Long-range charge order in the extended Holstein–Hubbard model

Tadahiro Miyao
Department of Mathematics, Hokkaido University,
Sapporo 060-0810, Japan
E-mail: miyao@math.sci.hokudai.ac.jp

Abstract

This study investigated the extended Holstein–Hubbard model at half-filling as a model for describing interplay of the electron-electron and electron-phonon couplings. When the electron-phonon and nearest-neighbor electron-electron interactions are strong, we prove the existence of long-range charge order at sufficiently low temperature in three or more dimensions. As a result, we rigorously justify the phase competition between the antiferromagnetic and charge orders.

1 Introduction

In the Bardeen–Cooper–Schrieffer theory, the electron-phonon coupling plays an essential role in the electron-pairing mechanism [1]. Recently, the strong electron-phonon coupling was observed in high-T_c cuprates [18]. In alkali-doped fullerides and aromatic superconductors, the electron-phonon interactions are reported to be strong [3, 14, 16, 27, 30]. These examples suggest that the electron-phonon coupling has received much attention in the field of superconductivity.

In the presence of strong electron-electron Coulomb and electron-phonon interactions, correlated electron systems provide an attractive field of study in which various phases compete with each other. While there has been extensive research regarding the competition between these phases, only few exact results are known. The Holstein–Hubbard model is a simple model which allows us to explore the interplay of electron-electron and electron-phonon interactions. Our aim in the present paper is to rigorously study the competition between the phases in the system described by the Holstein–Hubbard model.

Rigorous study of the Holstein model was initiated by Löwen [21]. Freericks and Lieb proved that the ground state of the Holstein model is unique and has a total spin $S = 0$ [6]. Remark that their studies focused on the electron-phonon interaction only and did not consider the interplay of electron-electron and electron-phonon interactions. Taking the interplay into account, Miyao proved the following in [24]:

- If the electron-phonon coupling is weak ($U_{\text{eff}} - \nu V > 0$), there is no long-range charge order in the Holstein–Hubbard system at half-filling.
- If the electron-phonon coupling is weak, the ground state of the Holstein–Hubbard model is unique and exhibits an antiferromagnetic order.

See Section 2 for precise statements. Our achivment in this paper is to prove that there exists a long-range charge order at sufficiently low temperature provided that the electron-phonon interaction is strong ($U_{\text{eff}} - \nu V < 0$). The obtained phase diagram is compatible with the previous results conjectured by heuristic arguments [2, 26]. To prove the main result, we apply the method of reflction positivity.

Reflection positivity originates from axiomatic quantum field theory [28]. Glimm, Jaffe and Spencer first applied reflection positivity to the rigorous study of the phase transition [10, 11]. This idea was further developed by Dyson, Fröhlich, Israel, Lieb, Simon and Spencer in [4, 7, 8, 9]. Applications of reflection positivity to the Hubbard model are given in [13, 15, 19]. In the present paper, we further develope the method in [8] in order to apply reflection positivity to the Holstein–Hubbard model which is more difficult to analyze than the Hubbard model. Usually, the hopping matrix elements of the Hubbard model are real numbers. Because of past successes in research of the Hubbard model, reflection positivity has been believed to be inapplicable to the case where the hopping matrix elements are *complex* numbers. In the study of the Holstein–Hubbard model, the Lang–Firsov transformation is known to be very useful. However, by this transformation, the hopping matrix elements change into complex numbers. Therefore, it appears that reflection positivity is unsuitable to study the Holstein–Hubbard model at a first glance. On the other hand, in a series of papers [23, 24, 25], Miyao shows that reflection positivity is still applicable to the case where the hopping matrix elements are complex. In the present paper, we further extend this idea and adapt reflection positivity to a rigorous analysis of the Holstein–Hubbard model.

The organization of the paper is as follows: In Section 2, we define the Holstein–Hubbard model and state the main results. We compare the obtained results with previous works as well. Section 3 is devoted to the proof of the main theorem. In Appendix A, we give an extension of the Dyson–Lieb–Simon inequality. In Appendix B, we prove a useful inequality.

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2 Main results

Let $\Lambda = [-L, L)^\nu \cap \mathbb{Z}^\nu$. The extended Holstein–Hubbard model on Λ is given by

$$\begin{aligned} H_\Lambda = &\sum_{\langle x;y\rangle} \sum_{\sigma=\uparrow,\downarrow} (-t)(c_{x\sigma}^* c_{y\sigma} + c_{y\sigma}^* c_{x\sigma}) \\ &+ U \sum_{x\in\Lambda} (n_x - \mathbb{1})^2 + V \sum_{\langle x;y\rangle} (n_x - \mathbb{1})(n_y - \mathbb{1}) \\ &+ g \sum_{x\in\Lambda} (n_x - \mathbb{1})(b_x + b_x^*) + \omega \sum_{x\in\Lambda} b_x^* b_x, \end{aligned} \tag{2.1}$$

where $n_x = n_{x\uparrow} + n_{x\downarrow}$ with $n_{x\sigma} = c_{x\sigma}^* c_{x\sigma}$. Here, $\langle x; y\rangle$ refers to a sum over nearest-neighbor pairs. We impose periodic boundary conditions, so $L \equiv -L$. H_Λ acts in the Hilbert space

$$\mathfrak{H} = \mathfrak{F} \otimes \mathfrak{P}. \tag{2.2}$$

The electrons live in the fermionic Fock space $\mathfrak{F}$ given by $\mathfrak{F} := \mathfrak{F}_{\rm as}(\ell^2_\uparrow(\Lambda) \oplus \ell^2_\downarrow(\Lambda)) := \bigoplus_{n\ge 0} \wedge^n(\ell^2_\uparrow(\Lambda) \oplus \ell^2_\downarrow(\Lambda))$, where $\ell^2_\uparrow(\Lambda) = \ell^2_\downarrow(\Lambda) = \ell^2(\Lambda)$, and $\wedge^n$ is the n-fold antisymmetric tensor product. The phonons live in the bosonic Fock space $\mathfrak{P}$ defined by $\mathfrak{P} = \bigoplus_{n\ge 0} \otimes^n_{\rm s} \ell^2(\Lambda)$, where $\otimes^n_{\rm s}$ is the n-fold symmetric tensor product. $c_{x\sigma}$ is the electron annihilation operator, b_x is the phonon annihilation operator. These operators satisfy the following relations:

$$\{c_{x\sigma}, c^*_{x'\sigma'}\} = \delta_{\sigma\sigma'}\delta_{xx'}, \quad [b_x, b^*_{x'}] = \delta_{xx'}. \tag{2.3}$$

t is the hopping matrix element, g is the strength of the electron-phonon interaction. An on-site and a nearest-neighbor repulsions are denoted by U and V, respectively. The phonons are assumed to be dispersionless with energy ω. Henceforth, we assume the following:

- $g \in \mathbb{R}, \quad t > 0, \quad U > 0, \quad V > 0, \quad \omega > 0.$
- L is an odd number[1].

The thermal expectation is defined by

$$\langle A\rangle_{\beta,\Lambda} = \mathrm{Tr}\big[A\, e^{-\beta H_\Lambda}\big]\Big/ Z_{\beta,\Lambda}, \quad Z_{\beta,\Lambda} = \mathrm{Tr}\big[e^{-\beta H_\Lambda}\big]. \tag{2.4}$$

We restrict ourselves to the half-filling case (indeed, we can check that $\langle n_x\rangle_{\beta,\Lambda} = 1$). Let $q_x = n_x - \mathbb{1}$. We define the two-point correlation function by

$$\langle q_x q_o\rangle_\beta = \lim_{L\to\infty} \langle q_x q_o\rangle_{\beta,\Lambda}. \tag{2.5}$$

The effective interaction strength is defined by

$$U_{\rm eff} = U - \frac{2g^2}{\omega}. \tag{2.6}$$

In [24], the following theorem is proven provided that $\nu V - U_{\rm eff} < 0$.

Theorem 2.1 [24] *Suppose that $\nu V - U_{\rm eff} < 0$. Then we have the following:*

(i) *For all $\beta \ge 0$, we have*

$$\lim_{\|x\|\to\infty} \langle q_x q_o\rangle_\beta = 0. \tag{2.7}$$

Hence, there is no long-range charge order.

(ii) *Let $\mathfrak{H}_M$ be the M-subspace[2] and let $H_{\Lambda,M} = H_\Lambda \restriction \mathfrak{H}_M$, the restriction of H_Λ to $\mathfrak{H}_M$. Then the ground state of $H_{\Lambda,M}$ is unique for all possible M.*

[1] This assumption is not essential. Indeed, by changing arguments in Section 3, we can prove our results even if L is even.

