theory of operator inequalities associated with Hilbert cones, which has been shown to be effective in studies of many-electron systems [21, 23, 24].

At first glance, it appears that the form of the Hamiltonian is unsuitable for application to operator inequalities because of the electron-phonon interaction term (the middle term in the RHS of (2)). To overcome this obstacle, we employ the Lang–Firsov transformation [16]. By this transformation, the electron-phonon interaction term in (3) disappears so that we can apply our theory of operator inequalities to the resulting Hamiltonian. This is the main reason why we use the Lang–Firsov transformation. Due to this transformation, the hopping matrix elements of the resulting Hamiltonian become *complex*-valued functions of the phonon coordinates [see (44)]. To the best of our knowledge, there has been no attempt, except Miyao [22], to show the uniqueness of the ground states of such a Hamiltonian. In the study by Miyao [22], the ground state properties of the Su–Schrieffer–Heeger (SSH) model [36] were investigated. The SSH model describes a one-dimensional many-electron system interacting with phonons⁴. A significant feature of this model is that its hopping matrix elements are *real*-valued functions of the phonon coordinates which makes our analysis complicated. Since the elements of the hopping matrix are complex in our case, the method in [22] cannot be applied directly. Therefore, we establish a more sophisticated analysis in this study.

Lieb’s results for the Hubbard model concern the ground state. On the other hand, Kubo and Kishi showed a finite temperature version of Lieb’s theorem [15]. They showed a uniform upper bound on the charge susceptibility of the Hubbard model at finite temperature, which implies the absence of charge long-range order. As the second achievement of this study, we extend their result to the extended Holstein–Hubbard model.

³To be precise, their results remain true if $U_x \leq 0$, but their method does not work if $U_x > 0$.

⁴The SSH Hamiltonian is concretely given by

$$H_{\text{SSH}} = - \sum_{j=1}^L \sum_{\sigma \in \{\uparrow, \downarrow\}} (q_j - q_{j+1}) t c_{j\sigma}^* c_{j+1\sigma} + \frac{1}{2} \sum_{j=1}^L U_j (n_j - \mathbb{1})^2 + \sum_{j=1}^L \omega_0 b_j^* b_j, \quad (4)$$

where $q_j = b_j - b_j^*$ and $t > 0$. Clearly, the hopping matrix element $t_j(\mathbf{q}) := -(q_j - q_{j+1})t$ depends on phonon coordinates, $\{q_j\}_{j \in \Lambda}$.

Our method requires a restriction on the electron-phonon coupling strength ($|g_0| \leq \sqrt{2U_0/\omega_0}$). We are aware of no rigorous results when the electron-phonon coupling strength is large enough ($|g_0| > \sqrt{2U_0/\omega_0}$).

1.2. The extended Holstein–Hubbard model

Let $G = (\Lambda, E)$ be a graph with vertex set Λ and edge collection E . We suppose that G is embedded in $\mathbb{R}^d$ and that Λ is a finite subset of $\mathbb{R}^d$. An edge with end-points x and y is denoted by $\{x, y\}$. We always assume that $\{x, x\} \notin E$ for any $x \in \Lambda$, i.e., any loops are excluded. Henceforth, we assume that

(G) G is bipartite⁵.

The Hamiltonian of the extended Holstein–Hubbard model is given by

$$\begin{aligned} H = & - \sum_{\substack{\{x,y\} \in E \\ \sigma \in \{\uparrow, \downarrow\}}} t_{xy} c_{x\sigma}^* c_{y\sigma} + \frac{1}{2} \sum_{x,y \in \Lambda} U_{xy} (n_x - \mathbb{1})(n_y - \mathbb{1}) \\ & + \sum_{x,y \in \Lambda} g_{xy} n_x (b_y^* + b_y) + \sum_{x \in \Lambda} \omega_0 b_x^* b_x, \end{aligned} \quad (5)$$

where $c_{x\sigma}$ is the electron annihilation operator at vertex x and b_x is the phonon annihilation operator at vertex x . These operators satisfy the following relations:

$$\{c_{x\sigma}, c_{x'\sigma'}^*\} = \delta_{\sigma\sigma'} \delta_{xx'}, \quad [b_x, b_{x'}^*] = \delta_{xx'}. \quad (6)$$

n_x is the fermionic number operator at vertex $x \in \Lambda$ defined by

$$n_x = \sum_{\sigma \in \{\uparrow, \downarrow\}} n_{x\sigma}, \quad n_{x\sigma} = c_{x\sigma}^* c_{x\sigma}. \quad (7)$$

t_{xy} is the hopping matrix element, U_{xy} is the energy of the Coulomb interaction, and g_{xy} is the strength of the electron-phonon interaction. We assume that

(I) $\{g_{xy}\}, \{t_{xy}\}$ and $\{U_{xy}\}$ are real symmetric $|\Lambda| \times |\Lambda|$ matrices⁶.

The phonons are assumed to be dispersionless with energy $\omega_0 > 0$. H acts in the Hilbert space

$$\mathfrak{E} \otimes \mathfrak{P}. \quad (8)$$

$\mathfrak{E}$ is defined by $\mathfrak{F}_e \otimes \mathfrak{F}_e$. $\mathfrak{F}_e$ is the fermionic Fock space over $\ell^2(\Lambda)$ given by $\mathfrak{F}_e = \bigoplus_{n=0}^{\infty} \wedge^n \ell^2(\Lambda)$, where $\wedge^n \ell^2(\Lambda)$ is the n -fold anti-symmetric tensor product of $\ell^2(\Lambda)$. $\mathfrak{P}$ is the bosonic Fock space over $\ell^2(\Lambda)$ defined by $\mathfrak{P} = \bigoplus_{n=0}^{\infty} \otimes_s^n \ell^2(\Lambda)$, where $\otimes_s^n \ell^2(\Lambda)$ is the n -fold symmetric tensor product. By

⁵A graph G is called *bipartite* if Λ admits a partition into two classes, such that every edge has its ends in different classes.

⁶Let $M = \{M_{xy}\}$ be a $|\Lambda| \times |\Lambda|$ matrix. M is called a *real symmetric matrix* if M_{xy} is real and $M_{xy} = M_{yx}$ for all $x, y \in \Lambda$.

the Kato–Rellich theorem, H is self-adjoint on $\text{dom}(N_p)$ and bounded from below⁷, where $N_p = \sum_{x \in \Lambda} b_x^* b_x$.

Let $N_e = \sum_{\sigma \in \{\uparrow, \downarrow\}} \sum_{x \in \Lambda} n_{x\sigma}$, the fermionic number operator. We are interested in the ground state properties of H at half-filling. Thus, we consider only the following subspace:

$$\mathfrak{H} = \mathfrak{E}_{|\Lambda|} \otimes \mathfrak{P}, \quad \mathfrak{E}_{|\Lambda|} = \ker(N_e - |\Lambda|). \quad (9)$$

Let $S^{(z)} = \frac{1}{2}(N_{e\uparrow} - N_{e\downarrow})$, where $N_{e\sigma} = \sum_{x \in \Lambda} n_{x\sigma}$, $\sigma \in \{\uparrow, \downarrow\}$. Since $S^{(z)}$ commutes with H , we have the following decompositions:

$$\mathfrak{H} = \bigoplus_{M=-|\Lambda|/2}^{|\Lambda|/2} \mathfrak{H}_M, \quad \mathfrak{H}_M = \left(\ker[S^{(z)} - M] \cap \mathfrak{E}_{|\Lambda|} \right) \otimes \mathfrak{P}, \quad (10)$$

$$H = \bigoplus_{M=-|\Lambda|/2}^{|\Lambda|/2} H_M, \quad H_M = H \upharpoonright \mathfrak{H}_M. \quad (11)$$

Here, $\mathfrak{H}_M$ is called the M -subspace.

1.3. Ground state properties

Before we state our first result, we need to introduce some definitions.

The effective Coulomb interaction is given by the following equation:

$$U_{\text{eff},xy} = U_{xy} - \frac{2}{\omega_0} \sum_{z \in \Lambda} g_{xz} g_{yz}. \quad (12)$$

In what follows, we assume that

(A. 1) $\sum_{x \in \Lambda} g_{xy}$ is a constant independent of $y \in \Lambda$.

Example 1. (i) An example satisfying **(A. 1)** is $g_{xy} = g_0 \delta_{xy}$, where δ_{xy} is the Kronecker delta.

(ii) Let us consider a linear chain of $2L$ atoms with periodic boundary conditions. In this case, $G = (\Lambda, E)$ is defined by $\Lambda = \{x_j\}_{j=1}^{2L}$, $x_j \in \mathbb{R}^2$ and $E = \{\{x_j, x_{j+1}\}, \{x_{j+1}, x_j\}\}_{j=1}^{2L}$ with $x_{2L+1} = x_1$. We denote the distance from atom i to atom j by $w_{i,j} = |x_i - x_j|$. Assume that $w_{j,j+1} = \text{constant}$ for all j . If g_{xy} is a function of $|x - y|$, i.e., $g_{xy} = f(|x - y|)$, then **(A. 1)** is satisfied. Similarly, if Λ has a symmetric structure, like C_{60} fullerene, then **(A. 1)** is fulfilled. $\diamond$

⁷To show self-adjointness, recall the well-known bounds: $\|b_x(N_p + \mathbb{1})^{-1/2}\| \leq 1$, $\|b_x^*(N_p + \mathbb{1})^{-1/2}\| \leq 1$. Thus, we see that

$$\left\| \sum_x g_{xy} n_x (b_y + b_y^*) \varphi \right\| \leq 4|\Lambda| \max_{x,y} |g_{xy}| \|(N_p + \mathbb{1})^{1/2} \varphi\|, \quad \varphi \in \text{dom}(N_p).$$

Since $\|(N_p + \mathbb{1})^{1/2} \varphi\|^2 \leq \varepsilon \|(N_p + \mathbb{1}) \varphi\|^2 + \frac{1}{4\varepsilon} \|\varphi\|^2$ for all $\varepsilon > 0$, the electron-phonon interaction term is infinitesimally N_p -bounded. Hence, we can apply the Kato–Rellich theorem [31].

Since G is bipartite, Λ can be divided into two disjoint sets Λ_e and Λ_o . Set

$$\tilde{S}_+ = \sum_{x \in \Lambda} \gamma_x c_{x\uparrow} c_{x\downarrow}, \quad \tilde{S}_- = \sum_{x \in \Lambda} \gamma_x c_{x\downarrow}^* c_{x\uparrow}^*, \quad \tilde{S}^{(z)} = \frac{1}{2}|\Lambda| - \frac{1}{2}(N_{e\uparrow} + N_{e\downarrow}), \quad (13)$$

where $\gamma_x = 1$ for $x \in \Lambda_e$, $\gamma_x = -1$ for $x \in \Lambda_o$. The pseudospin operator is defined by

$$\tilde{S}_{\text{tot}}^2 = \tilde{S}^{(z)2} + \frac{1}{2}\tilde{S}_+\tilde{S}_- + \frac{1}{2}\tilde{S}_-\tilde{S}_+. \quad (14)$$

Although $\tilde{S}_{\text{tot}}^2$ does not commute with H_M , it is still useful to study ground states of H_M .

Theorem 1.1. *Assume that $|\Lambda|$ is even. Assume (A. 1). Assume that U_{eff} is positive semi-definite⁸. Then for all $M \in \{-|\Lambda|/2, -|\Lambda|/2 + 1, \dots, |\Lambda|/2\}$, among all the ground states of H_M , there exists at least one ground state φ_M which satisfies the following:*

- (i) $\tilde{P}\varphi_M \neq 0$ holds, where $\tilde{P}$ is the orthogonal projection onto $\ker(\tilde{S}_{\text{tot}}^2)$.
- (ii) Let $S_{x+} = c_{x\uparrow}^* c_{x\downarrow}$ and $S_{x-} = (S_{x+})^*$. Then

$$\langle \varphi_M, S_{x+} S_{y-} \varphi_M \rangle \begin{cases} \geq 0 & \text{if } x, y \in \Lambda_e \text{ or } x, y \in \Lambda_o \\ \leq 0 & \text{otherwise.} \end{cases} \quad (16)$$

In other words, the magnetic structure of the ground state is antiferromagnetic.

Remark 1.2. In [26], it is pointed out that (16) can be regarded as the first Griffiths inequality. $\diamond$

Example 2. Let $U_{xy} = U_0 \delta_{xy}$ and $g_{xy} = g_0 \delta_{xy}$. Then $U_{\text{eff}, xy} = (U_0 - 2g_0^2/\omega_0) \delta_{xy}$. Thus, U_{eff} is positive semi-definite if and only if $|g_0| \leq \sqrt{2U_0/\omega_0}$. $\diamond$

Theorem 1.1 does not exclude the possibility that H_M has degenerate ground states. Our next result concerns the uniqueness of the ground state. To show it, we need an additional assumption:

(A. 2) G is connected⁹ and $t_{xy} \neq 0$ for all $\{x, y\} \in E$.

Let us introduce the total spin operator

$$S_{\text{tot}}^2 = S^{(z)2} + \frac{1}{2}S_+S_- + \frac{1}{2}S_-S_+, \quad (17)$$

⁸ U_{eff} is called *positive semi-definite*, if, for all $\{\xi_x\}_{x \in \Lambda} \in \mathbb{C}^{|\Lambda|}$,

$$\sum_{x, y \in \Lambda} \bar{\xi}_x \xi_y U_{\text{eff}, xy} \geq 0 \quad (15)$$

holds.

⁹The graph G is called *connected* if any of its vertices are linked by a path in G .

where

$$S_+ = \sum_{x \in \Lambda} c_{x\downarrow}^* c_{x\uparrow}, \quad S_- = \sum_{x \in \Lambda} c_{x\downarrow}^* c_{x\uparrow}. \quad (18)$$

Theorem 1.3. *Assume that $|\Lambda|$ is even. Assume (A. 1) and (A. 2). Assume that U_{eff} is positive definite¹⁰. For each $M \in \{-|\Lambda|/2, -|\Lambda|/2+1, \dots, |\Lambda|/2\}$, the ground state of H_M is unique. Let φ_M be the unique ground state of H_M . Then we have the following:*

- (i) $\tilde{P}\varphi_M \neq 0$.
- (ii) *There exists a unique number S such that $S \geq |M|$ and $S_{\text{tot}}^2 \varphi_M = S(S+1)\varphi_M$.*
- (iii)

$$\langle \varphi_M, S_{x+} S_{y-} \varphi_M \rangle \begin{cases} > 0 & \text{if } x, y \in \Lambda_e \text{ or } x, y \in \Lambda_o \\ < 0 & \text{otherwise.} \end{cases} \quad (20)$$

Remark 1.4. (20) means that the antiferromagnetic structure becomes sharper than (16) or a strict Griffiths inequality holds. $\diamond$

Example 3. Consider the case where $U_{xy} = U_0 \delta_{xy}$ and $g_{xy} = g_0 \delta_{xy}$. Then U_{eff} is positive definite if and only if $|g_0| < \sqrt{\omega_0 U_0/2}$. $\diamond$

1.4. Upper bounds on the charge susceptibility

We give a rigorous bound on the charge susceptibility of the Holstein–Hubbard model. For simplicity, we consider the d -dimensional simple cubic lattice $\mathbb{Z}^d$. For each $L \in \mathbb{N}$, the vertex set is given by

$$\Lambda = [-L, L]^d \cap \mathbb{Z}^d. \quad (21)$$

We impose a periodic boundary condition on the model. To be precise, the edge collection E is given by

$$E = \{ \{x, y\} \in \Lambda^2 \mid |x - y| = 1 \} \cup \partial, \quad (22)$$

where

$$\partial = \{ \{x, y\} \in \Lambda^2 \mid |x - y| = 2L - 1 \}. \quad (23)$$

We set $t_{xy} = t \neq 0$ for all $\{x, y\} \in E$.

Let $\delta n_x = n_x - \mathbb{1}$. Set

$$\widetilde{\delta n}_p = |\Lambda|^{-1/2} \sum_{x \in \Lambda} e^{-ix \cdot p} \delta n_x. \quad (24)$$

The charge susceptibility is defined by

$$\chi_\beta(p) = \lim_{L \rightarrow \infty} \beta(\widetilde{\delta n}_{-p}, \widetilde{\delta n}_p)_{\beta, \Lambda}, \quad p \in [-\pi, \pi]^d, \quad (25)$$

¹⁰ U_{eff} will be called *positive definite* if, for all $\{\xi_x\}_{x \in \Lambda} \in \mathbb{C}^{|\Lambda|} \setminus \{\mathbf{0}\}$,

$$\sum_{x, y \in \Lambda} \bar{\xi}_x \xi_y U_{\text{eff}, xy} > 0 \quad (19)$$

holds.

where

$$(A, B)_{\beta, \Lambda} = Z_{\beta, \Lambda}^{-1} \int_0^1 ds \text{Tr} \left[e^{-s\beta(H + \sum_{x \in \Lambda} \mu_x n_x)} A e^{-(1-s)\beta(H + \sum_{x \in \Lambda} \mu_x n_x)} B \right], \quad (26)$$

$$Z_{\beta, \Lambda} = \text{Tr} \left[e^{-\beta(H + \sum_{x \in \Lambda} \mu_x n_x)} \right]. \quad (27)$$

The local chemical potential is given by

$$\mu_x = \frac{2}{\omega_0} \sum_{y, z \in \Lambda} g_{xz} g_{zy}. \quad (28)$$

Note that if $g_{xy} = g_0 \delta_{xy}$, then $\mu_x = 2g_0^2/\omega_0$ for all $x \in \Lambda$. For any β and Λ , we can check that the thermal average density of the system satisfies $\langle n_o \rangle_{\beta, \Lambda} := Z_{\beta, \Lambda}^{-1} \text{Tr}[n_o e^{-\beta H}] = 1$, i.e., the system at half-filling is considered¹¹.

We assume the following:

- (B. 1) g_{xy} and U_{xy} are translation-invariant, i.e., $g_{xy} = g_{x-y, o}$ and $U_{xy} = U_{x-y, o}$ for all $x, y \in \Lambda$.
- (B. 2) Set $g(x) = g_{x, o}$ and $U(x) = U_{x, o}$. Then $g(x) \in \ell^2(\mathbb{Z}^d)$ and $U(x) \in \ell^1(\mathbb{Z}^d)$.
- (B. 3) For all $L > 0$, it holds that $\hat{U}_{\text{eff}, \Lambda}(p) \geq 0$, where $\hat{f}_\Lambda(p) = \sum_{x \in \Lambda} e^{-ix \cdot p} f(x)$.

