Ground state properties of the Holstein-Hubbard model

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Abstract

We study the ground state properties of the Holstein-Hubbard model on some bipartite lattices at half-filling; The ground state is proved to exhibit ferrimagnetism whenever the electron-phonon interaction is not so strong. In addition, the antiferromagnetic long range order is shown to exist in the ground state. In contrast to this, we prove the absence of the long range charge order.

1 Introduction and results

To explain ferromagnetism from the Hubbard model is known as a challenging problem. Since the discovery of the Nagaoka-Thouless ferromagnetism [15, 22], there have been significant developments in this field: The ground state of the Hubbard model on some bipartite lattices at half-filling is shown to exhibit ferrimagnetism by Lieb [7]; Mielke [8, 10, 11, 12] and Tasaki [19, 20, 21] constructed rigorous examples of ferromagnetic ground states in certain Hubbard models. However, the origin of ferromagnetism is still incompletely understood.

In the presence of electron-electron Coulomb and electron-phonon interaction, correlated electron systems provide an attractive field of study. The Holstein-Hubbard model is a simple model describing the interplay of electron-electron and electron-phonon interactions. Despite its importance, rigorous studies of magnetic properties of the Holstein-Hubbard model are rare; see, e.g. [2]. Recently, Miyao proved that the ground state of the
Holstein-Hubbard model on some bipartite lattices at half-filling is unique whenever the electron-phonon interaction is not so strong \[13\].

In the present paper, we prove that the unique ground state exhibits ferrimagnetism (Theorem 3) as an important consequence of \[13\]. As far as we know, this is a first rigorous example of ferrimagnetism in the Holstein-Hubbard model. The idea of our proof is to extend Lieb’s method in \[7\]. In addition, we prove the existence of antiferromagnetic long range order (Theorem 6) and absence of the long range charge order (Theorem 7) in the ground state.

The Hamiltonian of the Holstein–Hubbard model on a finite lattice \(\Lambda\) is given by

\[
H_{HH} = \sum_{x,y \in \Lambda} \sum_{\sigma \in \{\uparrow, \downarrow\}} t_{xy} c_{x\sigma}^* c_{y\sigma} + \sum_{x,y \in \Lambda} \frac{U_{xy}}{2} (n_x - 1)(n_y - 1)
\]
\[+ \sum_{x,y \in \Lambda} g_{xy} n_x (b_y^* + b_y) + \sum_{x \in \Lambda} \omega b_x^* b_x, \tag{1}\]

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

\[
\{c_{x\sigma}, c_{x'\sigma'}^*\} = \delta_{\sigma\sigma'} \delta_{xx'}, \quad [b_x, b_{x'}^*] = \delta_{xx'}, \tag{2}\]

where \(\delta_{xy}\) is the Kronecker delta. \(n_x\) is the fermionic number operator at site \(x \in \Lambda\) defined by \(n_x = \sum_{\sigma \in \{\uparrow, \downarrow\}} n_{x\sigma}\), \(n_{x\sigma} = c_{x\sigma}^* c_{x\sigma}\). \(t_{xy}\) 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 \(\{g_{xy}\}, \{t_{xy}\}\) and \(\{U_{xy}\}\) are real symmetric \(|\Lambda| \times |\Lambda|\) matrices. The phonons are assumed to be dispersionless with energy \(\omega > 0\).

\(H_{HH}\) acts in the Hilbert space \(\mathcal{E} \otimes \mathfrak{P}\), where \(\mathcal{E} = \bigoplus_{n \geq 0} \Lambda^n (\ell^2(\Lambda) \otimes \ell^2(\Lambda))\), the fermionic Fock space and \(\mathfrak{P} = \bigoplus_{n \geq 0} \otimes_s^n \ell^2(\Lambda)\), bosonic Fock space. Here, \(\Lambda^n (\ell^2(\Lambda) \otimes \ell^2(\Lambda))\) indicates the \(n\)-fold antisymmetric tensor product of \(\ell^2(\Lambda) \otimes \ell^2(\Lambda)\), while \(\otimes_s^n \ell^2(\Lambda)\) indicates the \(n\)-fold symmetric tensor product.

\(H_{HH}\) is self-adjoint on \(\text{dom}(N_b)\) and bounded from below, where \(N_b = \sum_{x \in \Lambda} b_x^* b_x\) and \(\text{dom}(A)\) is the domain of the linear operator \(A\).