[2] To be precise, $\mathfrak{H}_M$ is defined by

$$\mathfrak{H}_M = \{\psi \in \mathfrak{H} \,|\, N\psi = |\Lambda|\psi,\ S^3\psi = M\psi\}, \tag{2.8}$$

where $N = N_\uparrow + N_\downarrow$ and $S^3 = \frac{1}{2}(N_\uparrow - N_\downarrow)$ with $N_\sigma = \sum_{x\in\Lambda} n_{x\sigma}$. The condition $N\psi = |\Lambda|\psi$ indicates that we consider the half-filling case.

(iii) *Let*

$$S_x^+ = c_{x\uparrow}^* c_{x\downarrow}, \quad S_x^- = c_{x\downarrow}^* c_{x\uparrow}. \tag{2.9}$$

Let φ_M *be the ground state of* $H_{\Lambda,M}$. *Then we have*

$$(-1)^{\|x\|}\langle \varphi_M | S_x^+ S_o^- \varphi_M\rangle > 0 \tag{2.10}$$

for all $x \in \Lambda$, *where* $\|x\| = \sum_{j=1}^{\nu} |x_j|$. *This means that an antiferromagnetic order exists in the ground state.*

Considering this theorem, it is rogical as well as important to study the case where $\nu V - U_{\rm eff} > 0$. Our main result in this paper is the following:

Theorem 2.2 *Assume that* $\nu V - U_{\rm eff} > 0$. *For each* $\nu \ge 3$, *we have*

$$\lim_{\|x\|\to\infty} (-1)^{\|x\|}\langle q_x q_o\rangle_\beta \tag{2.11}$$

$$\ge 1 - \beta^{-1}(\nu V - U_{\rm eff})^{-1}\ln 4(1-e^{-\beta\omega})^{-1} - 8\nu t(\nu V - U_{\rm eff})^{-1} - \gamma_1 \int_{\mathbb{T}^\nu} dp E(p)^{-1} - \gamma_2, \tag{2.12}$$

where $\mathbb{T} = (-\pi, \pi)$ *and*

$$\gamma_1 = (2\pi)^{-\nu}\frac{1}{2}\Big\{(\beta V)^{-1} + \Big(\frac{t}{V}\Big)^{1/2}\Big\}, \quad \gamma_2 = \frac{1}{4}\Big(\frac{t}{V}\Big)^{1/2}. \tag{2.13}$$

Corollary 2.3 *Let* $\nu \ge 3$. *Assume that* $\nu V - U_{\rm eff} > 0$. *If* β, V, g *are sufficiently large such that the right hand side of (2.12) is strictly positive, then we have*

$$\lim_{\|x\|\to\infty} (-1)^{\|x\|}\langle q_x q_o\rangle_\beta > 0. \tag{2.14}$$

Thus, there is a staggered long-range charge order.

Remark 2.4 Our method can be applicable to several models. For instance, let us consider a crystal coupled to the quatized radiation field. The system's hamiltonian is given by

$$H_\Lambda = \sum_{\langle x;y\rangle}\sum_{\sigma=\uparrow,\downarrow}(-t)\exp\Big\{ie\int_{C_{xy}} dr\cdot A(r)\Big\}c_{x\sigma}^* c_{y\sigma} + \text{h.c.}$$
$$+ U\sum_{x\in\Lambda}(n_x - \mathbb{1})^2 + V\sum_{\langle x;y\rangle}(n_x - \mathbb{1})(n_y - \mathbb{1}) + \sum_{\lambda=1,2}\sum_{k\in V^*}\omega(k)a(k,\lambda)^* a(k,\lambda).$$

See [12, 25] for the precise definition of this model. In this case, we have the following:

Theorem 2.5 *Assume that* $\nu V - U > 0$. *For each* $\nu \ge 3$, *we have*

$$\lim_{\|x\|\to\infty} (-1)^{\|x\|}\langle q_x q_o\rangle_\beta$$
$$\ge 1 - \beta^{-1}(\nu V - U)^{-1}\ln 4 - \beta^{-1}(\nu V - U)^{-1}\int_{\mathbb{T}^\nu} dp \ln(1-e^{-\beta\omega(p)})^{-1} - 8\nu t(\nu V - U)^{-1}$$
$$- \gamma_1\int_{\mathbb{T}^\nu} dp E(p)^{-1} - \gamma_2.$$

If β, V *are sufficiently large, there is a staggered long-range charge order.*

3 Proof of Theorem 2.2

3.1 The Lang–Firsov transformation

We set $H_\Lambda = T + P + I + K$, where

$$T = \sum_{\langle x;y\rangle} \sum_{\sigma=\uparrow,\downarrow} (-t)\big(c_{x\sigma}^* c_{y\sigma} + c_{y\sigma}^* c_{x\sigma}\big), \tag{3.1}$$

$$P = U \sum_{x\in\Lambda} q_x^2 + V \sum_{\langle x;y\rangle} q_x q_y, \tag{3.2}$$

$$I = g \sum_{x\in\Lambda} q_x(b_x + b_x^*), \tag{3.3}$$

$$K = \omega \sum_{x\in\Lambda} b_x^* b_x. \tag{3.4}$$

For each $x \in \Lambda$, let

$$\phi_x = \sqrt{\frac{1}{2\omega}}(b_x^* + b_x), \quad \pi_x = i\sqrt{\frac{\omega}{2}}(b_x^* - b_x). \tag{3.5}$$

Both ϕ_x and π_x are essentially self-adjoint. We denote their closures by the same symbols. Next, let

$$L = -i\omega^{-3/2} g \sum_{x\in\Lambda} q_x \pi_x. \tag{3.6}$$

L is essentially antiself-adjoint. We also denote its closure by the same symbol. The *Lang-Firosov transformation* is a unitary operator defined by

$$\mathscr{U} = e^{-i\pi N_{\rm p}/2} e^{L}, \tag{3.7}$$

where $N_{\rm p} = \sum_{x\in\Lambda} b_x^* b_x$ [17]. We can check the following:

$$\mathscr{U} c_{x\sigma} \mathscr{U}^{-1} = e^{i\alpha\phi_x} c_{x\sigma}, \quad \alpha = \sqrt{2}\omega^{-3/2} g, \tag{3.8}$$

$$\mathscr{U} b_x \mathscr{U}^{-1} = b_x - \frac{g}{\omega} q_x. \tag{3.9}$$

By these formulas, we obtain the following:

Lemma 3.1 *Let $H'_\Lambda = \mathscr{U} H_\Lambda \mathscr{U}^{-1}$. We have*

$$H'_\Lambda = T' + P' + K, \tag{3.10}$$

where

$$T' = \sum_{\langle x;y\rangle} \sum_{\sigma=\uparrow,\downarrow} (-t)\Big(e^{-i\alpha(\phi_x-\phi_y)} c_{x\sigma}^* c_{y\sigma} + e^{+i\alpha(\phi_x-\phi_y)} c_{y\sigma}^* c_{x\sigma}\Big), \tag{3.11}$$

$$P' = U_{\rm eff} \sum_{x\in\Lambda} q_x^2 + V \sum_{\langle x;y\rangle} q_x q_y, \tag{3.12}$$

$$K = \frac{1}{2} \sum_{x\in\Lambda} (\pi_x^2 + \omega^2 \phi_x^2). \tag{3.13}$$

3.2 The Schrödinger representation

The bosonic Fock space can be identified as

$$\mathfrak{P} = L^2(\mathcal{Q}_\Lambda, d\mu_\Lambda), \tag{3.14}$$

where $\mathcal{Q}_\Lambda = \mathbb{R}^\Lambda$ and $d\mu_\Lambda = \prod_{x\in\Lambda} d\phi_x$, the $|\Lambda|$-dimensional Lebesgue measure. Moreover, each ϕ_x can be regarded as a multiplication operator by the *real*-valued function, and π_x can be regarded as a partial differential operator $-i\frac{\partial}{\partial\phi_x}$. This representation of the canonical commutation relations is called the Schrödinger representation. In what follows, we will switch to this representation.