Remark 1.5. (B. 3) implies that U_{eff} is positive semi-definite. $\diamond$

Theorem 1.6. Assume (B. 1), (B. 2), and (B. 3). For each $p \in [-\pi, \pi]^d$ such that $\hat{U}_{\text{eff}}(p) > 0$, we have

$$\chi_\beta(p) \leq \hat{U}_{\text{eff}}(p)^{-1}. \quad (29)$$

Here $\hat{f}(p) = \sum_{x \in \mathbb{Z}^d} e^{-ix \cdot p} f(x)$.

Remark 1.7. (i) By direct computation, we have $\hat{U}_{\text{eff}}(p) = \hat{U}(p) - 2\hat{g}(p)^2/\omega_0$.

(ii) This result is an extension of the Kubo–Kishi theorem [15] in the following way: (a) The electron-phonon interaction is taken into account. (b) Not only on-site but general Coulomb repulsion is considered.

(iii) In a companion paper [25], we obtain a similar bound on the Hubbard model coupled to a quantized radiation field. $\diamond$

Corollary 1.8. Assume (B. 1), (B. 2) and (B. 3). In addition, assume that there exists a constant $u_0 > 0$ such that $\hat{U}_{\text{eff}}(p) \geq u_0$ for all $p \in [-\pi, \pi]^d$. Then we have

$$\chi_\beta(p) \leq u_0^{-1}. \quad (30)$$

Thus, by the Falk–Bruch inequality [2, 4], there is no charge long-range order.

Remark 1.9. The existence of $u_0 > 0$ implies that U_{eff} is positive definite. $\diamond$

¹¹By $A := B$, we understand that A is defined in terms of B .

Example 4. For each $U_0, U_1, g_0 \geq 0$, let

$$U_{xy} = \begin{cases} U_0 & x = y \\ U_1/2d & |x - y| = 1, \\ 0 & \text{otherwise} \end{cases}, \quad g_{xy} = g_0 \delta_{xy}. \quad (31)$$

Clearly, **(B. 1)** and **(B. 2)** are satisfied. Then one sees $\hat{U}_{\text{eff}}(p) = (U_0 - U_1 - 2g_0^2/\omega_0) + \frac{U_1}{d} \sum_{j=1}^d (1 + \cos p_j)$. Thus, **(B. 3)** is satisfied whenever $U_0 - U_1 - 2g_0^2/\omega_0 \geq 0$. There is no charge long-range order if $U_0 - U_1 - 2g_0^2/\omega_0 > 0$. If $U_0 - U_1 - 2g_0^2/\omega_0 = 0$, then $\chi_\beta(p)$ could diverge at extreme points of $[-\pi, \pi]^d$. $\diamond$

Remark 1.10. In the case where $U_0 - U_1 - 2g^2/\omega_0 < 0$, the existence of charge long-range order is proved in [27]. $\diamond$

1.5. Organization

The organization of the paper is as follows: In Section 2, we introduce several operator inequalities related to Hilbert cones. These operator inequalities are very useful for our study. Sections 3–6 are devoted to proving the main results in Section 1.

In Section 3, we provide several expressions of the Hamiltonian (5) by performing the hole-particle and Lang–Firsov transformations. We then choose a suitable expression in each section below.

In Section 4, we show Theorem 1.1. By choosing a suitable Hilbert cone, we prove that the heat semi-group generated by the Hamiltonian preserves the positivity. Theorem 1.1 is a corollary of this fact.

In Section 5, proof of Theorem 1.3 is given. We show that the semi-group generated by the Hamiltonian improves the positivity with respect to the Hilbert cone constructed in Section 4. The uniqueness of ground states follows from Faris’ theorem, which is a generalization of the Perron–Frobenius theorem. By applying this fact, the some magnetic structures of the ground state are revealed.

Section 6 is devoted to the proof of Theorem 1.6. We obtain an upper bound on the charge susceptibility by extending the method of Gaussian domination established in [2, 8, 9].

In Appendices A and B, we give a list of basic facts that are used in the main sections.

In Appendix C, we give a proof of a technical proposition which is needed in Section 5.

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2. Preliminaries

2.1. Hilbert cones and their associated operator inequalities

Definition 2.1. Let $\mathfrak{X}$ be a complex Hilbert space. By a *convex cone*, we denote a closed convex set $\mathfrak{X}_+ \subseteq \mathfrak{X}$ such that $t\mathfrak{X}_+ \subseteq \mathfrak{X}_+$ for all $t \geq 0$ and $\mathfrak{X}_+ \cap (-\mathfrak{X}_+) = \{0\}$. In what follows, we always assume that $\mathfrak{X}_+ \neq \{0\}$. A convex cone, $\mathfrak{X}_+$ in $\mathfrak{X}$, is called a *Hilbert cone* if it satisfies the following¹²:

- (i) $\langle x, y \rangle \geq 0$ for all $x, y \in \mathfrak{X}_+$.
- (ii) Let $\mathfrak{X}_{\mathbb{R}}$ be a real subspace of $\mathfrak{X}$ generated by $\mathfrak{X}_+$. Then for all $x \in \mathfrak{X}_{\mathbb{R}}$, there exist $x_+, x_- \in \mathfrak{X}_+$ such that $x = x_+ - x_-$ and $\langle x_+, x_- \rangle = 0$.
- (iii) $\mathfrak{X} = \mathfrak{X}_{\mathbb{R}} + i\mathfrak{X}_{\mathbb{R}} = \{x + iy \mid x, y \in \mathfrak{X}_{\mathbb{R}}\}$.

A vector x is said to be *positive w.r.t. $\mathfrak{X}_+$* if $x \in \mathfrak{X}_+$. We write this as $x \geq 0$ w.r.t. $\mathfrak{X}_+$.

A vector $y \in \mathfrak{X}$ is called *strictly positive w.r.t. $\mathfrak{X}_+$* whenever $\langle x, y \rangle > 0$ for all $x \in \mathfrak{X}_+ \setminus \{0\}$. We write this as $x > 0$ w.r.t. $\mathfrak{X}_+$. $\diamond$

In subsequent sections, we will use the following operator inequalities:

Definition 2.2. We denote by $\mathcal{B}(\mathfrak{X})$ the set of all bounded linear operators on $\mathfrak{X}$. Let $A, B \in \mathcal{B}(\mathfrak{X})$.

- (i) If $A\mathfrak{X}_+ \subseteq \mathfrak{X}_+$ ¹³, we then write this as $A \trianglerighteq 0$ w.r.t. $\mathfrak{X}_+$ ¹⁴. In this case, we say that A *preserves the positivity w.r.t. $\mathfrak{X}_+$* . Suppose that $A\mathfrak{X}_{\mathbb{R}} \subseteq \mathfrak{X}_{\mathbb{R}}$ and $B\mathfrak{X}_{\mathbb{R}} \subseteq \mathfrak{X}_{\mathbb{R}}$. If $(A - B)\mathfrak{X}_+ \subseteq \mathfrak{X}_+$, then we write this as $A \trianglerighteq B$ w.r.t. $\mathfrak{X}_+$.
- (ii) We write $A \triangleright 0$ w.r.t. $\mathfrak{X}_+$, if $Ax > 0$ w.r.t. $\mathfrak{X}_+$ for all $x \in \mathfrak{X}_+ \setminus \{0\}$. In this case, we say that A *improves the positivity w.r.t. $\mathfrak{X}_+$* . $\diamond$

The following proposition is fundamental to this paper:

Proposition 2.3. Let $A, B, C, D \in \mathcal{B}(\mathfrak{X})$ and let $a, b \in \mathbb{R}$. We have the following:

- (i) If $A \trianglerighteq 0, B \trianglerighteq 0$ w.r.t. $\mathfrak{X}_+$ and $a, b \geq 0$, then $aA + bB \trianglerighteq 0$ w.r.t. $\mathfrak{X}_+$.
- (ii) If $A \trianglerighteq B \trianglerighteq 0$ and $C \trianglerighteq D \trianglerighteq 0$ w.r.t. $\mathfrak{X}_+$, then $AC \trianglerighteq BD \trianglerighteq 0$ w.r.t. $\mathfrak{X}_+$.

Proof. (i) is trivial.

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

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

This completes the proof. $\square$

In Appendix A, we give several crucial theorems on the operator inequalities associated with Hilbert cones.

¹² $\mathfrak{X}_+$ is a Hilbert cone if and only if $\mathfrak{X}_+$ is a self-dual cone [1, 21, 26].

¹³For each subset $\mathfrak{Y} \subseteq \mathfrak{X}$, $A\mathfrak{Y}$ is defined by $A\mathfrak{Y} = \{Ax \mid x \in \mathfrak{Y}\}$.

¹⁴This symbol was introduced by Miura [28], see also [14].

2.2. A canonical cone in $\mathcal{L}^2(\mathfrak{h})$

Let $\mathfrak{h}$ be a complex Hilbert space. The set of all Hilbert-Schmidt class operators on $\mathfrak{h}$ is denoted by $\mathcal{L}^2(\mathfrak{h})$, i.e., $\mathcal{L}^2(\mathfrak{h}) = \{\xi \in \mathcal{B}(\mathfrak{h}) \mid \text{Tr}[\xi^* \xi] < \infty\}$. Henceforth, we regard $\mathcal{L}^2(\mathfrak{h})$ as a Hilbert space equipped with the inner product $\langle \xi, \eta \rangle_{\mathcal{L}^2} = \text{Tr}[\xi^* \eta]$, $\xi, \eta \in \mathcal{L}^2(\mathfrak{h})$. For each $A \in \mathcal{B}(\mathfrak{h})$, the left multiplication operator is defined by

$$\mathcal{L}(A)\xi = A\xi, \quad \xi \in \mathcal{L}^2(\mathfrak{h}). \quad (32)$$

Similarly, the right multiplication operator is defined by

$$\mathcal{R}(A)\xi = \xi A, \quad \xi \in \mathcal{L}^2(\mathfrak{h}). \quad (33)$$

It is not hard to check that

$$\mathcal{L}(A)\mathcal{L}(B) = \mathcal{L}(AB), \quad \mathcal{R}(A)\mathcal{R}(B) = \mathcal{R}(BA), \quad A, B \in \mathcal{B}(\mathfrak{h}). \quad (34)$$

Definition 2.4. A canonical cone in $\mathcal{L}^2(\mathfrak{h})$ is given by

$$\mathcal{L}^2(\mathfrak{h})_+ = \left\{ \xi \in \mathcal{L}^2(\mathfrak{h}) \mid \xi \text{ is self-adjoint and } \xi \geq 0 \text{ as an operator on } \mathfrak{h} \right\}. \quad (35)$$

(Recall that a linear operator ξ on $\mathfrak{h}$ is said to be positive if $\langle x, \xi x \rangle_{\mathfrak{h}} \geq 0$ for all $x \in \mathfrak{h}$. We write this as $\xi \geq 0$.) $\diamond$

Proposition 2.5. $\mathcal{L}^2(\mathfrak{h})_+$ is a Hilbert cone in $\mathcal{L}^2(\mathfrak{h})$.

Proof. We will check conditions (i)-(iii) in Definition 2.1.

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

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

(iii) For each $\xi \in \mathcal{L}^2(\mathfrak{h})$, we have $\xi = \xi_R + i\xi_I$, where $\xi_R = (\xi + \xi^*)/2$ and $\xi_I = (\xi - \xi^*)/2i$. Trivially, $\xi_R, \xi_I \in \mathcal{L}^2(\mathfrak{h})_{\mathbb{R}}$. This completes the proof. $\square$

Lemma 2.6. Let $A \in \mathcal{B}(\mathfrak{h})$. We have $\mathcal{L}(A^*)\mathcal{R}(A) \supseteq 0$ w.r.t. $\mathcal{L}^2(\mathfrak{h})_+$.

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

3. Several expressions of the Hamiltonian, H

3.1. The Lang–Firsov transformation

Let

$$q_x = \frac{1}{\sqrt{2\omega_0}}(b_x^* + b_x), \quad p_x = i\sqrt{\frac{\omega_0}{2}}(b_x^* - b_x). \quad (36)$$

Both operators are essentially self-adjoint. We denote their closures by the same symbols. Let

$$L = -i\sqrt{2}\omega_0^{-3/2} \sum_{x,y \in \Lambda} g_{xy} n_x p_y. \quad (37)$$

L is essentially anti-self-adjoint. We also denote its closure by the same symbol. Hence, e^L is a unitary operator¹⁵. We see that

$$e^L c_{x\sigma} e^{-L} = \exp \left\{ i\sqrt{2}\omega_0^{-3/2} \sum_{y \in \Lambda} g_{xy} p_y \right\} c_{x\sigma}, \quad (38)$$

$$e^L b_x e^{-L} = b_x - \omega_0^{-1} \sum_{y \in \Lambda} g_{yx} n_y. \quad (39)$$

Let

$$V_{xy} = \sum_{z \in \Lambda} \frac{2}{\omega_0} g_{xz} g_{yz}. \quad (40)$$

Using the facts that

$$e^{-i\frac{\pi}{2}N_p} q_x e^{i\frac{\pi}{2}N_p} = \omega_0^{-1} p_x, \quad e^{-i\frac{\pi}{2}N_p} p_x e^{i\frac{\pi}{2}N_p} = \omega_0 q_x, \quad (41)$$

where $N_p = \sum_{x \in \Lambda} b_x^* b_x$, one arrives at the following:

Proposition 3.1. *Set $\mathcal{U} = e^{-i\frac{\pi}{2}N_p} e^L$. We define $\hat{H}_M$ by*

$$\hat{H}_M = \mathcal{U} H_M \mathcal{U}^* - \frac{1}{2} \sum_{x,y \in \Lambda} V_{xy} + \frac{g_*^2}{\omega_0^2} (|\Lambda| - 2M), \quad (42)$$

where $g_* = \sum_{x \in \Lambda} g_{xy}$ ¹⁶. Then we have

$$\hat{H}_M = -T_{-g,\uparrow} - T_{-g,\downarrow} + H_p + \mathbf{U}, \quad (43)$$

where

$$T_{\pm g,\sigma} = \sum_{\{x,y\} \in E} t_{xy} c_{x\sigma}^* c_{y\sigma} \exp \left\{ \pm i\Phi_{\{x,y\}} \right\}, \quad (44)$$

$$\Phi_{\{x,y\}} = \sqrt{2}\omega_0^{-1/2} \sum_{z \in \Lambda} (g_{xz} - g_{yz}) q_z, \quad (45)$$

$$H_p = \frac{1}{2} \sum_{x \in \Lambda} (p_x^2 + \omega_0^2 q_x^2), \quad (46)$$

$$\mathbf{U} = \frac{1}{2} \sum_{x,y \in \Lambda} U_{\text{eff},xy} (n_x - \mathbb{1})(n_y - \mathbb{1}), \quad (47)$$

$$U_{\text{eff},xy} = U_{xy} - V_{xy}. \quad (48)$$

¹⁵The unitary operator e^L was introduced by Lang and Firsov [16].

¹⁶By (A. 1), g_* is a constant independent of y .

Proof. We note the following:

$$\sum_{x,y \in \Lambda} V_{xy} n_{y\sigma} = \frac{2}{\omega_0} g_*^2 N_{e\sigma} = \frac{1}{\omega_0} g_*^2 (|\Lambda| - 2M) \quad \text{on } \mathfrak{H}_M. \quad (49)$$

Here, we used **(A. 1)**. Thus, the formula immediately follows from (38), (39) and (41). $\square$

3.2. Expression of the Hamiltonian in $(\mathfrak{F}_e \otimes \mathfrak{F}_e) \otimes \mathfrak{P}$

Note that

$$c_{x\uparrow} = c_x \otimes \mathbb{1}, \quad c_{x\downarrow} = (-\mathbb{1})^{N_e} \otimes c_x, \quad (50)$$

where c_x and c_x^* are the fermionic annihilation- and creation operators on $\mathfrak{F}_e$, and N_e is the fermionic number operator given by $N_e = \sum_{x \in \Lambda} n_x$ with $n_x = c_x^* c_x$. Thus, we have the following:

$$T_{\pm g, \uparrow} = \sum_{\{x,y\} \in E} t_{xy} c_x^* c_y \otimes \mathbb{1} \otimes \exp \left\{ \pm i\Phi_{\{x,y\}} \right\}, \quad (51)$$

$$T_{\pm g, \downarrow} = \sum_{\{x,y\} \in E} t_{xy} \mathbb{1} \otimes c_x^* c_y \otimes \exp \left\{ \pm i\Phi_{\{x,y\}} \right\}, \quad (52)$$

$$\mathbf{U} = \frac{1}{2} \sum_{x,y \in \Lambda} U_{\text{eff},xy} (n_x \otimes \mathbb{1} + \mathbb{1} \otimes n_x - \mathbb{1}) (n_y \otimes \mathbb{1} + \mathbb{1} \otimes n_y - \mathbb{1}) \otimes \mathbb{1}_{\mathfrak{P}}, \quad (53)$$

where $\mathbb{1}_{\mathfrak{P}}$ is the identity operator on $\mathfrak{P}$.