**Remark 1** At a first glance, it appears that the Coulomb interaction term in (1) is not standard; however, our Coulomb interaction coincides with the

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1 Let \(M = \{M_{xy}\}\) 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 \(x, y \in \Lambda\).
standard one when $\sum_{x \in \Lambda} U_{xy}$ is a constant independent of $y$; in this case, the Coulomb interaction in (1) becomes

$$\frac{1}{2} \sum_{x,y \in \Lambda} U_{xy}(n_x - 1)(n_y - 1) = \sum_{x \in \Lambda} U_{xx}n_x n_x + \frac{1}{2} \sum_{x \neq y} U_{xy}n_x n_y + \text{const.} \quad (3)$$

for every electron filling. A typical example satisfying the assumption about $U_{xy}$ is the case where $U_{xy} = U_0 \delta_{xy}$, see also Remark 5.

We say that there is a bond between $x$ and $y$ if $t_{xy} \neq 0$. We impose the following conditions on $\Lambda$:

(A. 1) $\Lambda$ is connected, namely, there is a connected path of bonds between every pair of sites.

(A. 2) $\Lambda$ is bipartite, namely, $\Lambda$ can be divided into two disjoint sites $A$ and $B$ such that $t_{xy} = 0$ whenever $x, y \in A$ or $x, y \in B$.

As to the electron-phonon interaction, we assume the following condition:

(A. 3) $\sum_{x \in \Lambda} g_{xy}$ is a constant independent of $y \in \Lambda$.

Remark 2

(i) A typical example satisfying (A. 3) is $g_{xy} = g_0 \delta_{xy}$, see also Remark 5.

(ii) Let us consider a linear chain of $2L$ atoms with periodic boundary conditions. We set $\Lambda = \{x_j\}_{j=1}^{2L}$. Assume that $|x_j - x_{j+1}|$ is constant for all $j$, where $x_{2L+1} = x_1$. If $g_{xy}$ is a function of $|x - y|$, i.e., $g_{xy} = f(|x - y|)$, then (A. 3) is satisfied. Similarly, if $\Lambda$ has a symmetric structure, like C$_{60}$ fullerene, then (A. 3) is fulfilled.

Let $N_{el}$ be the electron number operator given by $N_{el} = \sum_{x \in \Lambda} n_x$. Trivially, we have $\text{spec}(N_{el}) = \{0, 1, \ldots, 2|\Lambda|\}$, where $\text{spec}(N_{el})$ indicates the spectrum of $N_{el}$. We can decompose the Hilbert space $\mathcal{E} \otimes \mathcal{P}$ as

$$\mathcal{E} \otimes \mathcal{P} = \bigoplus_{n=0}^{2|\Lambda|} \mathcal{E}_n \otimes \mathcal{P}, \quad (4)$$

where $\mathcal{E}_n = \wedge^n(\ell^2(\Lambda) \oplus \ell^2(\Lambda))$, the $n$-electron subspace. Of course, $\mathcal{E}_n = \ker(N_{el} - n)$. The number of electron is conserved, i.e., $H_{HH}$ commutes with $N_{el}$. Hence, $H_{HH}$ can be decomposed as

$$H_{HH} = \bigoplus_{n=0}^{2|\Lambda|} H_{HH,n}, \quad H_{HH,n} = H_{HH} \upharpoonright \mathcal{E}_n \otimes \mathcal{P}, \quad (5)$$

More precisely, for any $x, y \in \Lambda$, there exist $x_1, \ldots, x_n$ such that $x_1 = x$, $x_n = y$ and $t_{x_1x_2}t_{x_2x_3} \cdots t_{x_{n-1}x_n} \neq 0$. 

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where $H_{\text{HH}} \mid \mathcal{E}_n \otimes \mathcal{P}$ is the restriction of $H_{\text{HH}}$ on $\mathcal{E}_n \otimes \mathcal{P}$. Because we are interested in the half-filled case, we will study the Hamiltonian

$$H := H_{\text{HH}, n = |\Lambda|}. \tag{6}$$

Let $S_x^{(+)} = c_x^+ c_x^\dagger$ and let $S_x^{(-)} = (S_x^{(+)})^*$. The spin operators are defined by

$$S(3) = \frac{1}{2} \sum_{x \in \Lambda} (n_x^\uparrow - n_x^\downarrow), \quad S^{(+)} = \sum_{x \in \Lambda} S_x^{(+)}, \quad S^{(-)} = \sum_{x \in \Lambda} S_x^{(-)}. \tag{7}$$

The total spin operator is defined by

$$S_{\text{tot}}^2 = (S^{(3)})^2 + \frac{1}{2} S^{(+)} S^{(-)} + \frac{1}{2} S^{(-)} S^{(+)} \tag{8}$$

with eigenvalues $S(S + 1)$. Let $\varphi$ be a vector in $\mathcal{E}_{n=|\Lambda|} \otimes \mathcal{P}$. If $\varphi$ is an eigenvector of $S_{\text{tot}}^2$ with $S_{\text{tot}}^2 \varphi = S(S + 1) \varphi$, then we say that $\varphi$ has total spin $S$. Main purpose in the present paper is to study the total spin $S$ for the ground states.