3.3 The zigzag transformation

Following [8], we introduce the *zigzag transformation* as follows: Let

$$v_{x\sigma} = \left[\prod_{z\neq x}(-1)^{n_{x\sigma}}\right](c_{x\sigma}^* + c_{x\sigma}). \tag{3.15}$$

It is not hard to check that

$$v_{x\sigma} c_{x'\sigma'} v_{x\sigma}^{-1} = \begin{cases} c_{x\sigma}^* & \text{if } (x,\sigma) = (x',\sigma') \\ c_{x'\sigma'} & \text{if } (x,\sigma) \neq (x',\sigma') \end{cases}. \tag{3.16}$$

Let $\Lambda_{\rm e} = \{x \in \Lambda \,|\, \|x\| \text{ is even}\}$ and let $\Lambda_{\rm o} = \{x \in \Lambda \,|\, \|x\| \text{ is odd}\}$. Now, we set

$$\mathscr{V} = \prod_{x\in\Lambda_{\rm o}} v_{x\uparrow} v_{x\downarrow}. \tag{3.17}$$

We observe that

$$\mathscr{V} c_{x\sigma} \mathscr{V}^{-1} = \begin{cases} c_{x\sigma}^* & \text{if } x \in \Lambda_{\rm o} \\ c_{x\sigma} & \text{if } x \in \Lambda_{\rm e} \end{cases}, \quad \mathscr{V} q_x \mathscr{V}^{-1} = (-1)^{\|x\|} q_x. \tag{3.18}$$

Lemma 3.2 *Let $H_\Lambda'' = \mathscr{V} H_\Lambda' \mathscr{V}^{-1}$. We have $H_\Lambda'' = T'' + P'' + K$, where*

$$T'' = \sum_{x\in\Lambda_{\rm e}} \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{\nu} \sum_{\varepsilon=\pm} (-t)\Big(e^{-i\alpha(\phi_x - \phi_{x+\varepsilon\delta_j})} c_{x\sigma}^* c_{x+\varepsilon\delta_j\sigma}^* + \text{h.c.}\Big), \tag{3.19}$$

$$P'' = U_{\rm eff} \sum_{x\in\Lambda} q_x^2 - V \sum_{\langle x;y\rangle} q_x q_y. \tag{3.20}$$

Proof. Let δ_j $(j = 1, \dots, \nu)$ be the unit vector in $\mathbb{Z}^\nu$ defined by $\delta_j = (0, \dots, 0, \underbrace{1}_{j-\text{th}}, 0, \dots, 0)$.

T' can be expressed as

$$T' = \sum_{x\in\Lambda_{\rm e}} \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{\nu} \sum_{\varepsilon=\pm 1} (-t)\Big(e^{-i\alpha(\phi_x - \phi_{x+\varepsilon\delta_j})} c_{x\sigma}^* c_{x+\varepsilon\delta_j\sigma} + \text{h.c.}\Big). \tag{3.21}$$

Thus, using (3.18), we obtain (3.19). Similarly, we have (3.20). □

To show the main theorem, we introduce the following modified hamiltonian:

Definition 3.3 For each $\mathbf{h} = \{h_x\}_{x\in\Lambda} \in \mathbb{R}^\Lambda$, we set

$$P''(\mathbf{h}) = (U_{\text{eff}} - \nu V)\sum_{x\in\Lambda} q_x^2 + \frac{V}{2}\sum_{\langle x;y\rangle}(q_x - h_x - q_y + h_y)^2 \tag{3.22}$$

and

$$H''_\Lambda(\mathbf{h}) = T'' + P''(\mathbf{h}) + K. \tag{3.23}$$

Trivially, we have $H''_\Lambda = H''_\Lambda(\mathbf{0})$. $\diamondsuit$

3.4 Reflection positivity

3.4.1 Preliminaries

We divide Λ as $\Lambda = \Lambda_L \cup \Lambda_R$, where

$$\Lambda_L = \{x = (x_1, \dots, x_\nu) \in \Lambda \,|\, x_1 < 0\}, \quad \Lambda_R = \{x = (x_1, \dots, x_\nu) \in \Lambda \,|\, x_1 \ge 0\}. \tag{3.24}$$

We also divide the single electron space $\ell^2(\Lambda)$ as

$$\ell^2(\Lambda) = \ell^2(\Lambda_L) \oplus \ell^2(\Lambda_R). \tag{3.25}$$

Hence, we have the following identifications:

$$\mathfrak{F} = \mathfrak{F}_L \otimes \mathfrak{F}_R, \tag{3.26}$$

where $\mathfrak{F}_L = \mathfrak{F}_{\text{as}}(\ell^2_\uparrow(\Lambda_L) \oplus \ell^2_\downarrow(\Lambda_L))$ and $\mathfrak{F}_R = \mathfrak{F}_{\text{as}}(\ell^2_\uparrow(\Lambda_R) \oplus \ell^2_\downarrow(\Lambda_R))$, and

$$\mathfrak{P} = \mathfrak{P}_L \otimes \mathfrak{P}_R, \tag{3.27}$$

where $\mathfrak{P}_L = \mathfrak{F}_{\text{s}}(\ell^2(\Lambda_L)) = L^2(\mathcal{Q}_{\Lambda_L}, d\mu_{\Lambda_L})$ and $\mathfrak{P}_R = \mathfrak{F}_{\text{s}}(\ell^2(\Lambda_R)) = L^2(\mathcal{Q}_{\Lambda_R}, d\mu_{\Lambda_R})$. Thus, the Hilbert space $\mathfrak{H}$ can be identified as follows:

$$\mathfrak{H} = \mathfrak{H}_L \otimes \mathfrak{H}_R, \tag{3.28}$$

where $\mathfrak{H}_L = \mathfrak{F}_L \otimes \mathfrak{P}_L$ and $\mathfrak{H}_R = \mathfrak{F}_R \otimes \mathfrak{P}_R$. Under this identification, we have the following identifications:

$$c_{x\sigma} = \begin{cases} c_{x\sigma} \otimes \mathbb{1} & \text{if } x \in \Lambda_L \\ (-1)^{N_L} \otimes c_{x\sigma} & \text{if } x \in \Lambda_R, \end{cases} \tag{3.29}$$

where $N_L = \sum_{x\in\Lambda_L} n_x$, and

$$\pi_x = \begin{cases} \pi_x \otimes \mathbb{1} & \text{if } x \in \Lambda_L \\ \mathbb{1} \otimes \pi_x & \text{if } x \in \Lambda_R \end{cases}, \quad \phi_x = \begin{cases} \phi_x \otimes \mathbb{1} & \text{if } x \in \Lambda_L \\ \mathbb{1} \otimes \phi_x & \text{if } x \in \Lambda_R \end{cases}. \tag{3.30}$$

Using these, we see the following lemmas.

Lemma 3.4 *Under the identification (3.28), we have* $T'' = T''_L \otimes \mathbb{1} + \mathbb{1} \otimes T''_R + T''_{LR}$*, where*

$$T''_L = \sum_{x\in\Lambda_{\rm e},\ x_1\le -2} \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{\nu} {\sum_{\varepsilon=\pm}}' (-t)\Big(e^{-i\alpha(\phi_x-\phi_{x+\varepsilon\delta_j})} c^*_{x\sigma} c^*_{x+\varepsilon\delta_j\sigma} + \text{h.c.}\Big), \tag{3.31}$$

$$T''_R = \sum_{x\in\Lambda_{\rm e},\ x_1\ge 0} \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{\nu} {\sum_{\varepsilon=\pm}}'' (-t)\Big(e^{-i\alpha(\phi_x-\phi_{x+\varepsilon\delta_j})} c^*_{x\sigma} c^*_{x+\varepsilon\delta_j\sigma} + \text{h.c.}\Big), \tag{3.32}$$

$$\begin{aligned} T''_{LR} = &\sum_{x\in\Lambda_{\rm e},\ x_1=0} \sum_{\sigma=\uparrow,\downarrow} (-t)\Big\{\Big[e^{i\alpha\phi_{x-\delta_1}}(-1)^{N_L} c^*_{x-\delta_1\sigma}\Big]\otimes\Big[e^{-i\alpha\phi_x} c^*_{x\sigma}\Big] + \text{h.c.}\Big\} \\ &+ \sum_{x\in\Lambda_{\rm e},\ x_1=L-1} \sum_{\sigma=\uparrow,\downarrow} (-t)\Big\{\Big[e^{i\alpha\phi_{x+\delta_1}}(-1)^{N_L} c^*_{x+\delta_1\sigma}\Big]\otimes\Big[e^{-i\alpha\phi_x} c^*_{x\sigma}\Big] + \text{h.c.}\Big\}. \end{aligned} \tag{3.33}$$

Here, ${\sum_{\varepsilon=\pm}}'$ *refers to a sum over pairs* $\langle x; x+\varepsilon\delta_j\rangle$ *such that* $x, x+\varepsilon\delta_j \in \Lambda_L$*. Similarly,* ${\sum_{\varepsilon=\pm}}''$ *refers to a sum over pairs* $\langle x; x+\varepsilon\delta_j\rangle$ *such that* $x, x+\varepsilon\delta_j \in \Lambda_R$*.*