3.3. The hole-particle transformation

The *hole-particle transformation* is a unitary operator $\mathcal{W}$ on $\mathfrak{E}_{|\Lambda|}$ such that

$$\mathcal{W} c_x \otimes \mathbb{1} \mathcal{W}^* = \gamma_x c_x^* \otimes \mathbb{1}, \quad \mathcal{W} c_x^* \otimes \mathbb{1} \mathcal{W}^* = \gamma_x c_x \otimes \mathbb{1}, \quad \mathcal{W} \mathbb{1} \otimes c_x \mathcal{W}^* = \mathbb{1} \otimes c_x. \quad (54)$$

Observe that $\mathcal{W} N_e \mathcal{W}^* = |\Lambda| - (N_e \otimes \mathbb{1} - \mathbb{1} \otimes N_e)$ and $\mathcal{W} S^{(z)} \mathcal{W}^* = \frac{1}{2} |\Lambda| - \frac{1}{2} (N_e \otimes \mathbb{1} + \mathbb{1} \otimes N_e)$. Hence, we have

$$\mathcal{W} \mathfrak{E}_{|\Lambda|} = \bigoplus_{n=0}^{|\Lambda|} \mathfrak{F}_{e,n} \otimes \mathfrak{F}_{e,n}, \quad \mathcal{W} \mathfrak{H}_M = \mathfrak{F}_{e, (|\Lambda|-2M)/2} \otimes \mathfrak{F}_{e, (|\Lambda|-2M)/2}, \quad (55)$$

where $\mathfrak{F}_{e,n} = \wedge^n \ell^2(\Lambda)$. In what follows, we set

$$M^\dagger = \frac{1}{2} (|\Lambda| - 2M). \quad (56)$$

Lemma 3.2. *We have the following:*

- (i) $\mathcal{W} T_{-g, \uparrow} \mathcal{W}^* = T_{+g, \uparrow}$.
- (ii) $\mathcal{W} T_{-g, \downarrow} \mathcal{W}^* = T_{-g, \downarrow}$.
- (iii) $\mathcal{W} \mathbf{U} \mathcal{W}^* = \tilde{\mathbf{U}}$, where

$$\tilde{\mathbf{U}} = \frac{1}{2} \sum_{x,y \in \Lambda} U_{\text{eff},xy} (n_x \otimes \mathbb{1} - \mathbb{1} \otimes n_x) (n_y \otimes \mathbb{1} - \mathbb{1} \otimes n_y) \otimes \mathbb{1}_{\mathfrak{P}}. \quad (57)$$

Proof. (i) By definition of $\mathcal{W}$, we have

$$\begin{aligned} & \mathcal{W} \sum_{\{x,y\} \in E} t_{xy} c_x^* c_y \otimes \mathbb{1} \otimes \exp \left\{ -i\Phi_{\{x,y\}} \right\} \mathcal{W}^* \\ &= \sum_{\{x,y\} \in E} t_{xy} \gamma_x \gamma_y c_x c_y^* \otimes \mathbb{1} \otimes \exp \left\{ -i\Phi_{\{x,y\}} \right\}. \end{aligned} \quad (58)$$

Since G is bipartite, $\gamma_x \gamma_y = -1$ holds for all $\{x, y\} \in E$. Consequently,

$$\text{RHS of (58)} = \sum_{\{x,y\} \in E} t_{xy} c_y^* c_x \otimes \mathbb{1} \otimes \exp \left\{ -i\Phi_{\{x,y\}} \right\} \quad (59)$$

$$\begin{aligned} &= \sum_{\{y,x\} \in E} t_{yx} c_x^* c_y \otimes \mathbb{1} \otimes \exp \left\{ -i\Phi_{\{y,x\}} \right\} \\ &= \sum_{\{x,y\} \in E} t_{xy} c_x^* c_y \otimes \mathbb{1} \otimes \exp \left\{ +i\Phi_{\{x,y\}} \right\}. \end{aligned} \quad (60)$$

Here, we used that $t_{xy} = t_{yx}$ and $\Phi_{\{y,x\}} = -\Phi_{\{x,y\}}$. Thus, we have (i). Similarly, one obtains that $\mathcal{W} T_{-g,\downarrow} \mathcal{W}^* = T_{-g,\downarrow}$.

(iii) Since $\mathcal{W} n_x \otimes \mathbb{1} \mathcal{W}^* = (\mathbb{1} - n_x) \otimes \mathbb{1}$ and $\mathcal{W} \mathbb{1} \otimes n_x \mathcal{W}^* = \mathbb{1} \otimes n_x$, we see that

$$\mathcal{W} \mathbf{U} \mathcal{W}^* = \tilde{\mathbf{U}}. \quad \square \quad (61)$$

Corollary 3.3. *Let $\mathbb{H}_M = \mathcal{W} \hat{H}_M \mathcal{W}^*$. Then we have*

$$\mathbb{H}_M = -T_{+g,\uparrow} - T_{-g,\downarrow} + \tilde{\mathbf{U}} + H_P. \quad (62)$$

3.4. Expression of the Hamiltonian in $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$

3.4.1. Natural identification $\mathfrak{F}_{e,M^\dagger} \otimes \mathfrak{F}_{e,M^\dagger}$ with $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})$. Let ϑ be an anti-linear involution on $\mathfrak{F}_{e,M^\dagger}$ defined by

$$\vartheta c_x \vartheta = c_x, \quad \vartheta \Omega = \Omega, \quad (63)$$

where Ω is the Fock vacuum in $\mathfrak{F}_e$. We define an isometric isomorphism from $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})$ onto $\mathfrak{F}_{e,M^\dagger} \otimes \mathfrak{F}_{e,M^\dagger}$ by

$$\Phi_\vartheta(|\varphi\rangle\langle\psi|) = \varphi \otimes \vartheta\psi. \quad (64)$$

Hence, we can identify $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})$ with $\mathfrak{F}_{e,M^\dagger} \otimes \mathfrak{F}_{e,M^\dagger}$ by Φ_ϑ . Moreover, one has

$$\Phi_\vartheta \mathcal{L}(A) \Phi_\vartheta^{-1} = A \otimes \mathbb{1}, \quad \Phi_\vartheta \mathcal{R}(\vartheta A^* \vartheta) \Phi_\vartheta^{-1} = \mathbb{1} \otimes A \quad (65)$$

for any bounded linear operator A on $\mathfrak{F}_{e,M^\dagger}$. To summarize, we have the following identifications:

$$\mathfrak{F}_{e,M^\dagger} \otimes \mathfrak{F}_{e,M^\dagger} = \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}), \quad (66)$$

$$\mathcal{L}(A) = A \otimes \mathbb{1}, \quad \mathcal{R}(\vartheta A^* \vartheta) = \mathbb{1} \otimes A. \quad (67)$$

3.4.2. The Schrödinger representation. Note the following identification:

$$\mathfrak{P} = L^2(\mathcal{Q}, d\mathbf{q}) = L^2(\mathcal{Q}), \quad (68)$$

where $\mathcal{Q} = \mathbb{R}^{|\Lambda|}$, $d\mathbf{q} = \prod_{x \in \Lambda} dq_x$ is the $|\Lambda|$ -dimensional Lebesgue measure on $\mathcal{Q}$, and $L^2(\mathcal{Q})$ is the Hilbert space of the square integrable functions on $\mathcal{Q}$. Under this identification, q_x and p_x can be viewed as multiplication and partial differential operators, respectively. Moreover, the phonon energy term can be expressed as

$$H_p = \frac{1}{2} \sum_{x \in \Lambda} \left(-\frac{\partial^2}{\partial q_x^2} + \omega_0^2 q_x^2 \right) - \frac{|\Lambda|}{2}. \quad (69)$$

3.4.3. Representation in $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$. By (66) and (68), we have the following identifications:

$$\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes \mathfrak{P} = \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q}) = \int_{\mathcal{Q}}^{\oplus} \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) d\mathbf{q}. \quad (70)$$

For each $\psi = \int_{\mathcal{Q}}^{\oplus} \psi(\mathbf{q}) d\mathbf{q} \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q}) = \int_{\mathcal{Q}}^{\oplus} \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) d\mathbf{q}$, let us define an isometric isomorphism $\Phi_{\vartheta}^{\oplus}$ from $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$ onto $[\mathfrak{F}_{e,M^\dagger} \otimes \mathfrak{F}_{e,M^\dagger}] \otimes L^2(\mathcal{Q})$ by

$$\Phi_{\vartheta}^{\oplus}(\psi) = \int_{\mathcal{Q}}^{\oplus} \Phi_{\vartheta}(\psi(\mathbf{q})) d\mathbf{q}. \quad (71)$$

Let $\mathbf{q} \mapsto A(\mathbf{q})$ be a $\mathcal{B}(\mathfrak{F}_{e,M^\dagger})$ -valued measurable map such that $\sup_{\mathbf{q}} \|A(\mathbf{q})\|_{\mathcal{B}} < \infty$. Using (65), we see that

$$\Phi_{\vartheta}^{\oplus} \int_{\mathcal{Q}}^{\oplus} \mathcal{L}(A(\mathbf{q})) d\mathbf{q} \Phi_{\vartheta}^{\oplus -1} = \int_{\mathcal{Q}}^{\oplus} A(\mathbf{q}) \otimes \mathbb{1} d\mathbf{q}, \quad (72)$$

$$\Phi_{\vartheta}^{\oplus} \int_{\mathcal{Q}}^{\oplus} \mathcal{R}(\vartheta A(\mathbf{q})^* \vartheta) d\mathbf{q} \Phi_{\vartheta}^{\oplus -1} = \int_{\mathcal{Q}}^{\oplus} \mathbb{1} \otimes A(\mathbf{q}) d\mathbf{q}. \quad (73)$$

Lemma 3.4. *Under identification (70), we have the following:*

(i)

$$T_{+g,\uparrow} = \int_{\mathcal{Q}}^{\oplus} \mathcal{L}(\mathbf{T}_{+g}(\mathbf{q})) d\mathbf{q}, \quad T_{-g,\downarrow} = \int_{\mathcal{Q}}^{\oplus} \mathcal{R}(\mathbf{T}_{+g}(\mathbf{q})) d\mathbf{q}, \quad (74)$$

where

$$\mathbf{T}_{\pm g}(\mathbf{q}) = \sum_{\{x,y\} \in E} t_{xy} c_x^* c_y \exp \left\{ \pm i \Phi_{\{x,y\}}(\mathbf{q}) \right\}, \quad (75)$$

$$\Phi_{\{x,y\}}(\mathbf{q}) = \sqrt{2} \omega_0^{-1/2} \sum_{z \in \Lambda} (g_{xz} - g_{yz}) q_z, \quad (76)$$

for each $\mathbf{q} = \{q_x\}_x \in \mathcal{Q}$.

(ii)

$$\tilde{\mathbf{U}} = \frac{1}{2} \sum_{x,y \in \Lambda} U_{\text{eff},xy} \{ \mathcal{L}(\mathbf{n}_x) - \mathcal{R}(\mathbf{n}_x) \} \{ \mathcal{L}(\mathbf{n}_y) - \mathcal{R}(\mathbf{n}_y) \} \otimes \mathbb{1}_{L^2}, \quad (77)$$

where $\mathbb{1}_{L^2}$ is the identity operator on $L^2(\mathcal{Q})$.

Proof. (i) Since $\mathcal{L}(\cdot)$ is linear, i.e., $\mathcal{L}(aX + bY) = a\mathcal{L}(X) + b\mathcal{L}(Y)$, we have

$$\begin{aligned} T_{+g,\uparrow} &= \int_{\mathcal{Q}}^{\oplus} \sum_{\{x,y\} \in E} t_{xy} \exp \left\{ i\Phi_{\{x,y\}}(\mathbf{q}) \right\} c_x^* c_y \otimes \mathbb{1} d\mathbf{q} \\ &= \int_{\mathcal{Q}}^{\oplus} \sum_{\{x,y\} \in E} t_{xy} \exp \left\{ i\Phi_{\{x,y\}}(\mathbf{q}) \right\} \mathcal{L}(c_x^* c_y) d\mathbf{q} \\ &= \int_{\mathcal{Q}}^{\oplus} \mathcal{L}(\mathbf{T}_{+g}(\mathbf{q})) d\mathbf{q}. \end{aligned} \quad (78)$$

Similarly, since $\mathcal{R}(\cdot)$ is linear and $\vartheta c_x \vartheta = c_x$, we have

$$\begin{aligned} T_{-g,\downarrow} &= \int_{\mathcal{Q}}^{\oplus} \sum_{\{x,y\} \in E} t_{xy} \exp \left\{ -i\Phi_{\{x,y\}}(\mathbf{q}) \right\} \mathbb{1} \otimes c_x^* c_y d\mathbf{q} \\ &= \int_{\mathcal{Q}}^{\oplus} \sum_{\{x,y\} \in E} t_{xy} \exp \left\{ -i\Phi_{\{x,y\}}(\mathbf{q}) \right\} \mathcal{R}(\vartheta(c_x^* c_y)^* \vartheta) d\mathbf{q} \\ &= \int_{\mathcal{Q}}^{\oplus} \sum_{\{x,y\} \in E} t_{xy} \exp \left\{ -i\Phi_{\{x,y\}}(\mathbf{q}) \right\} \mathcal{R}(c_y^* c_x) d\mathbf{q} \\ &= \int_{\mathcal{Q}}^{\oplus} \sum_{\{y,x\} \in E} t_{yx} \exp \left\{ -i\Phi_{\{y,x\}}(\mathbf{q}) \right\} \mathcal{R}(c_x^* c_y) d\mathbf{q} \\ &= \int_{\mathcal{Q}}^{\oplus} \mathcal{R}(\mathbf{T}_{+g}(\mathbf{q})) d\mathbf{q}. \end{aligned} \quad (79)$$

Here, we have used $t_{xy} = t_{yx}$ and $\Phi_{\{y,x\}}(\mathbf{q}) = -\Phi_{\{x,y\}}(\mathbf{q})$.

(ii) is immediate. $\square$

Corollary 3.5. *Under identification (70), we have*

$$\mathbb{H}_M = -\mathbb{T} - \mathbb{U} + H_p, \quad (80)$$

where

$$\mathbb{T} = \int_{\mathcal{Q}}^{\oplus} \mathcal{L}(\mathbf{T}_{+g}(\mathbf{q})) d\mathbf{q} + \int_{\mathcal{Q}}^{\oplus} \mathcal{R}(\mathbf{T}_{+g}(\mathbf{q})) d\mathbf{q}, \quad (81)$$

$$\mathbb{T}_{+g}(\mathbf{q}) = \mathbf{T}_{+g}(\mathbf{q}) + \frac{1}{2} \langle \mathbf{n}, \mathbf{U}_{\text{eff}} \mathbf{n} \rangle, \quad (82)$$

$$\mathbb{U} = \sum_{x,y \in \Lambda} U_{\text{eff},xy} \mathcal{L}(\mathbf{n}_x) \mathcal{R}(\mathbf{n}_y) \otimes \mathbb{1}_{L^2}. \quad (83)$$

Here, we use the following notation: $\langle \mathbf{n}, \mathbf{U}_{\text{eff}} \mathbf{n} \rangle := \sum_{x,y \in \Lambda} U_{\text{eff},xy} \mathbf{n}_x \mathbf{n}_y$.

3.5. Functional integral representation

Under identification (70), each $\psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$ can be expressed as $\psi = \int_{\mathcal{Q}}^\oplus \psi(\mathbf{q}) d\mathbf{q}$, where $\psi(\mathbf{q}) \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})$ for a.e. $\mathbf{q}$.

Definition 3.6. Let A be a bounded linear operator on $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$. If there exists a $\mathcal{B}(\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}))$ -valued map $(\mathbf{q}, \mathbf{q}') \mapsto K(\mathbf{q}, \mathbf{q}')$ such that

$$(A\psi)(\mathbf{q}) = \int_{\mathcal{Q}} K(\mathbf{q}, \mathbf{q}') \psi(\mathbf{q}') d\mathbf{q}' \quad \forall \psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q}), \quad (84)$$

then we say that A has a kernel operator K . We denote by $A(\mathbf{q}, \mathbf{q}')$ the kernel operator of A if it exists. Trivially, it holds that

$$\langle \varphi, A\psi \rangle = \int_{\mathcal{Q} \times \mathcal{Q}} d\mathbf{q} d\mathbf{q}' \langle \varphi(\mathbf{q}), A(\mathbf{q}, \mathbf{q}') \psi(\mathbf{q}') \rangle_{\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})}. \quad \diamond \quad (85)$$

In this subsection, we will express the kernel operator of $\exp\{-\beta(-\mathbb{T} + H_p)\}$ in terms of a functional integral representation.

In the remainder of this paper, we may assume that $\omega_0 = 1$ without loss of generality.

Set $A = C([0, \infty); \mathcal{Q})$, the set of all $\mathcal{Q}$ -valued continuous functions on $[0, \infty)$. Let $(A, \mathcal{B}(A), D\alpha)$ be the probability space for the $|\Lambda|$ -dimensional Brownian bridge $\{\alpha(s) \mid 0 \leq s \leq 1\} = \{\{\alpha_x(s)\}_{x \in \Lambda} \mid 0 \leq s \leq 1\}$, i.e., the Gaussian process with covariance

$$\int_A \alpha_x(s) \alpha_y(t) D\alpha = \delta_{xy} s(1-t) \quad (86)$$

for $0 \leq s \leq t \leq 1$ and $x, y \in \Lambda$. Define, for each $\mathbf{q}, \mathbf{q}' \in \mathcal{Q}$,

$$\omega(s) = (1 - \beta^{-1}s)\mathbf{q} + \beta^{-1}s\mathbf{q}' + \sqrt{\beta}\alpha(\beta^{-1}s). \quad (87)$$

The conditional Wiener measure $d\mu_{\mathbf{q}, \mathbf{q}'; \beta}$ is given by

$$d\mu_{\mathbf{q}, \mathbf{q}'; \beta} = P_\beta(\mathbf{q}, \mathbf{q}') D\alpha, \quad (88)$$

where $P_\beta(\mathbf{q}, \mathbf{q}') = (2\pi\beta)^{-1/2} \exp(-\frac{1}{2\beta}|\mathbf{q} - \mathbf{q}'|^2)$.

For each $\varphi \in A$, $\omega(\varphi)$ indicates a function $s \mapsto \omega(s)(\varphi)$, the sample path $\omega(\cdot)(\varphi)$ associated with φ . Let

$$G_\beta(\omega(\varphi)) = \prod_0^\beta e^{\mathbb{T} + g(\omega(s)(\varphi)) ds}, \quad (89)$$

where the RHS of (89) is the strong product integration (see Appendix B). Note that since $\omega(s)(\varphi)$ is continuous in s for all $\varphi \in A$, the RHS of (89) exists.

Proposition 3.7. *Let*

$$K_M = -\mathbb{T} + H_p. \quad (90)$$

Then $e^{-\beta K_M}$ has a kernel operator given by

$$e^{-\beta K_M}(\mathbf{q}, \mathbf{q}') = \int d\mu_{\mathbf{q}, \mathbf{q}'; \beta} \mathcal{L}[G_\beta(\omega)] \mathcal{R}[G_\beta(\omega)^*] e^{-\int_0^\beta ds \mathcal{V}(\omega(s))}, \quad (91)$$

where

$$\mathcal{V}(\mathbf{q}) = \frac{1}{2} \sum_{x \in \Lambda} \omega_0^2 q_x^2 - \frac{1}{2} |\Lambda|. \quad (92)$$

Proof. First, note that

$$\begin{aligned} & \left\langle f_0, e^{-\beta H_{\mathbb{P}}/n} f_1 e^{-\beta H_{\mathbb{P}}/n} f_2 \cdots f_n \right\rangle \\ &= \int_{\mathcal{Q} \times \mathcal{Q}} d\mathbf{q} d\mathbf{q}' \int d\mu_{\mathbf{q}, \mathbf{q}'; \beta} e^{-\int_0^\beta ds \mathcal{V}(\omega(s))} \\ & \quad \times f_0(\mathbf{q})^* f_1\left(\omega\left(\frac{\beta}{n}\right)\right) f_2\left(\omega\left(\frac{2\beta}{n}\right)\right) \cdots f_{n-1}\left(\omega\left(\frac{(n-1)\beta}{n}\right)\right) f_n(\mathbf{q}') \end{aligned} \quad (93)$$

for $f_0, f_n \in L^2(\mathcal{Q})$ and $f_1, \dots, f_{n-1} \in L^\infty(\mathcal{Q})$, see [33]. Let $\mathbb{T}(\mathbf{q}) = \mathcal{L}(\mathbb{T}_{+g}(\mathbf{q})) + \mathcal{R}(\mathbb{T}_{+g}(\mathbf{q}))$. By (93) and the Trotter–Kato product formula, we have

$$\begin{aligned} \langle \varphi, e^{-\beta K_M} \psi \rangle &= \lim_{n \rightarrow \infty} \left\langle \varphi, \left(e^{-\beta H_{\mathbb{P}}/n} e^{\beta \mathbb{T}/n} \right)^n \psi \right\rangle \\ &= \lim_{n \rightarrow \infty} \int_{\mathcal{Q} \times \mathcal{Q}} d\mathbf{q} d\mathbf{q}' \int d\mu_{\mathbf{q}, \mathbf{q}'; \beta} e^{-\int_0^\beta ds \mathcal{V}(\omega(s))} \\ & \quad \times \left\langle \varphi(\mathbf{q}), e^{\frac{\beta}{n} \mathbb{T}(\omega(\frac{\beta}{n}))} e^{\frac{\beta}{n} \mathbb{T}(\omega(\frac{2\beta}{n}))} \cdots e^{\frac{\beta}{n} \mathbb{T}(\omega(\frac{n\beta}{n}))} \psi(\mathbf{q}') \right\rangle_{\mathcal{L}^2(\mathfrak{F}_{e, M^\dagger})} \\ &= \lim_{n \rightarrow \infty} \int_{\mathcal{Q} \times \mathcal{Q}} d\mathbf{q} d\mathbf{q}' \int d\mu_{\mathbf{q}, \mathbf{q}'; \beta} e^{-\int_0^\beta ds \mathcal{V}(\omega(s))} \\ & \quad \times \left\langle \varphi(\mathbf{q}), \mathcal{L} \left[e^{\frac{\beta}{n} \mathbb{T}_{+g}(\omega(\frac{\beta}{n}))} \cdots e^{\frac{\beta}{n} \mathbb{T}_{+g}(\omega(\frac{n\beta}{n}))} \right] \right. \\ & \quad \times \left. \mathcal{R} \left[e^{\frac{\beta}{n} \mathbb{T}_{+g}(\omega(\frac{n\beta}{n}))} \cdots e^{\frac{\beta}{n} \mathbb{T}_{+g}(\omega(\frac{\beta}{n}))} \right] \psi(\mathbf{q}') \right\rangle_{\mathcal{L}^2(\mathfrak{F}_{e, M^\dagger})}. \end{aligned} \quad (94)$$

By the dominated convergence theorem, we conclude (91). $\square$

4. Proof of Theorem 1.1

4.1. Strategy

The main purpose of this section is to prove Theorem 4.1 below. As seen in Subsection 4.5, Theorem 1.1 is a corollary of Theorem 4.1.

Theorem 4.1. *Assume that $|\Lambda|$ is even. Assume **(A. 1)**. Assume that U_{eff} is positive semi-definite. Then for all $M \in \{-|\Lambda|/2, -|\Lambda|/2 + 1, \dots, |\Lambda|/2\}$, there exists a Hilbert cone $\mathfrak{H}_{M,+}$ such that $e^{-\beta H_M} \geq 0$ w.r.t. $\mathfrak{H}_{M,+}$ holds for all $\beta \geq 0$.*

In the remainder of this section, we will continue to assume **(A. 1)** and that $|\Lambda|$ is even.

4.2. Preliminaries

The canonical cone in $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$ is given by

$$\mathfrak{C}_M = \int_{\mathcal{Q}}^{\oplus} \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+ d\mathbf{q}, \quad (95)$$

where the direct integral of $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$ over $\mathcal{Q}$ is defined by

$$\begin{aligned} & \int_{\mathcal{Q}}^{\oplus} \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+ d\mathbf{q} \\ &= \left\{ \Psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q}) \mid \Psi(\mathbf{q}) \geq 0 \text{ w.r.t. } \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+ \text{ for a.e. } \mathbf{q} \right\}. \end{aligned} \quad (96)$$

Proposition 4.2. $\mathfrak{C}_M$ is a Hilbert cone in $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$.

Proof. We will check the conditions (i)-(iii) of Definition 2.1.

(i) For all $\Phi, \Psi \in \mathfrak{C}_M$, we know that $\langle \Phi(\mathbf{q}), \Psi(\mathbf{q}) \rangle_{\mathcal{L}^2} \geq 0$ for a.e. $\mathbf{q}$. Hence, $\langle \Phi, \Psi \rangle = \int_{\mathcal{Q}} \langle \Phi(\mathbf{q}), \Psi(\mathbf{q}) \rangle_{\mathcal{L}^2} d\mathbf{q} \geq 0$.

(ii) Let $\mathfrak{C}_{M,\mathbb{R}}$ be a real subspace generated by $\mathfrak{C}_M$. It is easy to see that $\mathfrak{C}_{M,\mathbb{R}} = \{\Psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q}) \mid \Psi(\mathbf{q}) \text{ is self-adjoint for a.e. } \mathbf{q}\}$. Let $\Psi \in \mathfrak{C}_{M,\mathbb{R}}$. Since $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$ is a Hilbert cone, we have a decomposition $\Psi(\mathbf{q}) = \Psi_+(\mathbf{q}) - \Psi_-(\mathbf{q})$ such $\Psi_\pm(\mathbf{q}) \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$ and $\langle \Psi_+(\mathbf{q}), \Psi_-(\mathbf{q}) \rangle_{\mathcal{L}^2} = 0$. Thus, (ii) is clear.

(iii) For each $\Psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$, we define $\Psi_R, \Psi_I \in \mathfrak{C}_{M,\mathbb{R}}$ by $\Psi_R(\mathbf{q}) = \frac{1}{2}(\Psi(\mathbf{q}) + \Psi(\mathbf{q})^*)$, $\Psi_I(\mathbf{q}) = \frac{1}{2i}(\Psi(\mathbf{q}) - \Psi(\mathbf{q})^*)$. Then $\Psi = \Psi_R + i\Psi_I$. $\square$

Lemma 4.3. Let $\Psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$. The following are equivalent:

- (i) $\Psi \in \mathfrak{C}_M$.
- (ii) $\forall \xi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+ \forall f \in L^2(\mathcal{Q})_+, \langle \Psi, \xi \otimes f \rangle \geq 0$.

Proof. To show that (i) $\Rightarrow$ (ii) is easy. Let us show the inverse. Set $g_\xi(\mathbf{q}) = \langle \Psi(\mathbf{q}), \xi \rangle_{\mathcal{L}^2}$. By (ii), we have

$$0 \leq \langle \Psi, \xi \otimes f \rangle = \int_{\mathcal{Q}} f(\mathbf{q}) g_\xi(\mathbf{q}) d\mathbf{q}. \quad (97)$$

From this, we conclude that $g_\xi(\mathbf{q}) \geq 0$ a.e. $\mathbf{q}$. Since ξ is arbitrary, we see that $\Psi \in \mathfrak{C}_{M,\mathbb{R}}$, otherwise, $g_\xi(\mathbf{q})$ becomes a complex-valued function for some ξ . Since $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$ is a Hilbert cone, we have the decomposition $\Psi(\mathbf{q}) = \Psi_+(\mathbf{q}) - \Psi_-(\mathbf{q})$, such that $\Psi_\pm(\mathbf{q}) \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$ and $\langle \Psi_+(\mathbf{q}), \Psi_-(\mathbf{q}) \rangle_{\mathcal{L}^2} = 0$. Since ξ is arbitrary, by taking $\xi = \Psi_-(\mathbf{q})$, we have

$$0 \leq g_\xi(\mathbf{q}) = -\|\Psi_-(\mathbf{q})\|^2 \leq 0, \quad (98)$$

which implies that $\Psi_-(\mathbf{q}) = 0$. Thus, $\Psi \in \mathfrak{C}_M$. $\square$

Lemma 4.4. Let $B : \mathcal{Q} \rightarrow \mathcal{B}(\mathfrak{F}_{e,M^\dagger})$; $\mathbf{q} \mapsto B(\mathbf{q})$ be strongly continuous. Then we have

$$\int_{\mathcal{Q}}^{\oplus} \mathcal{L}(B(\mathbf{q})^*) \mathcal{R}(B(\mathbf{q})) d\mathbf{q} \geq 0 \text{ w.r.t. } \mathfrak{C}_M. \quad (99)$$

In particular, $\mathcal{L}(C^*)\mathcal{R}(C) \otimes \mathbb{1}_{L^2} \geq 0$ w.r.t. $\mathfrak{C}_M$ for each $C \in \mathcal{B}(\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}))^{17}$.

Proof. For a.e. $\mathbf{q}$, we obtain $\mathcal{L}(B(\mathbf{q})^*)\mathcal{R}(B(\mathbf{q})) \geq 0$ w.r.t. $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$ by Lemma 2.6. Thus, $\int_Q^\oplus \mathcal{L}(B(\mathbf{q})^*)\mathcal{R}(B(\mathbf{q}))d\mathbf{q}$ leaves $\mathfrak{C}_M$ invariant. $\square$

Let $L^2(\mathcal{Q})_+$ be a Hilbert cone in $L^2(\mathcal{Q})$ defined by

$$L^2(\mathcal{Q})_+ = \{F \in L^2(\mathcal{Q}) \mid F(\mathbf{q}) \geq 0 \text{ a.e.}\}. \quad (100)$$

Then, the following lemma will be useful:

Lemma 4.5. *Let A be a bounded linear operator in $L^2(\mathcal{Q})$. If $A \geq 0$ w.r.t. $L^2(\mathcal{Q})_+$, then $\mathbb{1}_{\mathcal{L}^2} \otimes A \geq 0$ w.r.t. $\mathfrak{C}_M$.*

Proof. Let $f \in L^2(\mathcal{Q})_+$. Since $A \geq 0$ w.r.t. $L^2(\mathcal{Q})_+$, we know $Af \in L^2(\mathcal{Q})_+$. Thus, for each $\xi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$, it holds that $\xi \otimes Af \in \mathfrak{C}_M$. Hence, for each $\Psi \in \mathfrak{C}_M$, we have

$$\langle \mathbb{1}_{\mathcal{L}^2} \otimes A\Psi, \xi \otimes f \rangle = \langle \Psi, \xi \otimes Af \rangle \geq 0. \quad (101)$$

By Lemma 4.3, we obtain $\mathbb{1}_{\mathcal{L}^2} \otimes A\Psi \in \mathfrak{C}_M$, which means that $\mathbb{1}_{\mathcal{L}^2} \otimes A \geq 0$ w.r.t. $\mathfrak{C}_M$. $\square$

4.3. Lower bounds for the effective Coulomb interaction

Proposition 4.6. *We have the following:*

(i) *If U_{eff} is positive semi-definite, then*

$$\sum_{x,y \in \Lambda} U_{\text{eff},xy} \mathcal{L}(\mathbf{n}_x) \mathcal{R}(\mathbf{n}_y) \otimes \mathbb{1}_{L^2} \geq 0 \text{ w.r.t. } \mathfrak{C}_M. \quad (102)$$

(ii) *If U_{eff} is positive definite, then there exists a $U_0 > 0$ such that*

$$\sum_{x,y \in \Lambda} U_{\text{eff},xy} \mathcal{L}(\mathbf{n}_x) \mathcal{R}(\mathbf{n}_y) \otimes \mathbb{1}_{L^2} \geq U_0 \sum_{x \in \Lambda} \mathcal{L}(\mathbf{n}_x) \mathcal{R}(\mathbf{n}_x) \otimes \mathbb{1}_{L^2} \geq 0 \text{ w.r.t. } \mathfrak{C}_M. \quad (103)$$

Proof. (i) Let $\mathbf{M} = (M_{xy})$ be a $|\Lambda| \times |\Lambda|$ matrix defined by $M_{xy} = U_{\text{eff},xy}$ ($x, y \in \Lambda$). By assumption, $\mathbf{M}$ is positive semi-definite. Thus, there exists an orthogonal matrix $\mathbf{P}$ such that $\mathbf{M} = \mathbf{P}\mathbf{D}\mathbf{P}^T$, where $\mathbf{D} = \text{diag}(\lambda_x)$ is a diagonal matrix with $\lambda_x \geq 0$. Set $\mathbf{n} = \{\mathbf{n}_x\}_{x \in \Lambda}$ and set $\tilde{\mathbf{n}} = \mathbf{P}^T \mathbf{n}$. Denoting $\tilde{\mathbf{n}} = (\tilde{\mathbf{n}}_x)_{x \in \Lambda}$, we have

$$\begin{aligned} \sum_{x,y \in \Lambda} U_{\text{eff},xy} \mathcal{L}(\mathbf{n}_x) \mathcal{R}(\mathbf{n}_y) &= \langle \mathcal{L}(\mathbf{n}), \mathbf{M} \mathcal{R}(\mathbf{n}) \rangle = \langle \mathcal{L}(\tilde{\mathbf{n}}), \mathbf{D} \mathcal{R}(\tilde{\mathbf{n}}) \rangle \\ &= \sum_{x \in \Lambda} \lambda_x \mathcal{L}(\tilde{\mathbf{n}}_x) \mathcal{R}(\tilde{\mathbf{n}}_x). \end{aligned} \quad (104)$$

Clearly, the RHS of (104) is positive w.r.t. $\mathfrak{C}_M$ by Lemma 4.4.

¹⁷ $\mathcal{B}(\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}))$ is the set of all bounded linear operators in the Hilbert space $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})$,

(ii) By assumption, $\mathbf{M}$ is positive definite. Thus, the lowest eigenvalue of $\mathbf{M}$ is strictly positive: $U_0 := \min_x \lambda_x > 0$. Thus, by (104), one sees that

$$\begin{aligned}
 \sum_{x,y \in \Lambda} U_{\text{eff},xy} \mathcal{L}(\mathfrak{n}_x) \mathcal{R}(\mathfrak{n}_y) &= \sum_{x \in \Lambda} \lambda_x \mathcal{L}(\tilde{\mathfrak{n}}_x) \mathcal{R}(\tilde{\mathfrak{n}}_x) \\
 &\geq U_0 \sum_{x \in \Lambda} \mathcal{L}(\tilde{\mathfrak{n}}_x) \mathcal{R}(\tilde{\mathfrak{n}}_x) \\
 &= U_0 \sum_{x \in \Lambda} \mathcal{L}(\mathfrak{n}_x) \mathcal{R}(\mathfrak{n}_x) \\
 &\geq 0 \quad \text{w.r.t. } \mathcal{L}^2(\mathfrak{F}_{\text{e},M^\dagger})_+. \tag{105}
 \end{aligned}$$

By Lemma 4.4, we conclude our proof of (ii). $\square$

4.4. Completion of proof of Theorem 4.1

Proposition 4.7. *Assume that U_{eff} is positive semi-definite. For all $\beta \geq 0$ and $M^\dagger \in \{-|\Lambda|/2, -|\Lambda|/2 + 1, \dots, |\Lambda|/2\}$, we have $e^{-\beta \mathbb{H}_M} \geq 0$ w.r.t. $\mathfrak{C}_M$.*

Proof. Since $\mathbb{U} \geq 0$ w.r.t. $\mathfrak{C}_M$ by Proposition 4.6, we have

$$e^{\beta \mathbb{U}} = \sum_{n=0}^{\infty} \underbrace{\frac{\beta^n}{n!}}_{\geq 0} \underbrace{\mathbb{U}^n}_{\geq 0} \geq 0 \quad \text{w.r.t. } \mathfrak{C}_M \text{ for all } \beta \geq 0. \tag{106}$$

By (69) and Lemma 4.5, it holds that $e^{-\beta H_p} \triangleright 0$ w.r.t. $\mathfrak{C}_M$ for all $\beta \geq 0^{18}$. Denoting $K = H_p - \mathbb{U}$, we have $e^{-\beta K} = e^{-\beta H_p} e^{\beta \mathbb{U}} \geq 0$ w.r.t. $\mathfrak{C}_M$ for all $\beta \geq 0$.

By (81) and Lemma 4.4, we have

$$e^{\beta \mathbb{T}} = \int_{\mathcal{Q}}^{\oplus} \mathcal{L}\left(e^{\beta \mathbb{T}+g(\mathbf{q})}\right) \mathcal{R}\left(e^{\beta \mathbb{T}+g(\mathbf{q})}\right) d\mathbf{q} \geq 0 \quad \text{w.r.t. } \mathfrak{C}_M. \tag{107}$$

Combining these properties, we obtain

$$\left(\underbrace{e^{\beta \mathbb{T}/n}}_{\geq 0} \underbrace{e^{-\beta K/n}}_{\geq 0} \right)^n \geq 0 \quad \text{w.r.t. } \mathfrak{C}_M \text{ for all } \beta \geq 0. \tag{108}$$

Thus, the proposition follows from the Trotter–Kato formula. $\square$

4.5. Proof of Theorem 1.1

Let J be a conjugation defined by $(J\Psi)(\mathbf{q}) = \Psi^*(\mathbf{q})$ for each $\Psi \in \mathcal{L}^2(\mathfrak{F}_{\text{e},M^\dagger}) \otimes L^2(\mathcal{Q})$. Since $e^{-\beta \mathbb{H}_M}$ preserves the positivity w.r.t. $\mathfrak{C}_M$, $\mathbb{H}_M$ commutes with J . Let λ be an eigenvalue of $\mathbb{H}_M$ and let Ψ be a corresponding eigenvector. Set $\Psi_R = (\Psi + J\Psi)/2$ and $\Psi_I = (\Psi - J\Psi)/2i$. Then $\Psi_R(\mathbf{q})$ and $\Psi_I(\mathbf{q})$ are self-adjoint for a.e. $\mathbf{q}$. In addition, they are eigenvectors of $\mathbb{H}_M$ with an associated eigenvalue λ .