Lemma 3.5 *For each* $\mathbf{h} = \{h_x\}_{x\in\Lambda} \in \mathbb{R}^\Lambda$*, we set* $\mathbf{h}_L = \{h_x\}_{x\in\Lambda_L}$ *and* $\mathbf{h}_R = \{h_x\}_{x\in\Lambda_R}$*. We have* $P''(\mathbf{h}) = P''_L(\mathbf{h}_L)\otimes\mathbb{1} + \mathbb{1}\otimes P''_R(\mathbf{h}_R) + P''_{LR}(\mathbf{h})$*, where*

$$P''_L(\mathbf{h}_L) = (U_{\rm eff}-\nu V)\sum_{x\in\Lambda_L} q_x^2 + \frac{V}{2}\sum_{\langle x;y\rangle,\ x,y\in\Lambda_L} (q_x - h_x - q_y + h_y)^2, \tag{3.34}$$

$$P''_R(\mathbf{h}_R) = (U_{\rm eff}-\nu V)\sum_{x\in\Lambda_R} q_x^2 + \frac{V}{2}\sum_{\langle x;y\rangle,\ x,y\in\Lambda_R} (q_x - h_x - q_y + h_y)^2, \tag{3.35}$$

$$\begin{aligned} P''_{LR}(\mathbf{h}) = &-V\sum_{x\in\Lambda_{\rm e},\ x_1=0} (q_{x-\delta_1} - h_{x-\delta_1})\otimes(q_x - h_x) \\ &-V\sum_{x\in\Lambda_{\rm e},\ x_1=L-1} (q_{x+\delta_1} - h_{x+\delta_1})\otimes(q_x - h_x). \end{aligned} \tag{3.36}$$

Lemma 3.6 *We have* $K = K_L\otimes\mathbb{1} + \mathbb{1}\otimes K_R$*, where*

$$K_L = \frac{1}{2}\sum_{x\in\Lambda_L}(\pi_x^2 + \omega^2\phi_x^2), \quad K_R = \frac{1}{2}\sum_{x\in\Lambda_R}(\pi_x^2 + \omega^2\phi_x^2). \tag{3.37}$$

For all $x\in\Lambda_L$, we define

$$a_{x\sigma} = c_{x\sigma}(-1)^{N_L}. \tag{3.38}$$

In terms of $a_{x\sigma}$, T''_L and T''_{LR} can be expressed as follows.

Proposition 3.7 *We obtain the following:*

$$T_L'' = \sum_{x\in\Lambda_\mathrm{e},\ x_1\le -2}\ \sum_{\sigma=\uparrow,\downarrow}\sum_{j=1}^{\nu}\sum_{\varepsilon=\pm}{}' (+t)\Big(e^{-i\alpha(\phi_x-\phi_{x+\varepsilon\delta_j})}a_{x\sigma}^* a_{x+\varepsilon\delta_j\sigma}^* + \mathrm{h.c.}\Big), \tag{3.39}$$

$$\begin{aligned} T_{LR}'' = &\sum_{x\in\Lambda_\mathrm{e},\ x_1=0}\ \sum_{\sigma=\uparrow,\downarrow}(-t)\bigg\{\Big(e^{i\alpha\phi_{x-\delta_1}}a_{x-\delta_1\sigma}^*\Big)\otimes\Big(e^{-i\alpha\phi_x}c_{x\sigma}^*\Big)+\mathrm{h.c.}\bigg\}\\ &+\sum_{x\in\Lambda_\mathrm{e},\ x_1=L-1}\ \sum_{\sigma=\uparrow,\downarrow}(-t)\bigg\{\Big(e^{i\alpha\phi_{x+\delta_1}}a_{x+\delta_1\sigma}^*\Big)\otimes\Big(e^{-i\alpha\phi_x}c_{x\sigma}^*\Big)+\mathrm{h.c.}\bigg\}. \end{aligned}\tag{3.40}$$

Remark 3.8 Since $q_x = \sum_{\sigma=\uparrow,\downarrow} a_{x\sigma}^* a_{x\sigma} - \mathbb{1}$, expressions of $P_L''(\mathbf{h}_L)$ and $P_{LR}''(\mathbf{h})$ are unchanged if we write these in terms of $a_{x\sigma}$. $\diamondsuit$

3.4.2 Gaussian domination

We define the *reflection map* $r : \Lambda_R \to \Lambda_L$ by

$$r(x) = (-x_1 - 1, x_2, \dots, x_\nu), \quad x \in \Lambda_R. \tag{3.41}$$

Let ϑ be an antilinear unitary operator from $\mathfrak{H}_L$ to $\mathfrak{H}_R$ defined as

$$c_{x\sigma} = \vartheta a_{r(x)\sigma}\vartheta^{-1}, \quad \phi_x = \vartheta\phi_{r(x)}\vartheta^{-1}, \quad \pi_x = -\vartheta\pi_{r(x)}\vartheta^{-1}, \quad x\in\Lambda_R, \tag{3.42}$$

$$\vartheta\Omega_L = \Omega_R, \tag{3.43}$$

where Ω_L (resp. Ω_R) is the Fock vaccum $\Omega_\mathrm{f}\otimes\Omega_\mathrm{b}$ in $\mathfrak{H}_L$ (resp. $\mathfrak{H}_R$)[3].

Lemma 3.9 *We have the following:*

(i) $T_R'' = \vartheta T_L'' \vartheta^{-1}$.

(ii)

$$\begin{aligned} T_{LR}'' = &\sum_{x\in\Lambda_\mathrm{e},\ x_1=0}\ \sum_{\sigma=\uparrow,\downarrow}(-t)\bigg\{\Big(e^{i\alpha\phi_{x-\delta_1}}a_{x-\delta_1\sigma}^*\Big)\otimes\vartheta\Big(e^{i\alpha\phi_{x-\delta_1}}a_{x-\delta_1\sigma}^*\Big)\vartheta^{-1}+\mathrm{h.c.}\bigg\}\\ &+\sum_{x\in\Lambda_\mathrm{e},\ x_1=L-1}\ \sum_{\sigma=\uparrow,\downarrow}(-t)\bigg\{\Big(e^{i\alpha\phi_{x+\delta_1}}a_{x+\delta_1\sigma}^*\Big)\otimes\vartheta\Big(e^{i\alpha\phi_{x+\delta_1}}a_{x+\delta_1\sigma}^*\Big)\vartheta^{-1}+\mathrm{h.c.}\bigg\}. \end{aligned}\tag{3.44}$$

Proof. (ii) is trivial. As for (i), we have to take care. First, remark that T_L'' can be expressed as

$$T_L'' = \sum_{x\in\Lambda_\mathrm{o},\ x_1\le -1}\ \sum_{\sigma=\uparrow,\downarrow}\sum_{j=1}^{\nu}\sum_{\varepsilon=\pm}{}' (+t)\Big(e^{-i\alpha(\phi_{x+\varepsilon\delta_j}-\phi_x)}a_{x+\varepsilon\delta_j\sigma}^* a_{x\sigma}^* + \mathrm{h.c.}\Big). \tag{3.45}$$

[3] In the Schrödinger representation, $\Omega_\mathrm{b} = (\frac{1}{\pi})^{|\Lambda_L|/4}e^{-\sum_{x\in\Lambda_L}\phi_x^2/2}$. Ω_f is the standard Fock vacuum in $\mathfrak{F}_L$.

Hence, by (3.32), we see

$$
\begin{aligned}
T''_R &= \vartheta \sum_{x\in\Lambda_{\rm e},\ x_1\geq 0} \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{\nu} \sum_{\varepsilon=\pm}{}' (-t)\Big(e^{+i\alpha(\phi_{r(x)}-\phi_{r(x+\varepsilon\delta_j)})} a^*_{r(x)\sigma} a^*_{r(x+\varepsilon\delta_j)\sigma} + \text{h.c.}\Big)\vartheta^{-1} \\
&= \vartheta \sum_{X\in\Lambda_{\rm o},\ X_1\leq -1} \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{\nu} \sum_{\varepsilon=\pm}{}' (-t)\Big(e^{+i\alpha(\phi_X-\phi_{X+\varepsilon\delta_j})} a^*_{X\sigma} a^*_{X+\varepsilon\delta_j\sigma} + \text{h.c.}\Big)\vartheta^{-1} \\
&= \vartheta \sum_{X\in\Lambda_{\rm o},\ X_1\leq -1} \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{\nu} \sum_{\varepsilon=\pm}{}' (+t)\Big(e^{-i\alpha(\phi_{X+\varepsilon\delta_j}-\phi_X)} a^*_{X+\varepsilon\delta_j\sigma} a^*_{X\sigma} + \text{h.c.}\Big)\vartheta^{-1} \\
&= \vartheta T''_L \vartheta^{-1}. \qquad (3.46)
\end{aligned}
$$

Here, we used the fact that r maps even sites to odd sites, namely, if $x\in\Lambda_{\rm e}$, then $r(x)\in\Lambda_{\rm o}$. Besides, recall that ϑ is antilinear. □

Lemma 3.10 *For all* $\mathbf{h}_R\in\mathbb{R}^{\Lambda_R}$, *we define* $r(\mathbf{h}_R)=\{h_{r^{-1}(x)}\}_{x\in\Lambda_R}\in\mathbb{R}^{\Lambda_L}$. *We have the following:*

(i) $P''_R(\mathbf{h}_R)=\vartheta P''_L(r(\mathbf{h}_R))\vartheta^{-1}$.