Let ψ_M be a ground state of $\mathbb{H}_M$. ψ_M can be written as $\psi_M = \int_{\mathcal{Q}}^{\oplus} \psi_M(\mathbf{q}) d\mathbf{q}$ under identification (70). By the observation above, we may assume that $\psi_M(\mathbf{q})$ is self-adjoint for a.e. $\mathbf{q}$ without loss of generality. Let $\psi_{M,+}(\mathbf{q})$ (resp.

¹⁸To be precise, we know that $\exp\{-\beta \frac{1}{2} \sum_x (-\nabla_{q_x}^2 + \omega_0^2 q_x^2)\} \geq 0$ w.r.t. $L^2(\mathcal{Q})_+$. Thus, by Lemma 4.5, we have $e^{-\beta H_p} = \mathbb{1}_{\mathcal{L}^2} \otimes \exp\{-\beta \frac{1}{2} \sum_x (-\nabla_{q_x}^2 + \omega_0^2 q_x^2)\} \geq 0$ w.r.t. $\mathfrak{C}_M$.

$\psi_{M,-}(\mathbf{q})$ be the positive (resp. negative) part of $\psi_M(\mathbf{q})$ ¹⁹. Hence, it holds that $\psi_M = \psi_{M,+} - \psi_{M,-}$, $\psi_{M,\pm} \in \mathfrak{C}_M$ and $\langle \psi_{M,+}, \psi_{M,-} \rangle = 0$. By Proposition 4.7, we have

$$e^{-\beta E_M} = \langle \psi_M, e^{-\beta \mathbb{H}_M} \psi_M \rangle \leq \langle |\psi_M|, e^{-\beta \mathbb{H}_M} |\psi_M| \rangle, \quad (109)$$

where $|\psi_M| = \psi_{M,+} + \psi_{M,-}$. This means that $|\psi_M|$ is a ground state of $\mathbb{H}_M$ as well. We will show that $|\psi_M|$ satisfies properties (i) and (ii) in Theorem 1.1.

Using the notation in Subsection 5.2, we can express $|\psi_M|$ as

$$|\psi_M| = \sum_{x, Y \in \wedge^{M^\dagger} \Lambda} \int_{\mathcal{Q}}^{\oplus} |\psi_M|_{XY}(\mathbf{q}) |e_X\rangle \langle e_Y| d\mathbf{q}. \quad (110)$$

Since ψ_M is a non-zero vector, $|\psi_M|$ is non-zero as well. Thus, there exists an $X_0 \in \wedge^{M^\dagger} \Lambda$ and a measurable set $\mathcal{I} \subseteq \mathcal{Q}$ with $|\mathcal{I}| > 0$ such that $|\psi_M|_{X_0 X_0}(\mathbf{q}) \neq 0$ for all $\mathbf{q} \in \mathcal{I}$ (X_0 may depend on $\mathbf{q}$)²⁰. Observe that $S_{\text{tot}}^2 |e_{X_0}\rangle \langle e_{X_0}| = 0$. From this, it follows that $P_{S=0} \psi_M \neq 0$, where $P_{S=0}$ is the orthogonal projection onto $\ker[S_{\text{tot}}^2]$. Using the fact that $\mathcal{W}^* S_{\text{tot}}^2 \mathcal{W} = \tilde{S}^2$, we obtain (i).

Let φ_M be a positive ground state of H_M and let $\tilde{\varphi}_M$ be its representation in $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$. Note that $\mathcal{W} S_{x+} S_{y-} \mathcal{W}^* = \gamma_x \gamma_y \mathcal{L}(c_x c_y^*) \mathcal{R}((c_x c_y^*)^*)$. Hence,

$$\langle \varphi_M, S_{x+} S_{y-} \varphi_M \rangle = \gamma_x \gamma_y \langle \tilde{\varphi}_M, \mathcal{L}(c_x c_y^*) \mathcal{R}((c_x c_y^*)^*) \tilde{\varphi}_M \rangle. \quad (112)$$

Since $\tilde{\varphi}_M$ is positive and $\mathcal{L}(c_x c_y^*) \mathcal{R}((c_x c_y^*)^*) \geq 0$ w.r.t. $\mathfrak{C}_M$, we conclude our proof of (ii). $\square$

5. Proof of Theorem 1.3

5.1. Strategy

Our main purpose in this section is to show Theorem 5.1 below. To this end, recall the expression of $\mathbb{H}_M$ in Corollary 3.5.

Theorem 5.1. *Assume that $|\Lambda|$ is even. Assume (A. 1) and (A. 2). Assume that U_{eff} is positive definite. For all $\beta > 0$ and $M^\dagger \in \{-|\Lambda|/2, -|\Lambda|/2 + 1, \dots, |\Lambda|/2\}$, we have $e^{-\beta \mathbb{H}_M} \triangleright 0$ w.r.t. $\mathfrak{C}_M$.*

As a corollary, we obtain the following result by Theorem A.2.

¹⁹Precise definitions of $\psi_{M,\pm}(\mathbf{q})$ are given in the proof of Proposition 2.5.

²⁰Since $|\psi_M|$ is non-zero, there exists a measurable set $\mathcal{I}$ with $|\mathcal{I}| > 0$ such that $|\psi_M|(\mathbf{q}) \neq 0$ for all $\mathbf{q} \in \mathcal{I}$. For each $\mathbf{q} \in \mathcal{I}$, we observe that

$$0 < \text{Tr}[|\psi_M|(\mathbf{q})] = \sum_{X \in \wedge^{M^\dagger} \Lambda} |\psi_M|_{XX}(\mathbf{q}). \quad (111)$$

Hence, there exists an $X_0 \in \wedge^{M^\dagger} \Lambda$ such that $|\psi_M|_{X_0 X_0}(\mathbf{q}) \neq 0$.

Corollary 5.2. *Assume that $|\Lambda|$ is even. Assume (A. 1) and (A. 2). Assume that U_{eff} is positive definite. Let E_M be the ground state energy, i.e., the lowest eigenvalue of $\mathbb{H}_M$. For each $M^\dagger \in \{-|\Lambda|/2, -|\Lambda|/2 + 1, \dots, |\Lambda|/2\}$, E_M is nondegenerate and the corresponding eigenvector is strictly positive w.r.t. $\mathfrak{C}_M$.*

By this result, we see the uniqueness claimed in Theorem 1.3. Some additional observations tell us more detailed information about the ground state stated in Theorem 1.3; see Subsection 5.5.

In the remainder of this section, we continue to make every assumption named in Theorem 5.1.

Now, let us explain how to prove Theorem 5.1.

Proposition 5.3. *Let U_0 be a strictly positive constant given by Proposition 4.6. Let*

$$\mathbb{U}_0 = U_0 \sum_{x \in \Lambda} \mathcal{L}(\mathbf{n}_x) \mathcal{R}(\mathbf{n}_x) \otimes \mathbb{1}_{L^2}. \quad (113)$$

We define a new Hamiltonian $\mathbb{H}_M^{(0)}$ by

$$\mathbb{H}_M^{(0)} = K_M - \mathbb{U}_0. \quad (114)$$

If $e^{-\beta \mathbb{H}_M^{(0)}} \triangleright 0$ w.r.t. $\mathfrak{C}_M$ for all $\beta > 0$, then $e^{-\beta \mathbb{H}_M} \triangleright 0$ w.r.t. $\mathfrak{C}_M$ for all $\beta > 0$.

Proof. By Proposition 4.6, it holds that $\mathbb{U} \geq \mathbb{U}_0$ w.r.t. $\mathfrak{C}_M$. Hence, by applying Proposition A.1, we have $e^{-\beta \mathbb{H}_M} \geq e^{-\beta \mathbb{H}_M^{(0)}}$ w.r.t. $\mathfrak{C}_M$. Thus, if $e^{-\beta \mathbb{H}_M^{(0)}} \triangleright 0$ w.r.t. $\mathfrak{C}_M$, we conclude that $e^{-\beta \mathbb{H}_M} \triangleright 0$ w.r.t. $\mathfrak{C}_M$. $\square$

By Proposition 5.3, it is sufficient to prove that $e^{-\beta \mathbb{H}_M^{(0)}} \triangleright 0$ w.r.t. $\mathfrak{C}_M$ for all $\beta > 0$.

By the Duhamel formula, we have the following norm-convergent expansion:

$$e^{-\beta \mathbb{H}_M^{(0)}} = \sum_{n \geq 0} \mathcal{D}_{n, \beta}, \quad (115)$$

$$\mathcal{D}_{n, \beta} = \int_{S_n(\beta)} e^{-s_1 K_M} \mathbb{U}_0 e^{-s_2 K_M} \mathbb{U}_0 \dots e^{-s_n K_M} \mathbb{U}_0 e^{-(\beta - \sum_{j=1}^n s_j) K_M}, \quad (116)$$

where $\int_{S_n(\beta)} = \int_0^\beta dt_1 \int_0^{\beta-t_1} dt_2 \dots \int_0^{\beta - \sum_{j=1}^{n-1} t_j} dt_n$ and $\mathcal{D}_{0, \beta} = e^{-\beta K_M}$. In Subsection 5.3, we will prove the following:

Theorem 5.4. (Ergodicity) *$\{\mathcal{D}_{n, \beta}\}_{n \in \mathbb{N}_0}$ is ergodic in the sense that for each $\varphi, \psi \in \mathfrak{C}_M \setminus \{0\}$, there are $\beta > 0$ and $n \in \mathbb{N}_0 := \{0\} \cup \mathbb{N}$ such that $\langle \varphi, \mathcal{D}_{n, \beta} \psi \rangle > 0$.*

Assuming Theorem 5.4, we can prove Theorem 5.1.

Proof of Theorem 5.1 given Theorem 5.4

The basic idea originates from [7, 22]. Note that since $e^{\beta\mathbb{T}} \geq 0$ and $\mathbb{U}_0 \geq 0$ w.r.t. $\mathfrak{C}_M$, we see that $\mathcal{D}_{n,\beta} \geq 0$ w.r.t. $\mathfrak{C}_M$. Thus, for each $n \in \mathbb{N}_0$, one has

$$e^{-\beta\mathbb{H}_M^{(0)}} \geq \mathcal{D}_{n,\beta} \quad (117)$$

w.r.t. $\mathfrak{C}_M$. Take $\varphi, \psi \in \mathfrak{C}_M \setminus \{0\}$ arbitrarily. Then by Theorem 5.4, there exist $\beta > 0$ and $n \in \mathbb{N}_0$ such that $\langle \varphi, \mathcal{D}_{n,\beta} \psi \rangle > 0$. Hence, using (117), we have $\langle \varphi, e^{-\beta\mathbb{H}_M^{(0)}} \psi \rangle \geq \langle \varphi, \mathcal{D}_{n,\beta} \psi \rangle > 0$. To summarize, for each $\varphi, \psi \in \mathfrak{C}_M \setminus \{0\}$, there exists a $\beta > 0$ such that $\langle \varphi, e^{-\beta\mathbb{H}_M^{(0)}} \psi \rangle > 0$. This means that $e^{-\beta\mathbb{H}_M^{(0)}}$ improves the positivity w.r.t. $\mathfrak{C}_M$, according to Theorem A.2. $\square$

Conclusion: It suffices to show Theorem 5.4 to prove Theorem 1.3. $\diamond$

5.2. Preliminaries

Before we enter the proof of Theorem 5.4, we need to make some preparations.

Let $G = (\Lambda, E)$ be a connected graph. For each $0 \leq n \leq |\Lambda|$, we set

$$\Lambda^{(n)} = \{X = (x_1, \dots, x_n) \in \Lambda^n \mid x_1 \neq \dots \neq x_n\}. \quad (118)$$

Let $\mathfrak{S}_n$ be the permutation group on the set $\{1, \dots, n\}$. Let $(x_1, \dots, x_n), (y_1, \dots, y_n) \in \Lambda^{(n)}$. If there exists a $\sigma \in \mathfrak{S}_n$ such that $(x_{\sigma(1)}, \dots, x_{\sigma(n)}) = (y_1, \dots, y_n)$, then we write $(x_1, \dots, x_n) \sim (y_1, \dots, y_n)$. The binary relation “ $\sim$ ” on $\Lambda^{(n)}$ is an equivalence relation. We denote by $\wedge^n \Lambda$ the quotient set $\Lambda^{(n)} / \sim$. For notational simplicity, we denote by $(x_1, \dots, x_n)$ the equivalence class $[(x_1, \dots, x_n)]$ if no confusion occurs. We say that $X = (x_1, \dots, x_n), Y = (y_1, \dots, y_n) \in \wedge^n \Lambda$ are *neighbors* if there exists a unique j such that x_j and y_j are neighbors in G^{21} and $x_i = y_i$ holds for all $i \in \{1, \dots, n\} \setminus \{j\}$. For each $n \in \mathbb{N}_0$, we define a graph $\wedge^n G$ by

$$\wedge^n G = (\wedge^n \Lambda, \wedge^n E), \quad (119)$$

$$\wedge^n E = \{[X, Y] \in [\wedge^n \Lambda]^2 \mid X, Y \text{ are neighbors}\} \quad (120)$$

with $\wedge^0 G = (\emptyset, \emptyset)$, the empty graph, and $\wedge^1 G = G$. Remark that since $|\wedge^{|\Lambda|} \Lambda| = 1$, $\wedge^{|\Lambda|} G$ is trivial.

The following proposition is often useful:

Proposition 5.5. *If G is connected, then $\wedge^n G$ is connected for all $0 < n < |\Lambda|$.*

Proof. See [6, 22]. $\square$

A *path* in $\wedge^n G$ is a graph $P = (v, e) \subseteq \wedge^n G$ with $v = \{X_1, \dots, X_N\}$ and $e = \{\{X_1, X_2\}, \{X_2, X_3\}, \dots, \{X_{N-1}, X_N\}\}$, where all X_j are distinct. The path P is simply denoted by $P = X_1 X_2 \dots X_N$. The number $N - 1$ is called the *length of path* P and denoted by $|P|$. For each $X, Y \in \wedge^n \Lambda$, we denote by $\mathcal{P}_{XY}^{(n)}$ the set of all paths from X to Y . For each $L \in \mathbb{N}$, we set

$$\mathcal{P}_{XY}^{(n)}[L] = \{P \in \mathcal{P}_{XY}^{(n)} \mid |P| = L\}. \quad (121)$$

²¹ $x, y \in \Lambda$ is said to be *neighbors* if $\{x, y\} \in E$.

Clearly, it holds that $\mathcal{P}_{XY}^{(n)} = \bigcup_L \mathcal{P}_{XY}^{(n)}[L]$.

Let $e_x(y) = \delta_{xy}$. Then $\{e_x | x \in \Lambda\}$ is a complete orthonormal system(CONS) of $\ell^2(\Lambda)$. For each $X = (x_1, \dots, x_n) \in \wedge^n \Lambda$, we define

$$e_X = e_{x_1} \wedge \dots \wedge e_{x_n} \in \wedge^n \ell^2(\Lambda). \quad (122)$$

Then $\{e_X | X \in \wedge^n \Lambda\}$ is a CONS of $\wedge^n \ell^2(\Lambda)$ as well. Note that each $\psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$ can be expressed as

$$\psi = \sum_{X,Y \in \wedge^{M^\dagger} \Lambda} \int_{\mathcal{Q}}^{\oplus} \psi_{XY}(\mathbf{q}) |e_X\rangle \langle e_Y| d\mathbf{q}. \quad (123)$$

5.3. Proof of Theorem 5.4

We will prove Theorem 5.4 step-by-step.

Proposition 5.6. *Let*

$$\begin{aligned} \mathcal{C}_{n,\beta} &= \left(\mathbb{U}_0^{M^\dagger} e^{-\beta K_M / (n-1)} \right)^{n-1} \mathbb{U}_0^{M^\dagger} \\ &= \mathbb{U}_0^{M^\dagger} e^{\beta K_M / (n-1)} \mathbb{U}_0^{M^\dagger} \dots e^{\beta K_M / (n-1)} \mathbb{U}_0^{M^\dagger}. \end{aligned} \quad (124)$$

Suppose that $\{\mathcal{C}_{n,\beta}\}$ is ergodic in the sense that, for each $\varphi, \psi \in \mathfrak{C}_M \setminus \{0\}$, there exist $\beta > 0$ and $n \in \mathbb{N}_0$ such that $\langle \varphi, \mathcal{C}_{n,\beta} \psi \rangle > 0$. Then $\{\mathcal{D}_{n,\beta}\}$ is ergodic.

Proof. Set $N(n) = nM^\dagger + (n-1)$. It suffices to show that a subsequence $\{\mathcal{D}_{N(n),\beta}\}_{n,\beta}$ is ergodic. Let

$$F_n(s_1, \dots, s_n) = e^{-s_1 K_M} \mathbb{U}_0 e^{-s_2 K_M} \mathbb{U}_0 \dots e^{-s_n K_M} \mathbb{U}_0 e^{-(\beta - \sum_{j=1}^n s_j) K_M}. \quad (125)$$

By (116), it holds that

$$\mathcal{D}_{N(n),\beta} = \int_{S_{N(n)}(\beta)} F_{N(n)}(s_1, \dots, s_{N(n)}). \quad (126)$$

Remark that

$$\mathcal{C}_{n,\beta} = F_{N(n)} \left(\underbrace{0, \dots, 0}_{M^\dagger}, \beta/(n-1), \underbrace{0, \dots, 0}_{M^\dagger}, \dots, \beta/(n-1), \underbrace{0, \dots, 0}_{M^\dagger} \right). \quad (127)$$

In particular, $\mathcal{C}_{n,\beta} \geq 0$ w.r.t. $\mathfrak{C}_M$ for all $n \in \mathbb{N}_0$ and $\beta \geq 0$. Since $\{\mathcal{C}_{n,\beta}\}$ is ergodic, for each $\varphi, \psi \in \mathfrak{C}_M \setminus \{0\}$, there are $\beta > 0$ and $n \in \mathbb{N}_0$ such that $\langle \varphi, \mathcal{C}_{n,\beta} \psi \rangle > 0$. Let $f(s_1, \dots, s_{N(n)}) = \langle \varphi, F_{N(n)}(s_1, \dots, s_{N(n)}) \psi \rangle$. Then f is a non-zero positive function such that

$$f \left(\underbrace{0, \dots, 0}_{M^\dagger}, \beta/(n-1), \underbrace{0, \dots, 0}_{M^\dagger}, \dots, \beta/(n-1), \underbrace{0, \dots, 0}_{M^\dagger} \right) > 0 \quad (128)$$

by (127). Moreover, f is continuous in $s_1, \dots, s_{N(n)}$. Thus,

$$\langle \varphi, \mathcal{D}_{N(n),\beta} \psi \rangle = \int_{S_{N(n)}(\beta)} f(s_1, \dots, s_{N(n)}) > 0. \quad (129)$$

This means that $\{\mathcal{D}_{N(n),\beta}\}_{n,\beta}$ is ergodic. $\square$

In the remainder of this subsection, we will prove that $\{\mathcal{C}_{n,\beta}\}$ is ergodic. Henceforth, we may assume that

$$U_0 = 1 \quad (130)$$

without loss of generality. Let $\wedge^n G = (\wedge^n \Lambda, \wedge^n E)$ be the graph defined in Subsection 5.2.