(ii)

$$
\begin{aligned}
P''_{LR}(\mathbf{h}) = &-V\sum_{x\in\Lambda_{\rm e},\ x_1=0}(q_{x-\delta_1}-h_{x-\delta_1})\otimes\vartheta(q_{x-\delta_1}-h_x)\vartheta^{-1} \\
&-V\sum_{x\in\Lambda_{\rm e},\ x_1=L-1}(q_{x+\delta_1}-h_{x+\delta_1})\otimes\vartheta(q_{x+\delta_1}-h_x)\vartheta^{-1}. \qquad (3.47)
\end{aligned}
$$

Lemma 3.11 *We have* $K_R=\vartheta K_L\vartheta^{-1}$.

Proof. This immediately follows from (3.42). □

Proposition 3.12 *For all* $\mathbf{h}=(\mathbf{h}_L,\mathbf{h}_R)\in\mathbb{R}^{\Lambda}$, *let* $Z_\beta(\mathbf{h})=Z_\beta(\mathbf{h}_L,\mathbf{h}_R)=\text{Tr}[e^{-\beta H''_\Lambda(\mathbf{h})}]$. *Then we have*

$$
Z_\beta\big(\mathbf{h}_L,\mathbf{h}_R\big)^2\leq Z_\beta\big(\mathbf{h}_L,r^{-1}(\mathbf{h}_L)\big)Z_\beta\big(r(\mathbf{h}_R),\mathbf{h}_R\big). \qquad (3.48)
$$

Proof. Set

$$
\begin{aligned}
A &= T''_L+P''_L(\mathbf{h}_L)+K_L, \quad B=T''_L+P''_L(r(\mathbf{h}_R))+K_L, &(3.49)\\
C^{(1)}_{x,\pm} &= q_{x\pm\delta_1}-h_{x\pm\delta_1}, \quad D^{(1)}_{x,\pm}=q_{x\pm\delta_1}-h_x, &(3.50)\\
C^{(2)}_{x,\pm} &= D^{(2)}_{x,\pm}=e^{i\alpha\phi_{x\pm\delta_1}}a^*_{x\pm\delta_1\sigma} &(3.51)
\end{aligned}
$$

By Lemmas 3.9, 3.10 and 3.11, we see that $H''_\Lambda(\mathbf{h})$ has the form $A\otimes\mathbb{1}+\mathbb{1}\otimes\vartheta B\vartheta^{-1}-\sum_{x,\varepsilon,\sigma,\mu}\lambda_{x,\varepsilon,\mu}(C^{(\mu)}_{x,\varepsilon}\otimes\vartheta D^{(\mu)}_{x,\varepsilon}\vartheta^{-1}+C^{(\mu)*}_{x,\varepsilon}\otimes\vartheta D^{(\mu)*}_{x,\varepsilon}\vartheta^{-1})$ with $\lambda_{x,\varepsilon,\mu}\geq 0$. Thus, we can apply Theorem A.1. □

Corollary 3.13 *For all* $\mathbf{h}\in\mathbb{R}^{\Lambda}$, *we have* $Z_\beta(\mathbf{h})\leq Z_\beta(\mathbf{0})$.

Proof. We give a sketch only. First, let us clarify an instinctive meaning of the inequality (3.48), namely, the configurations $(\mathbf{h}_L, r^{-1}(\mathbf{h}_L))$ and $(r(\mathbf{h}_R), \mathbf{h}_R)$ are more "aligned" than the original configuration $\mathbf{h} = (\mathbf{h}_L, \mathbf{h}_R)$ because $(r(\mathbf{h}_R), \mathbf{h}_R)$ and $(\mathbf{h}_L, r^{-1}(\mathbf{h}_L))$ are invariant under the r-reflection.

For simplicity, assume that $Z_\beta\big(\mathbf{h}_L, r^{-1}(\mathbf{h}_L)\big) > Z_\beta\big(r(\mathbf{h}_R), \mathbf{h}_R\big)$. Proposition 3.12 concerns the reflection map r with respect to a plane $x_1 = -1/2$. However, there are many reflection maps with respect to other planes. Thus, we can apply similar arguments associated with another reflection map to $Z_\beta(\mathbf{h}_L, r^{-1}(\mathbf{h}_L))$. Then we obtain an inequality similar to (3.48): $Z_\beta(\mathbf{h}_L, r^{-1}(\mathbf{h}_L))^2 \le Z_\beta(\mathbf{h}_1)Z_\beta(\mathbf{h}_2)$. Point is that resulting configurations $\mathbf{h}_1$ and $\mathbf{h}_2$ are more aligned than $(\mathbf{h}_L, r^{-1}(\mathbf{h}_L))$. Repeating these procedures, we finally arrive at the most aligned configuration $\mathbf{h}_0 = \text{const.}$. Since $Z_\beta(\mathbf{h}_0) = Z_\beta(\mathbf{0})$, we obtain the result (see [4, 7] for details). □

3.4.3 Infrared bound

Let Δ be the discrete Laplacian on Λ given by

$$(\Delta \mathbf{h})_x = \sum_{j=1}^{\nu} (h_{x+\delta_j} + h_{x-\delta_j}) - 2\nu h_x \tag{3.52}$$

for all $\mathbf{h} = \{h_x\}_{x\in\Lambda} \in \mathbb{C}^\Lambda$. The following quantities will play essential roles:

$$g = \Big\langle \langle \mathbf{q}|(-\Delta)\mathbf{h}\rangle^* \langle \mathbf{q}|(-\Delta)\mathbf{h}\rangle \Big\rangle''_{\beta,\Lambda}, \tag{3.53}$$

$$b = \Big(\langle \mathbf{q}|(-\Delta)\mathbf{h}\rangle, \langle \mathbf{q}|(-\Delta)\mathbf{h}\rangle \Big)''_{\beta,\Lambda}, \tag{3.54}$$

$$c = \beta \Big\langle \Big[\langle \mathbf{q}|(-\Delta)\mathbf{h}\rangle, \Big[H''_\Lambda, \langle \mathbf{q}|(-\Delta)\mathbf{h}\rangle^* \Big]\Big] \Big\rangle''_{\beta,\Lambda}. \tag{3.55}$$

Here, we used the following notations:

- $\langle\cdot\rangle''_{\beta,\Lambda}$ is the thermal expectation associated with H''_Λ.
- $(A, B)''_{\beta,\Lambda}$ is the Duhamel two-point function associated with H''_Λ. Namely,

$$(A, B)''_{\beta,\Lambda} = (Z''_\beta)^{-1} \int_0^1 dx \mathrm{Tr}\big[e^{-x\beta H''_\Lambda} A^* e^{-(1-x)\beta H''_\Lambda} B\big], \tag{3.56}$$

$$Z''_\beta = \mathrm{Tr}\big[e^{-\beta H''_\Lambda}\big]. \tag{3.57}$$

- $\langle \mathbf{q}|(-\Delta)\mathbf{h}\rangle = \sum_{x\in\Lambda} q_x(-\Delta\mathbf{h})_x$.

First of all, we begin with the following lemma.

Lemma 3.14 *For all $\mathbf{h} \in \mathbb{C}^\Lambda$, we have*

$$b \le b_0, \tag{3.58}$$

where $b_0 = \dfrac{(\beta V)^{-1}}{2} \langle \mathbf{h}|(-\Delta)\mathbf{h}\rangle$. Here, $\langle\cdot|\cdot\rangle$ is the standard inner product on $\mathbb{C}^\Lambda$.

Proof. By Corollary 3.13, we have $d^2 Z_\beta(\lambda\mathbf{h})\Big/ d\lambda^2\Big|_{\lambda=0} \le 0$. Thus, we obtain (3.58) for all $\mathbf{h} \in \mathbb{R}^\Lambda$. Using the well-known fact $(A^*, A)''_{\beta,\Lambda} = (A_R, A_R)''_{\beta,\Lambda} + (A_I, A_I)''_{\beta,\Lambda}$ with $A_R = (A + A^*)/2$ and $A_I = (A - A^*)/2i$, we can extend (3.58) to complex $\mathbf{h}$. □

Lemma 3.15 *Let τ be a unitary operator on $\mathbb{C}^\Lambda$ given by $(\tau\mathbf{h})_x = \{(-1)^{\|x\|} h_x\}_{x\in\Lambda}$. For all $\mathbf{h} \in \mathbb{C}^\Lambda$, we have*

$$c \le c_0 \tag{3.59}$$

where $c_0 = 4\beta t\Big\langle(-\Delta)\mathbf{h}\Big|\tau(-\Delta)\tau^{-1}(-\Delta)\mathbf{h}\Big\rangle$.

Proof. Let $M = \tau(-\Delta)$. By direct computation, we have

$$\begin{aligned}&\Big[\langle\mathbf{q}|(-\Delta)\mathbf{h}\rangle, \Big[H''_\Lambda, \langle\mathbf{q}|(-\Delta)\mathbf{h}\rangle^*\Big]\Big]\\ &= \sum_{\langle x;y\rangle}\sum_{\sigma=\uparrow,\downarrow}(-t)\Big|(M\mathbf{h})_x - (M\mathbf{h})_y\Big|^2\big(e^{-i\alpha(\phi_x-\phi_y)}c^*_{x\sigma}c^*_{y\sigma} + \text{h.c.}\big).\end{aligned}$$

Hence, we have $c \le 4t\beta\langle(M\mathbf{h})|(-\Delta)(M\mathbf{h})\rangle = c_0$. This completes the proof. □

Proposition 3.16 *For all $\mathbf{h} \in \mathbb{C}^\Lambda$, we have*

$$g \le (2\pi)^{\nu/2}\gamma_1\langle\mathbf{h}|(-\Delta)\mathbf{h}\rangle + (2\pi)^{-\nu/2}\gamma_2\big\langle(-\Delta)\mathbf{h}|\tau^{-1}(-\Delta)\tau(-\Delta)\mathbf{h}\big\rangle. \tag{3.60}$$

Proof. Applying the Falk–Bruch inequality [5, 29], we have

$$g \le \frac{1}{2}\sqrt{bc}\coth\sqrt{\frac{c}{4b}}. \tag{3.61}$$

Since $\coth x \le 1 + \dfrac{1}{x}$, we have

$$g \le \frac{1}{2}\sqrt{bc} + b. \tag{3.62}$$

By Lemmas 3.14 and 3.15, it holds that

$$\sqrt{bc} \le \Big(\frac{t}{V}\Big)^{1/2}\langle\mathbf{h}|(-\Delta)\mathbf{h}\rangle + \frac{1}{2}\Big(\frac{t}{V}\Big)^{1/2}\big\langle(-\Delta)\mathbf{h}|\tau^{-1}(-\Delta)\tau(-\Delta)\mathbf{h}\big\rangle. \tag{3.63}$$

Thus, we obtain the desired result. □

Theorem 3.17 *Let $(2\pi)^{-\nu/2}c_\beta = \lim_{\|x\|\to\infty}\langle q_x q_o\rangle''_\beta$. We have*

$$\langle q_o^2\rangle''_\beta \le (2\pi)^{-\nu/2}c_\beta + \gamma_1\int_{\mathbb{T}^\nu}\frac{dp}{E(p)} + \gamma_2. \tag{3.64}$$

Proof. Let $G_{\beta,\Lambda}(x-y) = \langle q_x q_y \rangle''_{\beta,\Lambda}$. Let $E(p) = \sum_{j=1}^{\nu}(1-\cos p_j)$ and let $F(p) = \sum_{j=1}^{\nu}(1+\cos p_j)$. By the Fourier transformation, we see that

$$g = \frac{(2\pi)^\nu}{|\Lambda|}\sum_{p\in B_L} E(p)^2\Big\{(2\pi)^{\nu/2}\hat{G}_{\beta,\Lambda}(p)\Big\}|\hat{h}(p)|^2, \tag{3.65}$$

$$\langle \mathbf{h}|(-\Delta)\mathbf{h}\rangle = \frac{(2\pi)^\nu}{|\Lambda|}\sum_{p\in B_L} E(p)|\hat{h}(p)|^2, \tag{3.66}$$

$$\big\langle(-\Delta)\mathbf{h}|\tau^{-1}(-\Delta)\tau(-\Delta)\mathbf{h}\big\rangle = \frac{(2\pi)^\nu}{|\Lambda|}\sum_{p\in B_L} E(p)^2F(p)|\hat{h}(p)|^2, \tag{3.67}$$

where $\hat{h}(p) = (2\pi)^{-\nu/2}\sum_{x\in\Lambda}e^{-ix\cdot p}h_x$.

By inserting these formulas into (3.60) and taking $L\to\infty$, we obtain

$$\begin{aligned}&\int_{\mathbb{T}^\nu} dpE(p)^2(2\pi)^{\nu/2}\hat{G}_\beta(p)|\hat{h}(p)|^2\\ &\le (2\pi)^{\nu/2}\gamma_1\int_{\mathbb{T}^\nu} dpE(p)|\hat{h}(p)|^2 + (2\pi)^{-\nu/2}\gamma_2\int_{\mathbb{T}^\nu} dpF(p)E(p)^2|\hat{h}(p)|^2.\end{aligned} \tag{3.68}$$

From this, we know that $\hat{G}_\beta$ has the following form

$$\hat{G}_\beta(p) = a_\beta\delta(p) + I_\beta(p), \tag{3.69}$$

where $I_\beta(p)$ satisfies

$$I_\beta(p) \le \gamma_1\frac{1}{E(p)} + (2\pi)^{-\nu}\gamma_2F(p). \tag{3.70}$$

On the other hand, we have

$$\langle q_o^2\rangle''_\beta = (2\pi)^{-\nu/2}\int_{\mathbb{T}^\nu} dp\,\hat{G}_\beta(p) = (2\pi)^{-\nu/2}a_\beta + (2\pi)^{-\nu/2}\int_{\mathbb{T}^\nu} dpI_\beta(p). \tag{3.71}$$

Combining this with (3.70), we obtain

$$\langle q_o^2\rangle''_\beta \le (2\pi)^{-\nu/2}a_\beta + \gamma_1\int_{\mathbb{T}^\nu}\frac{dp}{E(p)} + \gamma_2. \tag{3.72}$$

Finally, we show that $a_\beta = c_\beta$. To this end, we observe that

$$\langle q_x q_o\rangle''_\beta = (2\pi)^{-\nu/2}\int_{\mathbb{T}^\nu} dpe^{-ix\cdot p}\hat{G}_\beta(p) = (2\pi)^{-\nu/2}a_\beta + (2\pi)^{-\nu/2}\int_{\mathbb{T}^\nu} dp\,e^{ip\cdot x}I_\beta(p). \tag{3.73}$$

By the Riemann–Lebesgue lemma, we know that $\lim_{\|x\|\to\infty}\int_{\mathbb{T}^\nu} dp\,e^{ix\cdot p}I_\beta(p) = 0$. Thus, we have $a_\beta = c_\beta$. □

3.5 Lower bound for $\langle q_o^2 \rangle''_\beta$

Lemma 3.18 *Assume that* $\nu V - U_{\rm eff} > 0$*. Let* $M_\Lambda = H''_\Lambda - K$*. We have*

$$\Big\langle -\frac{M_\Lambda}{|\Lambda|}\Big\rangle''_{\beta,\Lambda} \le 8\nu t + (\nu V - U_{\rm eff})\langle q_o^2 \rangle''_{\beta,\Lambda}. \tag{3.74}$$

Proof. First, remark that

$$-M_\Lambda = -T'' + (\nu V - U_{\rm eff})\sum_{x\in\Lambda} q_x^2 - \frac{1}{2}\sum_{\langle x;y\rangle} V(q_x - q_y)^2. \tag{3.75}$$

Since

$$\Bigg\langle \sum_{\langle x;y\rangle}(q_x - q_y)^2 \Bigg\rangle''_{\beta,\Lambda} \ge 0, \tag{3.76}$$

$$\langle q_x^2 \rangle''_{\beta,\Lambda} = \langle q_o^2 \rangle''_{\beta,\Lambda},\ \forall x \in \Lambda, \tag{3.77}$$

$$\big|\langle T'' \rangle''_{\beta,\Lambda}\big| \le 2t \sum_{\langle x;y\rangle}\sum_{\sigma} 1 = 8\nu t|\Lambda|, \tag{3.78}$$

we obtain the assertion in the lemma. □

Lemma 3.19 *We have*

$$\ln \mathrm{Tr}[e^{-\beta H''_\Lambda}] \ge \beta(\nu V - U_{\rm eff})|\Lambda|. \tag{3.79}$$