Lemma 5.7. *Let $E_X = |e_X\rangle\langle e_X|$ for each $X \in \wedge^{M^\dagger} \Lambda$. We have*

$$\mathbb{U}_0^{M^\dagger} \supseteq \sum_{X \in \wedge^{M^\dagger} \Lambda} \mathcal{L}(E_X) \mathcal{R}(E_X) \otimes \mathbb{1}_{L^2} \quad \text{w.r.t. } \mathfrak{C}_M. \quad (131)$$

Proof. Since $|\wedge^{M^\dagger} \Lambda| \geq |\wedge^{M^\dagger} \Lambda|$ and $E_X = \mathbf{n}_{x_1} \cdots \mathbf{n}_{x_{M^\dagger}}$ for each $X = (x_1, \dots, x_{M^\dagger}) \in \wedge^{M^\dagger} \Lambda$, we obtain, by Lemma 4.4,

$$\begin{aligned} \mathbb{U}_0^{M^\dagger} &= \sum_{(x_1, \dots, x_{M^\dagger}) \in \wedge^{M^\dagger} \Lambda} \mathcal{L}(\mathbf{n}_{x_1} \cdots \mathbf{n}_{x_{M^\dagger}}) \mathcal{R}(\mathbf{n}_{x_1} \cdots \mathbf{n}_{x_{M^\dagger}}) \otimes \mathbb{1}_{L^2} \\ &\supseteq \sum_{X \in \wedge^{M^\dagger} \Lambda} \mathcal{L}(E_X) \mathcal{R}(E_X) \otimes \mathbb{1}_{L^2} \end{aligned} \quad (132)$$

w.r.t. $\mathfrak{C}_M$. $\square$

We introduce the following notation:

$$\begin{aligned} &\int d\nu_{\mathbf{q}, \mathbf{q}'; \beta}^{(n-1)} F(\boldsymbol{\omega}_1, \dots, \boldsymbol{\omega}_{n-1}) \\ &:= \int_{\mathcal{Q}^{n-2}} \prod_{j=1}^{n-2} d\mathbf{q}_j \int d\mu_{\mathbf{q}, \mathbf{q}_1; \beta}(\boldsymbol{\varphi}_1) d\mu_{\mathbf{q}_1, \mathbf{q}_2; \beta}(\boldsymbol{\varphi}_2) \cdots d\mu_{\mathbf{q}_{n-2}, \mathbf{q}'; \beta}(\boldsymbol{\varphi}_{n-1}) \\ &\quad \times \exp \left[- \sum_{j=1}^{n-1} \int_0^\beta ds \mathcal{V}(\boldsymbol{\omega}_j(s)(\boldsymbol{\varphi}_j)) \right] F(\boldsymbol{\omega}_1(\boldsymbol{\varphi}_1), \dots, \boldsymbol{\omega}_{n-1}(\boldsymbol{\varphi}_{n-1})). \end{aligned} \quad (133)$$

Remark 5.8. Using the Brownian bridge $\boldsymbol{\alpha}_j$ ($j = 1, \dots, n$), $\boldsymbol{\omega}_j$ can be expressed as

$$\boldsymbol{\omega}_j(s)(\boldsymbol{\varphi}_j) = (1 - \beta^{-1}s)\mathbf{q}_{j-1} + \beta^{-1}s\mathbf{q}_j + \sqrt{\beta}\boldsymbol{\alpha}_j(\beta^{-1}s)(\boldsymbol{\varphi}_j). \quad \diamond \quad (134)$$

Proposition 5.9. *For each $P = X_1 X_2 \cdots X_{|P|+1} \in \mathcal{P}_{XY}^{(M^\dagger)}$ and $\boldsymbol{\varphi}_1, \dots, \boldsymbol{\varphi}_{|P|} \in A$, let*

$$\mathcal{G}_\beta^{(M^\dagger)} \left(P, \{\boldsymbol{\omega}_j(\boldsymbol{\varphi}_j)\}_{j=1}^{|P|} \right) = \prod_{j=1}^{|P|} E_{X_j} G_\beta(\boldsymbol{\omega}_j(\boldsymbol{\varphi}_j)) E_{X_{j+1}}, \quad (135)$$

where $\prod_{j=1}^n A_j := A_1 A_2 \cdots A_n$, the ordered product. Set $\tilde{\beta} = \beta/(n-1)$. The kernel operator of $\mathcal{C}_{n,\beta}$ satisfies the following operator inequality :

$$\begin{aligned} \mathcal{C}_{n,\beta}(\mathbf{q}, \mathbf{q}') \supseteq & \sum_{X_1, X_n \in \wedge^{M^\dagger} \Lambda} \sum_{P \in \mathcal{P}_{X_1 X_n}^{(M^\dagger)}[n-1]} \int d\nu_{\mathbf{q}, \mathbf{q}'; \tilde{\beta}}^{(n-1)} \\ & \times \mathcal{L} \left[\mathcal{G}_{\tilde{\beta}}^{(M^\dagger)} \left(P, \{\omega_j\}_{j=1}^{n-1} \right) \right] \mathcal{R} \left[\left\{ \mathcal{G}_{\tilde{\beta}}^{(M^\dagger)} \left(P, \{\omega_j\}_{j=1}^{n-1} \right) \right\}^* \right] \end{aligned} \quad (136)$$

w.r.t. $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$.

Proof. First, we note the following fact: Let A, B be bounded operators on $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger}) \otimes L^2(\mathcal{Q})$. Suppose that A and B have kernel operators. If $A \supseteq B$ w.r.t. $\mathfrak{C}_M$, then $A(\mathbf{q}, \mathbf{q}') \supseteq B(\mathbf{q}, \mathbf{q}')$ w.r.t. $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$ for a.e. $\mathbf{q}, \mathbf{q}'^{22}$.

By Proposition 3.7 and Lemma 5.7, we have

$$\begin{aligned} & \mathcal{C}_{n,\beta}(\mathbf{q}, \mathbf{q}') \\ \supseteq & \sum_{X_1, \dots, X_n \in \wedge^{M^\dagger} \Lambda} \int d\nu_{\mathbf{q}, \mathbf{q}'; \tilde{\beta}}^{(n-1)} \\ & \times \mathcal{L} \left[E_{X_1} G_{\tilde{\beta}}(\omega_1) E_{X_2} \cdots G_{\tilde{\beta}}(\omega_{n-1}) E_{X_n} \right] \\ & \times \mathcal{R} \left[E_{X_n} G_{\tilde{\beta}}(\omega_{n-1})^* E_{X_{n-1}} \cdots G_{\tilde{\beta}}(\omega_1)^* E_{X_1} \right] \\ \supseteq & \sum_{X_1, X_n \in \wedge^{M^\dagger} \Lambda} \sum_{P = X_1 \cdots X_n \in \mathcal{P}_{X_1 X_n}^{(M^\dagger)}[n-1]} \int d\nu_{\mathbf{q}, \mathbf{q}'; \tilde{\beta}}^{(n-1)} \\ & \times \mathcal{L} \left[E_{X_1} G_{\tilde{\beta}}(\omega_1) E_{X_2} \cdots G_{\tilde{\beta}}(\omega_{n-1}) E_{X_n} \right] \\ & \times \mathcal{R} \left[E_{X_n} G_{\tilde{\beta}}(\omega_{n-1})^* E_{X_{n-1}} \cdots G_{\tilde{\beta}}(\omega_1)^* E_{X_1} \right] \end{aligned} \quad (137)$$

w.r.t. $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$. $\square$

²²The proof of this fact is as follows. Since $A \supseteq B$ w.r.t. $\mathfrak{C}_M$, we have $\langle \varphi \otimes f, A\psi \otimes g \rangle \geq \langle \varphi \otimes f, B\psi \otimes g \rangle$ for all $f, g \in L^2(\mathcal{Q})_+$ and $\varphi, \psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$. This means that $\int f(\mathbf{q})g(\mathbf{q}') \langle \varphi, A(\mathbf{q}, \mathbf{q}')\psi \rangle d\mathbf{q}d\mathbf{q}' \geq \int f(\mathbf{q})g(\mathbf{q}') \langle \varphi, B(\mathbf{q}, \mathbf{q}')\psi \rangle d\mathbf{q}d\mathbf{q}'$. Thus, $\langle \varphi, A(\mathbf{q}, \mathbf{q}')\psi \rangle \geq \langle \varphi, B(\mathbf{q}, \mathbf{q}')\psi \rangle$ holds for a.e. $\mathbf{q}, \mathbf{q}'$. Since $\varphi, \psi \in \mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$, we conclude that $A(\mathbf{q}, \mathbf{q}') \supseteq B(\mathbf{q}, \mathbf{q}')$ w.r.t. $\mathcal{L}^2(\mathfrak{F}_{e,M^\dagger})_+$ for a.e. $\mathbf{q}, \mathbf{q}'$.

Let $\psi, \varphi \in \mathfrak{C}_M \setminus \{0\}$. By (123), we can express these as

$$\begin{aligned}\psi &= \sum_{X,Y \in \wedge^{M^\dagger} \Lambda} \int_{\mathcal{Q}}^{\oplus} \psi_{XY}(\mathbf{q}) |e_X\rangle \langle e_Y| d\mathbf{q}, \\ \varphi &= \sum_{X,Y \in \wedge^{M^\dagger} \Lambda} \int_{\mathcal{Q}}^{\oplus} \varphi_{XY}(\mathbf{q}) |e_X\rangle \langle e_Y| d\mathbf{q}.\end{aligned}$$

Since $\psi \geq 0, \varphi \geq 0$ w.r.t. $\mathfrak{C}_M$, one obtains $\psi_{XX}(\mathbf{q}) = \langle e_X, \psi(\mathbf{q}) e_X \rangle_{\mathfrak{F}_{e,M^\dagger}} \geq 0$ and $\varphi_{XX}(\mathbf{q}) = \langle e_X, \varphi(\mathbf{q}) e_X \rangle_{\mathfrak{F}_{e,M^\dagger}} \geq 0$ for all $X \in \wedge^{M^\dagger} \Lambda$ which imply $\psi_{XX}(\mathbf{q}) \geq 0$ and $\varphi_{XX}(\mathbf{q}) \geq 0$ for all $X \in \wedge^{M^\dagger} \Lambda$ and a.e. $\mathbf{q}$. In particular, since both ψ and φ are non-zero, there exist $X, Y \in \wedge^{M^\dagger} \Lambda$ and $\mathcal{S}_X, \mathcal{S}_Y \subseteq \mathcal{Q}$ with non-vanishing Lebesgue measures such that $\psi_{XX}(\mathbf{q}) > 0$ on $\mathcal{S}_X$ and $\varphi_{YY}(\mathbf{q}) > 0$ on $\mathcal{S}_Y$ ²³. Then one obtains the following:

Corollary 5.10. *It holds that*

$$\begin{aligned}\langle \varphi, \mathcal{C}_{n,\beta} \psi \rangle &\geq \sum_{P \in \mathcal{P}_{YX}^{(M^\dagger)}[n-1]} \int_{\mathcal{S}_Y \times \mathcal{S}_X} d\mathbf{q} d\mathbf{q}' \int d\nu_{\mathbf{q},\mathbf{q}';\tilde{\beta}}^{(n-1)} \varphi_{YY}(\mathbf{q}) \psi_{XX}(\mathbf{q}') \\ &\quad \times \left| \left\langle e_Y, \mathcal{G}_{\tilde{\beta}}^{(M^\dagger)} \left(P, \{\omega_j\}_{j=1}^{n-1} \right) e_X \right\rangle_{\mathfrak{F}_{e,M^\dagger}} \right|^2.\end{aligned}\tag{138}$$

Proof. By (136), we have

$$\begin{aligned}&\langle \varphi, \mathcal{C}_{n,\beta} \psi \rangle \\ &\geq \sum_{X_1, X_n \in \wedge^{M^\dagger} \Lambda} \sum_{P \in \mathcal{P}_{X_1 X_n}^{(M^\dagger)}[n-1]} \int_{\mathcal{Q} \times \mathcal{Q}} d\mathbf{q} d\mathbf{q}' \int d\nu_{\mathbf{q},\mathbf{q}';\tilde{\beta}}^{(n-1)} \varphi_{X_1 X_1}(\mathbf{q}) \psi_{X_n X_n}(\mathbf{q}') \\ &\quad \times \left| \left\langle e_{X_1}, \mathcal{G}_{\tilde{\beta}}^{(M^\dagger)} \left(P, \{\omega_j\}_{j=1}^{n-1} \right) e_{X_n} \right\rangle_{\mathfrak{F}_{e,M^\dagger}} \right|^2 \\ &\geq \text{RHS of (138)}. \quad \square\end{aligned}\tag{139}$$

Conclusion: By Corollary 5.10, to show that $\{\mathcal{C}_{n,\beta}\}$ is ergodic, it suffices to find some n and β such that the RHS of (138) is strictly positive. $\diamond$

For all $\{x, y\} \in E$ and $z \in \Lambda$, set

$$a_z = a_z(\{x, y\}) = \sqrt{2} \omega_0^{-1/2} (g_{xz} - g_{yz}).\tag{140}$$

²³Assume that $\psi_{XX}(\cdot) = 0$ for all $X \in \wedge^{M^\dagger} \Lambda$ as a vector in $L^2(\mathcal{Q})$. Then we have $\text{Tr}[\psi(\mathbf{q})] = \sum_{X \in \wedge^{M^\dagger} \Lambda} \psi_{XX}(\mathbf{q}) = 0$, which implies that $\psi = 0$. This is a contradiction. Thus, there exists an $X \in \wedge^{M^\dagger} \Lambda$ such that $\psi_{XX}(\cdot) \neq 0$ as a vector in $L^2(\mathcal{Q})$. Thus, there exists a measurable set $\mathcal{S}_X$ with $|\mathcal{S}_X| > 0$ such that $\psi_{XX}(\mathbf{q}) > 0$ for all $\mathbf{q} \in \mathcal{S}_X$.

Let

$$\mathcal{Y} = \left\{ (\mathbf{q}, \mathbf{q}') \in \mathcal{Q} \times \mathcal{Q} \mid \exists \{x, y\} \in E \text{ s.t. } \sum_{z \in \Lambda} a_z(\{x, y\})(q_z - q'_z) \in 2\pi\mathbb{Z} \right\}. \quad (141)$$

Clearly, $\mathcal{Y}$ is a set of Lebesgue measure 0. Let

$$W_\beta = \left\{ \boldsymbol{\varphi} \in A \mid \max_{s \in [0,1]} |\boldsymbol{\alpha}(s)(\boldsymbol{\varphi})| \leq \beta^{-1/4} \right\}. \quad (142)$$

Note that $\int_{W_\beta} D\boldsymbol{\alpha} > 0$ for sufficiently small $\beta > 0$, since $\cup_{\beta>0} W_\beta = A$. In Appendix C, we will show the following:

Proposition 5.11. (*Connectivity*) *Let $P \in \mathcal{P}_{XY}^{(M^\dagger)}[L]$. Let $(\mathbf{q}, \mathbf{q}_1), (\mathbf{q}_1, \mathbf{q}_2), \dots, (\mathbf{q}_{L-1}, \mathbf{q}') \in \mathcal{Y}^c$, the complement of $\mathcal{Y}$. Then there exist $\beta_* > 0$ and $\Gamma_* > 0$ such that for all $\beta \in (0, \beta_*)$ and $\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \dots, \boldsymbol{\varphi}_L \in W_\beta$, we have*

$$\left| \beta^{-L} \left\langle e_X, \mathcal{G}_\beta^{(M^\dagger)} \left(P, \{\boldsymbol{\omega}_j(\boldsymbol{\varphi}_j)\}_{j=1}^L \right) e_Y \right\rangle_{\mathfrak{F}_{e, M^\dagger}} \right| \geq \Gamma_*. \quad (143)$$

Note that β_* and Γ_* depend on $\mathbf{q}, \mathbf{q}_1, \dots, \mathbf{q}_{L-1}, \mathbf{q}'$.

Proof. See Appendix C. $\square$

5.4. Completion of proof of Theorem 5.4

By Proposition 5.5, we can take $n \in \mathbb{N}$ such that $\mathcal{P}_{YX}^{(M^\dagger)}[n-1] \neq \emptyset$. Let $(\mathbf{q}, \mathbf{q}_1), \dots, (\mathbf{q}_{n-2}, \mathbf{q}') \in \mathcal{Y}^c$. For all $P \in \mathcal{P}_{YX}^{(M^\dagger)}[n-1]$, $\beta \in (0, \beta_*)$ and $\boldsymbol{\varphi}_1, \dots, \boldsymbol{\varphi}_{n-1} \in W_\beta$, the term

$$\left| \left\langle e_Y, \mathcal{G}_\beta^{(M^\dagger)} \left(P, \{\boldsymbol{\omega}_j(\boldsymbol{\varphi}_j)\}_{j=1}^{n-1} \right) e_X \right\rangle_{\mathfrak{F}_{e, M^\dagger}} \right|^2$$

is strictly positive by Proposition 5.11. Thus, it holds that

$$\begin{aligned} & \int_0^1 d\beta \int d\mu_{\mathbf{q}, \mathbf{q}_1; \beta}(\boldsymbol{\varphi}_1) d\mu_{\mathbf{q}_1, \mathbf{q}_2; \beta}(\boldsymbol{\varphi}_2) \cdots d\mu_{\mathbf{q}_{n-2}, \mathbf{q}'; \beta}(\boldsymbol{\varphi}_{n-1}) \\ & \times \exp \left[- \sum_{j=1}^{n-1} \int_0^\beta ds \mathcal{V}(\boldsymbol{\omega}_j(s)(\boldsymbol{\varphi}_j)) \right] \left| \left\langle e_Y, \mathcal{G}_\beta^{(M^\dagger)} \left(P, \{\boldsymbol{\omega}_j(\boldsymbol{\varphi}_j)\}_{j=1}^{n-1} \right) e_X \right\rangle_{\mathfrak{F}_{e, M^\dagger}} \right|^2 \\ & > 0 \end{aligned} \quad (144)$$

for all $(\mathbf{q}, \mathbf{q}_1), \dots, (\mathbf{q}_{n-2}, \mathbf{q}') \in \mathcal{Y}^c$. Let $\mathcal{K}_{n, \beta}$ be the RHS of (138). By (133) and (144), we have $\int_0^1 \mathcal{K}_{n, \beta} d\beta > 0$. Since $\mathcal{K}_{n, \beta}$ is continuous in β , there exists a $\beta_0 > 0$ such that $\mathcal{K}_{n, \beta_0}$ is strictly positive. Hence, $\{\mathcal{C}_{n, \beta}\}$ is ergodic. $\square$

5.5. Proof of Theorem 1.3

By Corollary 5.2 and Theorem A.2, the ground state of $\mathbb{H}_M$ is unique and strictly positive w.r.t. $\mathfrak{C}_M$.

(i) immediately follows from Theorem 1.1.

Because H_M commutes with S_{tot}^2 and because the ground state of H_M is unique, we obtain (ii).

By an argument similar to that for (112), we have

$$\langle \psi_M, S_{x+} S_{y-} \psi_M \rangle = \gamma_x \gamma_y \langle \psi_M, \mathcal{L}(c_x c_y^*) \mathcal{R}((c_x c_y^*)^*) \psi_M \rangle. \quad (145)$$

Since ψ_M is strictly positive and $\mathcal{L}(c_x c_y^*) \mathcal{R}((c_x c_y^*)^*) \geq 0$ w.r.t. $\mathfrak{C}_M$, we conclude (iii). $\square$

6. Proof of Theorem 1.6

6.1. Gaussian domination

In this section, we assume (B. 1), (B. 2) and (B. 3).

In the previous sections, we considered the Hamiltonian in the M -subspace. Here, we will study the Hamiltonian in the full space $\mathfrak{E} \otimes \mathfrak{P}$. In this case, we can still define the Lang–Firsov transformation $\mathcal{U}$ and the hole-particle transformation $\mathcal{W}$ as before. Let us define $\mathbb{H}$ by

$$\mathbb{H} = \mathcal{W} \mathcal{U} H \mathcal{U}^* \mathcal{W}^* + \sum_{x \in \Lambda} \mu_x n_x - \frac{1}{2} \sum_{x, y \in \Lambda} V_{xy}. \quad (146)$$

We can confirm that

$$\mathbb{H} = -T_{+, \uparrow} - T_{-, \downarrow} + \tilde{\mathbf{U}} + H_{\mathfrak{p}}, \quad (147)$$

where $T_{\pm, \sigma}$ and $\tilde{\mathbf{U}}$ are given in Subsections 3.1 and 3.3, respectively.

For each $\mathbf{h} = \{h_x\}_{x \in \Lambda} \in \mathbb{R}^{|\Lambda|}$, let

$$\tilde{\mathbf{U}}(\mathbf{h}) = \frac{1}{2} \sum_{x, y \in \Lambda} U_{\text{eff}, xy} (n_{x\uparrow} - n_{x\downarrow} + h_x) (n_{y\uparrow} - n_{y\downarrow} + h_y). \quad (148)$$

We introduce a new Hamiltonian given by the following:

$$\mathbb{H}(\mathbf{h}) = -T_{+, \uparrow} - T_{-, \downarrow} + \tilde{\mathbf{U}}(\mathbf{h}) + H_{\mathfrak{p}}. \quad (149)$$

Note that

$$\mathbb{H} = \mathbb{H}(\mathbf{0}). \quad (150)$$

The main purpose in this subsection is to show the following:

Theorem 6.1. *Let $\mathcal{Z}_{\beta, \varepsilon}(\mathbf{h}) = \text{Tr} \left[e^{-\beta \mathbb{H}(\mathbf{h})} e^{-\varepsilon H_{\mathfrak{p}}} \right]$. We have $\mathcal{Z}_{\beta, \varepsilon}(\mathbf{h}) \leq \mathcal{Z}_{\beta, \varepsilon}(\mathbf{0})$ for all $\mathbf{h} \in \mathbb{R}^{|\Lambda|}$ and $\varepsilon > 0$.*

Remark 6.2. We introduced $e^{-\varepsilon H_{\mathfrak{p}}}$ in $\mathcal{Z}_{\beta, \varepsilon}(\mathbf{h})$ for the following reason: the factor $e^{-\varepsilon H_{\mathfrak{p}}}$ enables us to interchange a limit operation and a trace operation in the final step of the proof. $\diamond$

6.1.1. Auxiliary lemmas. Let $T = T_{+g,\uparrow} + T_{-g,\downarrow}$. Under the identification

$$\mathfrak{E} \otimes \mathfrak{P} = \int_{\mathcal{Q}}^{\oplus} \mathfrak{F}_e \otimes \mathfrak{F}_e d\mathbf{q}, \quad (151)$$

we have

$$T = \int_{\mathcal{Q}}^{\oplus} T(\mathbf{q}) d\mathbf{q}, \quad T(\mathbf{q}) = \mathbf{T}_{+g}(\mathbf{q}) \otimes \mathbb{1} + \mathbb{1} \otimes \mathbf{T}_{-g}(\mathbf{q}), \quad (152)$$

where $\mathbf{T}_{\pm g}(\mathbf{q})$ is defined by (75).

Lemma 6.3. *Let $K = -T + H_p$. Let*

$$\mathcal{Z}_{\beta,n,\varepsilon}(\mathbf{h}) = \text{Tr} \left[\left(e^{-\beta K/n} e^{-\beta \tilde{\mathbf{U}}(\mathbf{h})/n} \right)^n e^{-\varepsilon H_p} \right], \quad n \in \mathbb{N}, \quad \varepsilon > 0. \quad (153)$$

Let us introduce the following notation:

$$\begin{aligned} & \int d\nu_{\mathbf{q},\mathbf{q}';\beta,\varepsilon}^{(n+1)} F(\boldsymbol{\omega}_1, \dots, \boldsymbol{\omega}_{n+1}) \\ &:= \int_{\mathcal{Q}^n} \prod_{j=1}^n d\mathbf{q}_j \int d\mu_{\mathbf{q},\mathbf{q}_1;\beta} \int d\mu_{\mathbf{q}_1,\mathbf{q}_2;\beta} \cdots \int d\mu_{\mathbf{q}_{n-1},\mathbf{q}_n;\beta} \int d\mu_{\mathbf{q}_n,\mathbf{q}';\varepsilon} \\ & \times \exp \left\{ - \sum_{j=1}^n \int_0^\beta ds \mathcal{V}(\boldsymbol{\omega}_j(s)) - \int_0^\varepsilon ds \mathcal{V}(\boldsymbol{\omega}_{n+1}(s)) \right\} F(\boldsymbol{\omega}_1, \dots, \boldsymbol{\omega}_{n+1}). \end{aligned} \quad (154)$$

Then, setting $\tilde{\beta} = \beta/n$, we have

$$\begin{aligned} & \mathcal{Z}_{\beta,n,\varepsilon}(\mathbf{h}) \\ &= (4\pi)^{-n|\Lambda|/2} \int_{\mathbb{R}^{n|\Lambda|}} \prod_{j=1}^n d\mathbf{k}_j \int_{\mathcal{Q}} d\mathbf{q} \int d\nu_{\mathbf{q},\mathbf{q}';\beta,\varepsilon}^{(n+1)} e^{-i \sum_{j=1}^n \mathbf{k}_j \cdot \mathbf{h}} e^{-\sum_{j=1}^n \mathbf{k}_j^2/4} \\ & \times \text{Tr}_{\mathfrak{F}_e \otimes \mathfrak{F}_e} \left[\prod_{j=1}^n \left(\prod_0^{\tilde{\beta}} e^{T(\boldsymbol{\omega}_j(s)) ds} e^{i \sum_{x,y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff},xy}(\mathbf{n}_y \otimes \mathbb{1} - \mathbb{1} \otimes \mathbf{n}_y)} \right) \right]. \end{aligned} \quad (155)$$

Proof. By the Trotter–Kato product formula, we have

$$e^{-\beta K}(\mathbf{q}, \mathbf{q}') = \int d\mu_{\mathbf{q},\mathbf{q}';\beta} \left(\prod_0^{\beta} e^{T(\boldsymbol{\omega}(s)) ds} \right) e^{-\int_0^\beta ds \mathcal{V}(\boldsymbol{\omega}(s))}. \quad (156)$$

Let

$$\mathcal{I}_{n,\beta,\varepsilon} = \left(e^{-\beta K/n} e^{-\beta \tilde{\mathbf{U}}(\mathbf{h})/n} \right)^n e^{-\varepsilon H_p}. \quad (157)$$

By (156), the kernel operator of $\mathcal{J}_{n,\beta,\varepsilon}$ is obtained by the following observation:

$$\begin{aligned}
& \mathcal{J}_{n,\beta,\varepsilon}(\mathbf{q}_0, \mathbf{q}_{n+1}) \\
&= \int_{\mathcal{Q}^n} \prod_{j=1}^n d\mathbf{q}_j \left(\prod_{j=1}^n e^{-\beta K/n}(\mathbf{q}_{j-1}, \mathbf{q}_j) e^{-\beta \tilde{\mathbf{U}}(\mathbf{h})/n} \right) e^{-\varepsilon H_{\mathbf{p}}(\mathbf{q}_n, \mathbf{q}_{n+1})} \\
&= \int_{\mathcal{Q}^n} \prod_{j=1}^n d\mathbf{q}_j \int d\mu_{\mathbf{q}_0, \mathbf{q}_1; \tilde{\beta}} \cdots \int d\mu_{\mathbf{q}_n, \mathbf{q}_{n+1}; \varepsilon} e^{-\sum_{j=1}^n \int_0^{\tilde{\beta}} ds \mathcal{V}(\boldsymbol{\omega}_j(s)) - \int_0^{\varepsilon} ds \mathcal{V}(\boldsymbol{\omega}_{n+1}(s))} \\
&\quad \times \prod_{j=1}^n \left\{ \left(\prod_0^{\tilde{\beta}} e^{T(\boldsymbol{\omega}_j(s)) ds} \right) e^{-\tilde{\beta} \tilde{\mathbf{U}}(\mathbf{h})} \right\} \\
&= \int d\nu_{\mathbf{q}_0, \mathbf{q}_{n+1}; \beta, \varepsilon}^{(n+1)} \prod_{j=1}^n \left\{ \left(\prod_0^{\tilde{\beta}} e^{T(\boldsymbol{\omega}_j(s)) ds} \right) e^{-\tilde{\beta} \tilde{\mathbf{U}}(\mathbf{h})} \right\}. \tag{158}
\end{aligned}$$

Thus, we have

$$\begin{aligned}
\mathcal{Z}_{\beta, n, \varepsilon}(\mathbf{h}) &= \text{Tr}[\mathcal{J}_{n, \beta, \varepsilon}] = \int_{\mathcal{Q}} d\mathbf{q} \text{Tr}_{\mathfrak{F}_e \otimes \mathfrak{F}_e} \left[\mathcal{J}_{n, \beta, \varepsilon}(\mathbf{q}, \mathbf{q}) \right] \\
&= \int_{\mathcal{Q}} d\mathbf{q} \int d\nu_{\mathbf{q}, \mathbf{q}; \beta, \varepsilon}^{(n+1)} \text{Tr}_{\mathfrak{F}_e \otimes \mathfrak{F}_e} \left[\prod_{j=1}^n \left\{ \left(\prod_0^{\tilde{\beta}} e^{T(\boldsymbol{\omega}_j(s)) ds} \right) e^{-\tilde{\beta} \tilde{\mathbf{U}}(\mathbf{h})} \right\} \right]. \tag{159}
\end{aligned}$$

Finally, applying the following identity

$$e^{-\tilde{\beta} \tilde{\mathbf{U}}(\mathbf{h})} = (4\pi)^{-|\Lambda|/2} \int_{\mathbb{R}^{|\Lambda|}} d\mathbf{k} e^{-i\mathbf{h} \cdot \mathbf{k}} e^{-\mathbf{k}^2/4} e^{i \sum_{x, y \in \Lambda} \tilde{\beta} U_{\text{eff}, xy} \mathbf{k}_x (n_{y\uparrow} - n_{y\downarrow})}, \tag{160}$$

we obtain the assertion in the lemma. $\square$

Lemma 6.4. *We have*

$$\begin{aligned}
& \mathcal{Z}_{\beta, n, \varepsilon}(\mathbf{h}) \\
&= (4\pi)^{-n|\Lambda|/2} \int_{\mathbb{R}^{n|\Lambda|}} \prod_{j=1}^n d\mathbf{k}_j \int_{\mathcal{Q}} d\mathbf{q} \int d\nu_{\mathbf{q}, \mathbf{q}; \beta, \varepsilon}^{(n+1)} e^{-i \sum_{j=1}^n \mathbf{k}_j \cdot \mathbf{h}} e^{-\sum_{j=1}^n \mathbf{k}_j^2/4} \\
&\quad \times \left| \text{Tr}_{\mathfrak{F}_e} \left[\prod_{j=1}^n \left(\prod_0^{\tilde{\beta}} e^{T_{+g}(\boldsymbol{\omega}_j(s)) ds} e^{i \sum_{x, y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff}, xy} \mathbf{n}_y} \right) \right] \right|^2. \tag{161}
\end{aligned}$$

Proof. Note that $\text{Tr}[A \otimes B] = \text{Tr}[A]\text{Tr}[B]$. By Lemma 6.3, we immediately have

$$\begin{aligned} & \mathcal{Z}_{\beta,n,\varepsilon}(\mathbf{h}) \\ &= (4\pi)^{-n|\Lambda|/2} \int_{\mathbb{R}^{n|\Lambda|}} \prod_{j=1}^n d\mathbf{k}_j \int_{\mathcal{Q}} d\mathbf{q} \int d\nu_{\mathbf{q},\mathbf{q};\beta,\varepsilon}^{(n+1)} e^{-i\sum_{j=1}^n \mathbf{k}_j \cdot \mathbf{h}} e^{-\sum_{j=1}^n \mathbf{k}_j^2/4} \\ & \quad \times \text{Tr}_{\mathfrak{F}_e} \left[\prod_{j=1}^n \left(\prod_0^{\tilde{\beta}} e^{T_{+g}(\omega_j(s))ds} e^{+i\sum_{x,y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff},xy} n_y} \right) \right] \\ & \quad \times \text{Tr}_{\mathfrak{F}_e} \left[\prod_{j=1}^n \left(\prod_0^{\tilde{\beta}} e^{T_{-g}(\omega_j(s))ds} e^{-i\sum_{x,y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff},xy} n_y} \right) \right]. \end{aligned} \quad (162)$$

Let Θ be a conjugation in $\mathfrak{F}_e$ defined by $\Theta c_{x_1}^* \cdots c_{x_N}^* \Omega = c_{x_1}^* \cdots c_{x_N}^* \Omega$, where Ω is the Fock vacuum in $\mathfrak{F}_e$. Noting that $\Theta c_x \Theta = c_x$, we have $\Theta T_{-g}(\omega(s)) \Theta = T_{+g}(\omega(s))$ and $\Theta n_x \Theta = n_x$. Thus, it holds that

$$\Theta \prod_0^{\tilde{\beta}} e^{T_{-g}(\omega(s))ds} \Theta = \prod_0^{\tilde{\beta}} e^{T_{+g}(\omega(s))ds}, \quad (163)$$

$$\Theta e^{-i\sum_{x,y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff},xy} n_y} \Theta = e^{+i\sum_{x,y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff},xy} n_y}. \quad (164)$$

Hence, using the fact that $\text{Tr}[A] = (\text{Tr}[\Theta A \Theta])^*$, we observe that

$$\begin{aligned} & \text{Tr}_{\mathfrak{F}_e} \left[\prod_{j=1}^n \left(\prod_0^{\tilde{\beta}} e^{T_{-g}(\omega(s))ds} e^{-i\sum_{x,y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff},xy} n_y} \right) \right] \\ &= \left\{ \text{Tr}_{\mathfrak{F}_e} \left[\Theta \prod_{j=1}^n \left(\prod_0^{\tilde{\beta}} e^{T_{-g}(\omega(s))ds} e^{-i\sum_{x,y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff},xy} n_y} \right) \Theta \right] \right\}^* \\ &= \left\{ \text{Tr}_{\mathfrak{F}_e} \left[\prod_{j=1}^n \left(\prod_0^{\tilde{\beta}} e^{T_{+g}(\omega(s))ds} e^{+i\sum_{x,y \in \Lambda} \tilde{\beta} k_{jx} U_{\text{eff},xy} n_y} \right) \right] \right\}^*. \end{aligned} \quad (165)$$

This completes the proof. $\square$

6.1.2. Proof of Theorem 6.1. Remark that except for $e^{-i\sum_{j=1}^n \mathbf{k}_j \cdot \mathbf{h}}$, all factors of the integrand in (161) are positive. Thus, $|\mathcal{Z}_{\beta,n,\varepsilon}(\mathbf{h})| \leq \mathcal{Z}_{\beta,n,\varepsilon}(\mathbf{0})$. As $n \rightarrow \infty$, $\mathcal{Z}_{\beta,n,\varepsilon}(\mathbf{h})$ converges to $\mathcal{Z}_{\beta,\varepsilon}(\mathbf{h})$ by Lemma 6.5 below. Thus, we have $\mathcal{Z}_{\beta,\varepsilon}(\mathbf{h}) \leq \mathcal{Z}_{\beta,\varepsilon}(\mathbf{0})$. $\square$

Lemma 6.5. *We denote by $\mathcal{L}^1(\mathfrak{X})$ the ideal of all trace class operators on a Hilbert space $\mathfrak{X}$. Let $A_n, A \in \mathcal{B}(\mathfrak{X})$ and $B_n, B \in \mathcal{L}^1(\mathfrak{X})$ such that A_n converges to A strongly and $\|B_n - B\|_1 \rightarrow 0$ as $n \rightarrow \infty$, where $\|\cdot\|_1$ is the trace norm. Then $\|A_n B_n - AB\|_1 \rightarrow 0$ as $n \rightarrow \infty$.*

Proof. See [34, Chap. 2, Example 3]. $\square$

6.2. Completion of proof of Theorem 1.6

We define the Duhamel two-point function as

$$((A, B))_{\beta, \Lambda} = \mathcal{Z}_{\beta}^{-1} \int_0^1 dx \operatorname{Tr} \left[e^{-x\beta\mathbb{H}} A e^{-(1-x)\beta\mathbb{H}} B \right]. \quad (166)$$

Theorem 6.6. *Let $\sigma_x = n_{x\uparrow} - n_{x\downarrow}$. For all $\mathbf{h} \in \mathbb{C}^{|\Lambda|}$, we have*

$$\left(\left(\langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle^*, \langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle \right) \right)_{\beta, \Lambda} \leq \beta^{-1} \langle \mathbf{h}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle, \quad (167)$$

where $\langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle = \sum_{x, y \in \Lambda} U_{\text{eff}, xy} \sigma_x h_y$.