Proof. Let

$$\Psi = \Bigg[\prod_{x\in\Lambda} c_{x\uparrow}^* c_{x\downarrow}^* \tilde{\Omega}_{\rm f}\Bigg] \otimes \tilde{\Omega}_{\rm b}, \tag{3.80}$$

where $\tilde{\Omega}_{\rm f}$ (resp. $\tilde{\Omega}_{\rm b}$) is the Fock vacuum in $\mathfrak{F}$ (resp. $\mathfrak{P}$). Then we have

$$\langle \Psi | H''_\Lambda \Psi \rangle = -(\nu V - U_{\rm eff})|\Lambda|. \tag{3.81}$$

By the Peierls–Bogoliubov inequality [29], we have

$$\mathrm{Tr}[e^{-\beta H''_\Lambda}] \ge e^{-\beta\langle \Psi | H''_\Lambda \Psi\rangle} = e^{\beta(\nu V - U_{\rm eff})|\Lambda|}. \tag{3.82}$$

This completes the proof. □

Proposition 3.20 *We have*

$$\langle q_o^2 \rangle''_{\beta,\Lambda} \ge 1 - 8\nu t(\nu V - U_{\rm eff})^{-1} - (\nu V - U_{\rm eff})^{-1} \ln 4(1 - e^{-\beta\omega})^{-1}. \tag{3.83}$$

Proof. By Lemma B.1, we have

$$\ln \mathrm{Tr}[e^{-\beta H''_\Lambda}] \le \langle (-\beta M_\Lambda) \rangle''_{\beta,\Lambda} + \ln \mathrm{Tr}[e^{-\beta K}]. \tag{3.84}$$

Note that $\mathrm{Tr}[e^{-\beta K}] = 4^{|\Lambda|}(1 - e^{-\beta\omega})^{-|\Lambda|}$. Combining this with Lemmas 3.18 and 3.19, we obtain the desired result. □

3.6 Completion of proof of Theorem 2.2

By (3.64), (3.83) and the fact $\langle q_x q_o \rangle''_\beta = (-1)^{\|x\|} \langle q_x q_o \rangle_\beta$, we obtain the assertion in the theorem. □

A The Dyson–Lieb–Simon inequality

Let $\mathfrak{X}$ be a complex Hilbert space and let ϑ be an antilinear unitary operator in $\mathfrak{X}$. Let $A, B, C_j, D_j, j = 1, \dots, n$ be linear operators in $\mathfrak{X}$. Suppose that A and B are self-adjoint and bounded from below. Suppose that C_j and D_j are bounded. We will study the following Hamiltonian:

$$H(A, B, \mathbf{C}, \mathbf{D}) = H_0 - V, \tag{A.1}$$

$$H_0 = A \otimes \mathbb{1} + \mathbb{1} \otimes \vartheta B \vartheta^{-1}, \tag{A.2}$$

$$V = \sum_{j=1}^{n} \lambda_j (C_j \otimes \vartheta D_j \vartheta^{-1} + C_j^* \otimes \vartheta D_j^* \vartheta^{-1}). \tag{A.3}$$

$H(A, B, \mathbf{C}, \mathbf{D})$ is a self-adjoint operator bounded from below and acts in $\mathfrak{X} \otimes \mathfrak{X}$.

Theorem A.1 *Assume that* $e^{-\beta A}$ *and* $e^{-\beta B}$ *are trace class operators for all* $\beta > 0$*. Assume that* $\lambda_j \geq 0$ *for all* $j \in \{1, \dots, n\}$*. Let* $Z_\beta(A, B, \mathbf{C}, \mathbf{D}) = \mathrm{Tr}\big[e^{-\beta H(A,B,\mathbf{C},\mathbf{D})}\big]$, $\beta > 0$*. We have*

$$Z_\beta(A, B, \mathbf{C}, \mathbf{D})^2 \leq Z_\beta(A, A, \mathbf{C}, \mathbf{C}) Z_\beta(B, B, \mathbf{D}, \mathbf{D}). \tag{A.4}$$

Remark A.2 In [4], all matrix elements of A, B, C_j, D_j are assumed to be *real*. However, as pointed out in [20, 22], this assumption is unnecessary. This point is essential in the present paper. ♢

Proof. This theorem is proven in [22]. However, we present a sketch of proof for reader's convenience.

It sufficies to show the assertion when $\dim \mathfrak{X} < \infty$. For notational simplicity, we assume that C_j and D_j are self-adjoint and assume that $\lambda_j = 1/2$. By the Duhamel formula,

$$e^{-\beta H(A,B;\mathbf{C},\mathbf{D})} = \sum_{N \geq 0} \mathscr{D}_{N,\beta}(A, B; \mathbf{C}, \mathbf{D}), \tag{A.5}$$

$$\mathscr{D}_{N,\beta}(A, B; \mathbf{C}, \mathbf{D}) = \int_{S_N(\beta)} e^{-t_1 H_0} V e^{-t_2 H_0} \cdots e^{-t_N H_0} V e^{-(\beta - \sum_{j=1}^{N} t_j) H_0}, \tag{A.6}$$

where $\int_{S_N(\beta)} = \int_0^\beta \mathrm{d}t_1 \int_0^{\beta - t_1} \mathrm{d}t_2 \cdots \int_0^{\beta - \sum_{j=1}^{N-1} t_j} \mathrm{d}t_N$. Observe that

$$\begin{aligned} &\mathscr{D}_{N,\beta}(A, B; \mathbf{C}, \mathbf{D}) \\ &= \sum_{k_1, \dots, k_N \geq 1} \int_{S_N(\beta)} \Big[\mathscr{L}_{A;\mathbf{C}}\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big)\Big] \otimes \vartheta \Big[\mathscr{L}_{B;\mathbf{D}}\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big)\Big] \vartheta^{-1}, \end{aligned} \tag{A.7}$$

where $\mathbf{k}_{(N)} = (k_1, \dots, k_N) \in \mathbb{N}^N$, $\mathbf{t}_{(N)} = (t_1, \dots, t_N) \in \mathbb{R}_+^N$ and

$$\mathscr{L}_{X;\mathbf{Y}}\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big) = e^{-t_1 X} Y_{k_1} e^{-t_2 X} \cdots e^{-t_N X} Y_{k_N} e^{-(\beta - \sum_{j=1}^N t_j) X} \tag{A.8}$$

with $\mathbf{Y} = \{Y_j\}_j$. Note that

$$\mathrm{Tr}_{\mathfrak{X}\otimes\mathfrak{X}}[A \otimes \vartheta B \vartheta^{-1}] = \mathrm{Tr}_{\mathfrak{X}}[A]\big(\mathrm{Tr}_{\mathfrak{X}}[B]\big)^*. \tag{A.9}$$

By this fact, we obtain

$$\begin{aligned}
&\mathrm{Tr}_{\mathfrak{X}\otimes\mathfrak{X}}\Big[E \otimes \vartheta F \vartheta^{-1} \mathscr{D}_{N,\beta}(A, B; \mathbf{C}, \mathbf{D})\Big] \\
&= \sum_{k_1, \dots, k_N \geq 1} \int_{S_N(\beta)} \Big\{\mathrm{Tr}_{\mathfrak{X}}\Big[E \mathscr{L}_{A;\mathbf{C}}\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big)\Big]\Big\} \times \Big\{\mathrm{Tr}_{\mathfrak{X}}\Big[F \mathscr{L}_{B;\mathbf{D}}\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big)\Big]\Big\}^*.
\end{aligned} \tag{A.10}$$

Let us introduce an inner product by

$$\langle F, G \rangle_{N,\beta} = \sum_{k_1, \dots, k_N \geq 1} \int_{S_N(\beta)} F\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big) G\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big)^*. \tag{A.11}$$

In terms of this inner product, we have

$$\mathrm{Tr}_{\mathfrak{X}\otimes\mathfrak{X}}\Big[E \otimes \vartheta F \vartheta^{-1} \mathscr{D}_{N,\beta}(A, B; \mathbf{C}, \mathbf{D})\Big] = \Big\langle F^{(N)}_{A;\mathbf{C};E}, F^{(N)}_{B;\mathbf{D};F} \Big\rangle_{N,\beta}, \tag{A.12}$$

where

$$F^{(N)}_{X;\mathbf{Y};Z}\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big) = \mathrm{Tr}_{\mathfrak{X}}\Big[Z \mathscr{L}_{X;\mathbf{Y}}\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big)\Big]. \tag{A.13}$$

By the Schwartz inequality, we have

$$\begin{aligned}
\Big|\mathrm{Tr}_{\mathfrak{X}}\Big[E \otimes \vartheta F \vartheta^{-1}\, \mathrm{e}^{-\beta H(A,B,\mathbf{C},\mathbf{D})}\Big]\Big|^2 &= \Big|\sum_{N \geq 0} \Big\langle F^{(N)}_{A;\mathbf{C};E}, F^{(N)}_{B;\mathbf{D};F} \Big\rangle_{N,\beta}\Big|^2 \\
&\leq \Big(\sum_{N \geq 0} \|F^{(N)}_{A;\mathbf{C};E}\|^2_{N,\beta}\Big)\Big(\sum_{N \geq 0} \|F^{(N)}_{B;\mathbf{D};F}\|^2_{N,\beta}\Big).
\end{aligned} \tag{A.14}$$