Proof. Let $\lambda \in \mathbb{R}$. We note

$$\mathbb{H}(\lambda \mathbf{h}) = \mathbb{H} + \delta \tilde{\mathbf{U}}(\lambda \mathbf{h}), \quad (168)$$

$$\delta \tilde{\mathbf{U}}(\lambda \mathbf{h}) = \tilde{\mathbf{U}}(\lambda \mathbf{h}) - \tilde{\mathbf{U}}(\mathbf{0}) = \lambda \langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle + \frac{\lambda^2}{2} \langle \mathbf{h}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle. \quad (169)$$

By the Duhamel formula, we have the norm-convergent expansion:

$$e^{-\beta\mathbb{H}(\lambda \mathbf{h})} = \sum_{n=0}^{\infty} \mathcal{D}_n(\lambda), \quad (170)$$

$$\mathcal{D}_n(\lambda) = (-\beta)^n \int_{S_n(1)} e^{-s_1\beta\mathbb{H}} \delta \tilde{\mathbf{U}}(\lambda \mathbf{h}) \cdots e^{-s_n\beta\mathbb{H}} \delta \tilde{\mathbf{U}}(\lambda \mathbf{h}) e^{-(1-\sum_{j=1}^n s_j)\beta\mathbb{H}}. \quad (171)$$

By Lemma 6.5, we have

$$\mathcal{Z}_{\beta, \varepsilon}(\lambda \mathbf{h}) = \sum_{n=0}^{\infty} \operatorname{Tr} \left[\mathcal{D}_n(\lambda) e^{-\varepsilon H_p} \right]. \quad (172)$$

Note that

$$\operatorname{Tr} \left[\mathcal{D}_1(\lambda) e^{-\varepsilon H_p} \right] = \frac{\lambda^2}{2} \langle \mathbf{h}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle \operatorname{Tr} \left[e^{-\beta\mathbb{H}} e^{-\varepsilon H_p} \right] \quad (173)$$

and, by Theorem 6.1,

$$\frac{\mathcal{Z}_{\beta, \varepsilon}(\mathbf{0}) - \mathcal{Z}_{\beta, \varepsilon}(\lambda \mathbf{h})}{\lambda^2} \geq 0. \quad (174)$$

Hence, letting $\lambda \rightarrow 0$, it follows that

$$\begin{aligned} & \frac{\beta}{2} \langle \mathbf{h}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle \operatorname{Tr} \left[e^{-\beta\mathbb{H}} e^{-\varepsilon H_p} \right] \\ & - \beta^2 \int_0^1 ds_1 \int_0^{1-s_1} ds_2 \operatorname{Tr} \left[e^{-s_1\beta\mathbb{H}} \langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle e^{-s_2\beta\mathbb{H}} \langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle \right. \\ & \quad \left. \times e^{-(1-s_1-s_2)\beta\mathbb{H}} e^{-\varepsilon H_p} \right] \geq 0. \end{aligned} \quad (175)$$

By applying Lemma 6.5 again, we have $\lim_{\varepsilon \rightarrow +0} \operatorname{Tr} [e^{-\beta\mathbb{H}} e^{-\varepsilon H_p}] = \mathcal{Z}_{\beta}$ and the second term in (175)

$$\rightarrow \frac{\beta^2}{2} \int_0^1 dx \operatorname{Tr} \left[\langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle e^{-x\beta\mathbb{H}} \langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle e^{-(1-x)\beta\mathbb{H}} \right] \text{ as } \varepsilon \rightarrow +0. \quad (176)$$

Thus, we obtain (167) for $\mathbf{h}$ real-valued. To extend this to complex-valued $\mathbf{h}$'s, we just note that, if $A = A_R + iA_I$ with $A_R^* = A_R$, $A_I^* = A_I$, we have $((A^*, A))_{\beta, \Lambda} = ((A_R, A_R))_{\beta, \Lambda} + ((A_I, A_I))_{\beta, \Lambda}$. $\square$

To finish proof of Theorem 1.6, we note that

$$\left(\langle \delta \mathbf{n}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle^*, \langle \delta \mathbf{n}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle \right)_{\beta, \Lambda} = \left(\left(\langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle^*, \langle \boldsymbol{\sigma}, \mathbf{U}_{\text{eff}} \mathbf{h} \rangle \right) \right)_{\beta, \Lambda}. \quad (177)$$

Thus, by the Fourier transformation, we obtain Theorem 1.6. $\square$

Appendix A. Operator inequalities associated with the Hilbert cone

Let $\mathfrak{X}$ be a complex Hilbert space and $\mathfrak{X}_+$ be a Hilbert cone in $\mathfrak{X}$.

Proposition A.1. *Let A, B be self-adjoint positive operators on $\mathfrak{X}$. Suppose that*

- (i) $e^{-\beta A} \geq 0$ w.r.t. $\mathfrak{X}_+$ for all $\beta \geq 0$;
- (ii) $A \geq B$ w.r.t. $\mathfrak{X}_+$;
- (iii) $C = A - B$ is bounded.

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

Proof. By (ii), $C \geq 0$ w.r.t. $\mathfrak{X}_+$ and $B = A - C$. By the Duhamel formula, we have the following norm-convergent expansion:

$$e^{-\beta B} = \sum_{n=0}^{\infty} D_n(\beta), \quad (178)$$

$$D_n(\beta) = \int_{S_n(\beta)} e^{-s_1 A} C e^{-s_2 A} C \dots e^{-s_n A} C e^{-(\beta - \sum_{j=1}^n s_j) A}, \quad (179)$$

where $\int_{S_n(\beta)} = \int_0^\beta ds_1 \int_0^{\beta-s_1} ds_2 \dots \int_0^{\beta-\sum_{j=1}^{n-1} s_j} ds_n$ and $D_0(\beta) = e^{-\beta A}$. Since $C \geq 0$ and $e^{-tA} \geq 0$ w.r.t. $\mathfrak{X}_+$, it holds that $D_n(\beta) \geq 0$ w.r.t. $\mathfrak{X}_+$ for all $n \geq 0$. Thus, by (178), we have $e^{-\beta B} \geq D_0(\beta) = e^{-\beta A}$ w.r.t. $\mathfrak{X}_+$ for all $\beta \geq 0$. $\square$

The following theorem plays an important role:

Theorem A.2. (Perron–Frobenius–Faris) *Let A be a positive self-adjoint operator on $\mathfrak{X}$. Suppose that $0 \leq e^{-tA}$ w.r.t. $\mathfrak{X}_+$ for all $t \geq 0$ and $\inf \text{spec}(A)$ is an eigenvalue. Let P_A be the orthogonal projection onto the closed subspace spanned by eigenvectors associated with $\inf \text{spec}(A)$. Then the following are equivalent:*

- (i) $\dim \text{ran } P_A = 1$ and $P_A \triangleright 0$ w.r.t. $\mathfrak{X}_+$.
- (ii) $0 \triangleleft e^{-tA}$ w.r.t. $\mathfrak{X}_+$ for all $t > 0$.
- (iii) For each $x, y \in \mathfrak{X}_+ \setminus \{0\}$, there exists a $t > 0$ such that $\langle x, e^{-tA} y \rangle > 0$.

Proof. See [5, 21, 31]. $\square$

Appendix B. Strong product integration

Let $\mathbb{C}_{n \times n}$ be the space of $n \times n$ matrices with complex entries. Let $A(\cdot) : [0, a] \rightarrow \mathbb{C}_{n \times n}$ be continuous. Let $P = \{s_0, s_1, \dots, s_n\}$ be a partition of $[0, a]$ and $\mu(P) = \max_j \{s_j - s_{j-1}\}$. The *strong product integration* of A is defined by

$$\prod_0^a e^{A(s)ds} := \lim_{\mu(P) \rightarrow 0} e^{A(s_1)(s_1-s_0)} e^{A(s_2)(s_2-s_1)} \dots e^{A(s_n)(s_n-s_{n-1})}. \quad (180)$$

Note that the limit is independent of any partition P .

Theorem B.1. *It holds that*

$$\left\| \prod_0^a e^{A(s)ds} - \mathbb{1} - \int_0^a ds A(s) \right\| \leq e^{\int_0^a ds \|A(s)\|} - 1 - \int_0^a ds \|A(s)\|. \quad (181)$$

Proof. See [3]. $\square$

Appendix C. Proof of Proposition 5.11

To show Proposition 5.11, we need two technical lemmas.

Recall the definition of $\Phi_{\{x,y\}}(\cdot)$ given by (45).

Lemma C.1. *Let $(\mathbf{q}, \mathbf{q}') \in \mathcal{Y}^c$, the complement of $\mathcal{Y}$. There exist $\beta_0 > 0$ and $C > 0$ such that, for all $\beta \in (0, \beta_0)$ and $\boldsymbol{\varphi} \in W_\beta$,*

$$\left| \beta^{-1} \int_0^\beta ds \exp \left\{ i \Phi_{\{x,y\}}(\boldsymbol{\omega}(s)(\boldsymbol{\varphi})) \right\} \right| \geq \gamma_{xy} - C\beta^{1/4}, \quad (182)$$

where

$$\gamma_{xy} = 2 \left| \frac{\sin \theta_{xy}}{\theta_{xy}} \right|, \quad \theta_{xy} = \frac{1}{2} \sum_{z \in \Lambda} a_z(\{x, y\})(q'_z - q_z). \quad (183)$$

Note that $\gamma_{xy} > 0$ for all $(\mathbf{q}, \mathbf{q}') \in \mathcal{Y}^c$ and β_0 depends on $(\mathbf{q}, \mathbf{q}')$.

Proof. Let

$$K_{xy} = \frac{1}{2\theta_{xy}} e^{i \sum_{z \in \Lambda} a_z q_z} \left(e^{2i\theta_{xy}} - 1 \right). \quad (184)$$

Note that $|K_{xy}| = \gamma_{xy}$ and

$$K_{xy} = \beta^{-1} \int_0^\beta ds \exp \left\{ i \Phi_{\{x,y\}} \left((1 - \beta^{-1}s)q_z + \beta^{-1}s q'_z \right) \right\}. \quad (185)$$

Thus, since $|e^{ia} - 1| \leq |a|$, we have

$$\begin{aligned}
& \left| \beta^{-1} \int_0^\beta ds \exp \left\{ i\Phi_{\{x,y\}}(\omega(s)(\varphi)) \right\} - K_{xy} \right| \\
&= \left| \beta^{-1} \int_0^\beta ds \exp \left\{ i\Phi_{\{x,y\}} \left((1 - \beta^{-1}s)q_z + \beta^{-1}s q'_z \right) \right\} \right. \\
&\quad \times \left. \left(\exp \left\{ i\sqrt{\beta}\Phi_{\{x,y\}}(\alpha(s)(\varphi)) \right\} - 1 \right) \right| \\
&\leq \max_{s \in [0,\beta]} \left| \sqrt{\beta}\Phi_{\{x,y\}}(\alpha(s)(\varphi)) \right| \\
&\leq \beta^{1/4} \sum_{z \in \Lambda} |a_z(\{x,y\})|. \tag{186}
\end{aligned}$$

This completes the proof. $\square$

Lemma C.2. *Let $(\mathbf{q}, \mathbf{q}') \in \mathcal{Y}^c$. Let $\{X, Y\} \in \wedge^{M^\dagger} E$. There exist $\beta_0 > 0$ and $\gamma > 0$ such that, for all $\beta \in (0, \beta_0)$ and $\varphi \in W_\beta$, we have*

$$\left| \left\langle e_X, \beta^{-1} \int_0^\beta ds \mathbb{T}_{+g}(\omega(s)(\varphi)) e_Y \right\rangle \right| \geq \gamma. \tag{187}$$

Note that β_0 and $\gamma = \gamma(\mathbf{q}, \mathbf{q}')$ depend on $(\mathbf{q}, \mathbf{q}')$.

Proof. Using standard notation of the second quantization²⁴, we can write

$$\mathbb{T}_{+g}(\mathbf{q}) = d\Gamma(\mathcal{T}_{+g}(\mathbf{q}))_{M^\dagger}, \tag{190}$$

$$\mathcal{T}_{+g}(\mathbf{q}) = \sum_{\{x,y\} \in E} t_{xy} \exp \{ i\Phi_{\{x,y\}}(\mathbf{q}) \} |e_x\rangle \langle e_y| \tag{191}$$

for all $\mathbf{q} \in \mathcal{Q}$.

Write X, Y as $X = (x_1, \dots, x_{M^\dagger})$ and $Y = (y_1, \dots, y_{M^\dagger})$. Then, there exists a unique j such that $\{x_j, y_j\} \in E$ and $x_i = y_i$ holds for all $i \neq j$. By

²⁴Let A be a bounded self-adjoint operator on $\ell^2(\Lambda)$. The second quantization of A is defined by

$$d\Gamma(A)_N = \sum_{j=1}^N \mathbb{1} \otimes \cdots \otimes \underbrace{A}_{j\text{th}} \otimes \cdots \otimes \mathbb{1}. \tag{188}$$

$d\Gamma(A)_N$ acts in $\wedge^N \ell^2(\Lambda)$. Set $a_{xy} = \langle e_x, A e_y \rangle$. Then $d\Gamma(A)_N$ can be expressed as

$$d\Gamma(A)_N = \sum_{x,y \in \Lambda} a_{xy} c_x^* c_y. \tag{189}$$

(190), it indicates the following:

$$\begin{aligned} \left\langle e_X, \int_0^\beta ds \mathbb{T}_{+g}(\omega(s)(\varphi)) e_Y \right\rangle &= \left\langle e_{x_j}, \int_0^\beta ds \mathbb{T}_{+g}(\omega(s)(\varphi)) e_{y_j} \right\rangle \\ &= \int_0^\beta ds t_{x_j y_j} \exp \left\{ i \Phi_{\{x_j, y_j\}}(\omega(s)(\varphi)) \right\}. \end{aligned} \quad (192)$$

By (192) and Lemma C.1, we have

$$\begin{aligned} &\left| \left\langle e_X, \beta^{-1} \int_0^\beta ds \mathbb{T}_{+g}(\omega(s)(\varphi)) e_Y \right\rangle \right| \\ &= |t_{x_j y_j}| \left| \beta^{-1} \int_0^\beta ds \exp \left\{ i \Phi_{\{x_j, y_j\}}(\omega(s)(\varphi)) \right\} \right| \\ &\geq |t_{x_j y_j}| (\gamma_{x_j y_j} - C\beta^{1/4}). \end{aligned} \quad (193)$$

Thus, we have the desired assertion. $\square$

Completion of proof of Proposition 5.11

For each $P = X_1 X_2 \cdots X_{L+1} \in \mathcal{P}_{XY}^{M^\dagger}[L]$, let

$$\tau_\beta^{(M^\dagger)}(P, \{\omega_j(\varphi_j)\}_{j=1}^L) = \prod_{j=1}^L E_{X_j} \int_0^\beta ds_j \mathbb{T}_{+g}(\omega_j(s_j)(\varphi_j)) E_{X_{j+1}}. \quad (194)$$

We claim that

$$\mathcal{G}_\beta^{(M^\dagger)}(P, \{\omega_j(\varphi_j)\}_{j=1}^L) = \tau_\beta^{(M^\dagger)}(P, \{\omega_j(\varphi_j)\}_{j=1}^L) + \mathcal{O}(\beta^{L+1}). \quad (195)$$

Here, the error term $\mathcal{O}(\beta^{L+1})$ satisfies $\|\mathcal{O}(\beta^{L+1})\| \leq C\beta^{L+1}$, where C is independent of φ_j . To see this, we observe that, by Theorem B.1,

$$\begin{aligned} &\left\| E_{X_j} \left[G_\beta(\omega_j(s_j)(\varphi_j)) - \int_0^\beta ds \mathbb{T}_{+g}(\omega_j(s)(\varphi_j)) \right] E_{X_{j+1}} \right\| \\ &= \left\| E_{X_j} \left[G_\beta(\omega_j(s_j)(\varphi_j)) - \mathbb{1} - \int_0^\beta ds \mathbb{T}_{+g}(\omega_j(s)(\varphi_j)) \right] E_{X_{j+1}} \right\| \\ &\leq \left(\int_0^\beta ds \|\mathbb{T}_{+g}(\omega_j(s)(\varphi_j))\| \right)^2 \\ &\leq \beta^2 C(M^\dagger)^2 (\max_{x,y} |t_{xy}|)^2. \end{aligned} \quad (196)$$

Here, we have used the fact that $E_{X_j} E_{X_{j+1}} = 0$.

Denote $X_0 = X$ and $X_{L+1} = Y$. By Lemma C.2, we have

$$\begin{aligned} & \left| \beta^{-L} \left\langle e_X, \tau_\beta^{M^\dagger} \left(P, \{\omega_j(\varphi_j)\}_{j=1}^L \right) e_Y \right\rangle \right| \\ &= \prod_{j=1}^{L+1} \left| \left\langle e_{X_{j-1}}, \beta^{-1} \int_0^\beta ds \mathbb{T}_{+g}(\omega_j(s)(\varphi_j)) e_{X_j} \right\rangle \right| \\ &\geq \gamma(\mathbf{q}, \mathbf{q}_1) \gamma(\mathbf{q}_1, \mathbf{q}_2) \cdots \gamma(\mathbf{q}_{L-1}, \mathbf{q}'), \end{aligned} \quad (197)$$

where $\gamma(\mathbf{q}, \mathbf{q}')$ is given by Lemma C.2. By combining this and (195), we obtain the desired result. $\square$

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