Finally, we remark that

$$\begin{aligned}
\sum_{N \geq 0} \|F^{(N)}_{A;\mathbf{C};E}\|^2_{N,\beta} &= \sum_{N \geq 0} \sum_{k_1, \dots, k_N \geq 1} \int_{S_N(\beta)} \Big|\mathrm{Tr}_{\mathfrak{X}}\Big[E \mathscr{L}_{A;\mathbf{C}}\big(\mathbf{k}_{(N)}; \mathbf{t}_{(N)}\big)\Big]\Big|^2 \\
&= \sum_{N \geq 0} \mathrm{Tr}_{\mathfrak{X}\otimes\mathfrak{X}}\Big[E \otimes \vartheta E \vartheta^{-1} \mathscr{D}_{N,\beta}(A, A; \mathbf{C}, \mathbf{C})\Big] \\
&= \mathrm{Tr}_{\mathfrak{X}\otimes\mathfrak{X}}\Big[E \otimes \vartheta E \vartheta^{-1} e^{-\beta H(A,A;\mathbf{C},\mathbf{C})}\Big].
\end{aligned} \tag{A.15}$$

Combining (A.14) and (A.15), we obtain the assertion. □

B A useful lemma

Lemma B.1 *Let B, C be self-adjoint operators. Suppose that e^{-C} is a trace class operator and suppose that B is bounded. We have*

$$\ln \mathrm{Tr}\big[e^{-(B+C)}\big] \le \langle -B\rangle + \ln \mathrm{Tr}\big[e^{-C}\big], \tag{B.1}$$

where

$$\langle X\rangle = \mathrm{Tr}\big[Xe^{-(B+C)}\big] \Big/ \mathrm{Tr}\big[e^{-(B+C)}\big]. \tag{B.2}$$

Proof. For all $\lambda \ge 0$, let

$$f(\lambda) = \ln \mathrm{Tr}\big[e^{-(\lambda B+C)}\big]. \tag{B.3}$$

We have

$$f'(\lambda) = \langle -B\rangle_\lambda, \quad f''(\lambda) = (B, B)_\lambda - \langle B\rangle_\lambda^2, \tag{B.4}$$

where $\langle X\rangle_\lambda$ and $(X, Y)_\lambda$ are the thermal expectation and the Duhamel two-point function associated with $\lambda B + C$, respectively. Since $f''(\lambda) \ge 0$ by the basic property of the Duhamel two-point function, we have $f(1) \le f'(1) + f(0)$. □

References

[1] J. Bardeen, L. N. Cooper, J. R. Schrieffer, Theory of Superconductivity. Phys. Rev. 108 (1957), 1175-1204.

[2] R. A. Bari, Effects of short-range interactions on electron-charge ordering and lattice distortions in the localized state. Phys. Rev. B 3 (1971), 2662-2670.

[3] M. Capone, M. Fabrizio, C. Castellani, E. Tosatti, Colloquium: Modeling the unconventional superconducting properties of expanded A_3C_{60} fullerides. Rev. Mod. Phys. 81 (2009), 943-958.

[4] F. J. Dyson, E. H. Lieb, B. Simon, Phase transitions in quantum spin systems with isotropic and nonisotropic interactions. J. Stat. Phys. 18 (1978), 335-383.

[5] H. Falk, L. W. Bruch, Susceptibility and Fluctuation. Phys. Rev. 180 (1969), 442-444.

[6] J. K. Freericks, E. H. Lieb, Ground state of a general electron-phonon Hamiltonian is a spin singlet. Phys. Rev. B 51 (1995), 2812-2821.

[7] J. Fröhlich, R. Israel, E. H. Lieb, B. Simon, Phase transitions and reflection positivity. I. General theory and long range lattice models. Comm. Math. Phys. 62 (1978), 1-34.

[8] J. Fröhlich, R. Israel, E. H. Lieb, B. Simon, Phase transitions and reflection positivity. II. Lattice systems with short-range and Coulomb interactions. J. Stat. Phys. 22 (1980), 297-347.

[9] J. Fröhlich, B. Simon, T. Spencer, Infrared bounds, phase transitions and continuous symmetry breaking. Comm. Math. Phys. 50 (1976), 79-95.

[10] J. Glimm, A. Jaffe, T. Spencer, Phase transitions for φ_2^4 quantum fields. Comm. Math. Phys. 45 (1975), 203-216.

[11] J. Glimm, A. Jaffe, *Quantum physics. A functional integral point of view. Second edition.* Springer-Verlag, New York, 1987.

[12] A. Giuliani, V. Mastropietro, M. Porta, Universality of conductivity in interacting graphene. Comm. Math. Phys. 311 (2012), 317-355.

[13] J. Jedrzejewski, Electron charge ordering in the extended Hubbard model. Z. Phys. B Condensed Matter 48 (1982), 219-225.

[14] T. Kosugi, T. Miyake, S. Ishibashi, R. Arita, H. Aoki, First-principles structural optimization and electronic structure of the superconductor picene for various potassium doping levels. Phys. Rev. B 84 (2011), 214506.

[15] K. Kubo, T. Kishi, Rigorous bounds on the susceptibilities of the Hubbard model. Phys. Rev. B 41 (1990), 4866-4868.

[16] Y. Kubozono, H. Mitamura, X. Lee, X. He, Y. Yamanari, Y. Takahashi, Y. Suzuki, Y. Kaji, R. Eguchi, K. Akaike, T. Kambe, H. Okamoto, A. Fujiwara, T. Kato, T. Kosugi, H. Aoki, Metal-intercalated aromatic hydrocarbons: a new class of carbon-based superconductors. Phys. Chem. Chem. Phys. 13 (2011), 16476-16493

[17] I. G. Lang, Y. A. Firsov, Kinetic theory of semiconductors with low mobility. Sov. Phys. JETP 16 (1963), 1301.

[18] A. Lanzara, P. V. Bogdanov, X. J. Zhou, S. A. Kellar, D. L. Feng, E. D. Lu, T. Yoshida, H. Eisaki, A. Fujimori, K. Kishio, J.-I. Shimoyama, T. Noda, S. Uchida, Z. Hussain, Z.-X. Shen, Evidence for ubiquitous strong electron-phonon coupling in high-temperature superconductors. Nature 412 (2001), 510-514.

[19] E. H. Lieb, Two theorems on the Hubbard model. Phys. Rev. Lett. 62 (1989), 1201-1204.

[20] E. H. Lieb, B. Nachtergaele, Stability of the Peierls instability for ring-shaped molecules. Phys. Rev. B 51 (1995), 4777-4791.

[21] H. Löwen, Absence of phase transitions in Holstein systems. Phys. Rev. B 37 (1988), 8661-8667.

[22] T. Miyao, Self-dual cone analysis in condensed matter physics. Rev. Math. Phys. 23 (2011), 749-822.

[23] T. Miyao, Ground state properties of the SSH model. J. Stat. Phys. 149 (2012), 519-550.

[24] T. Miyao, Some rigorous results on the Holstein–Hubbard model. arXiv:1402.5202

[25] T. Miyao, Upper bounds on the charge susceptibility of many-electron systems coupled to the quantized radiation field. Lett. Math. Phys. 105 (2015), 1119-1133.

[26] Y. Murakami, P. Werner, N. Tsuji, H. Aoki, Ordered phases in the Holstein-Hubbard model: Interplay of strong Coulomb interaction and electron-phonon coupling. Phys. Rev. B 88 (2013), 125126.

[27] Y. Nomura, K. Nakamura, R. Arita, Ab initio derivation of electronic low-energy models for C_{60} and aromatic compounds. Phys. Rev. B 85 (2012), 155452.

[28] K. Osterwalder, R. Schrader, Axioms for Euclidean Green's functions. Comm. Math. Phys. 31 (1973), 83-112. Axioms for Euclidean Green's functions. II. With an appendix by Stephen Summers. Comm. Math. Phys. 42 (1975), 281-305.

[29] B. Simon, *The Statistical Mechanics of Lattice Gases, Volume I.* Princeton Univ Press, 1993

[30] Y. Takabayashi, A. Y. Ganin, P. Jegli, D. Aron, T. Takano, Y. Iwasa, Y. Ohishi, M. Takata, N. Takeshita, K. Prassides, M. J. Rosseinsky, The Disorder-Free Non-BCS Superconductor Cs_3C_{60} Emerges from an Antiferromagnetic Insulator Parent State. Science 323 (2009), 1585-1590.