To state our results, we introduce the effective Coulomb interaction by

$$U_{\text{eff}, xy} = U_{xy} - \frac{2}{\omega} \sum_{z \in \Lambda} g_{xz} g_{yz}. \tag{9}$$

**Theorem 3** Assume that $|\Lambda|$ is even. Assume (A. 1) — (A. 3). Assume that $\{U_{\text{eff}, xy}\}$ is positive definite. Then the ground state of $H$ has total spin $S = \frac{1}{2} ||\Lambda|| - |A|$ and is unique apart from the trivial $(2S + 1)$-degeneracy.

**Remark 4**

(i) In general, the positive definitness of $\{U_{\text{eff}, xy}\}$ implies that the electron-phonon interaction is not so strong. To see this, consider the case where $U_{xy} = U_0 \delta_{xy}$ and $g_{xy} = g_0 \delta_{xy}$. In this case, $H$ becomes the standard Holstein-Hubbard model. $\{U_{\text{eff}, xy}\}$ is positive definite if and only if $|g_0| < \sqrt{\omega U_0/2}$, namely, the electron-phonon interaction is not so strong.

(ii) Theorem 3 claims that Lieb’s ferrimagnetism (Theorem 10) is stable whenever the electron-phonon interaction is not so strong.

(iii) Recently, Nagaoka’s theorem in the Hubbard model is extended to the Holstein-Hubbard model [14]. Theorem 3 is consistent with this result.

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A matrix $\{M_{xy}\}$ will be called positive definite if $\sum_{x,y \in \Lambda} \xi_x \xi_y M_{xy} > 0$ (strict inequality) holds for all $\{\xi_x\}_{x \in \Lambda} \in \mathbb{C}^{||\Lambda||} \setminus \{0\}$.
Remark 5 Let $\mathcal{P}$ be a Bravais lattice with the set of primitive vectors $\{a_1, \ldots, a_d\}$ ($d = 2, 3$). If $\Lambda$ is a subset of $\mathcal{P}$, then the positive definiteness of $\{U_{xy}\}$ can be expressed as follows: Let $\{b_1, \ldots, b_d\}$ be the set of primitive vectors of the reciprocal lattice of $\mathcal{P}$, i.e., $a_i \cdot b_j = 2\pi\delta_{ij}$. We set $\Lambda = \left\{ \sum_{j=1}^{d} n_j a_j \mid n_j = -L + 1, \ldots, L \right\}$ and $\Lambda^* = \left\{ \sum_{j=1}^{d} \ell_j b_j / L \mid \ell_j = -L + 1, \ldots, L \right\}$. Suppose that $g_{xy}$ and $U_{xy}$ are given by

$$g_{xy} = \frac{1}{L^d} \sum_{k \in \Lambda^*} G(k) e^{i k \cdot (x-y)}, \quad U_{xy} = \frac{1}{L^d} \sum_{k \in \Lambda^*} U(k) e^{i k \cdot (x-y)},$$

(10)

where $G(k)$ and $U(k)$ are real-valued continuous functions on $T_d = \left\{ \sum_{j=1}^{d} \theta_j b_j \mid 1 \leq \theta_j \leq 1 \right\}$ with $G(-k) = G(k)$ and $U(-k) = U(k)$. Since $\sum_{x \in \Lambda} g_{xy} = G(0)$ for all $y \in \Lambda$, (A. 3) is satisfied. In this case, we obtain

$$U_{\text{eff},xy} = \frac{1}{L^d} \sum_{k \in \Lambda^*} \left\{ U(k) - \frac{2}{\omega} G(k)^2 \right\} e^{i k \cdot (x-y)}.$$

(11)

If $U(k) > \frac{2}{\omega} G(k)^2$ for all $k \in T_d$, then $U_{\text{eff},xy}$ is positive definite for all $L \in \mathbb{N}$. It is noteworthy that this condition is uniform in the size. ♦

Let

$$\hat{S}_0^{(+)}, \quad \hat{S}_{Q}^{(+)}, \quad \hat{S}_{Q}^{(+)} = |\Lambda|^{-1/2} \sum_{x \in \Lambda} \gamma(x) S_{x}^{(+)},$$

(12)

where $\gamma(x) = 1$ if $x \in A$, $\gamma(x) = -1$ if $x \in B$. The correlation functions are given by

$$m(k) = \left\langle \hat{S}_k^{(+)}(\hat{S}_k^{(+)})^* \right\rangle$$

(13)

for $k = 0$ or $Q$, where $\langle \cdot \rangle$ is the ground state expectation.

**Theorem 6** Assume that $|\Lambda|$ is even. Assume (A. 1)—(A. 3). Assume that $\{U_{\text{eff},xy}\}$ is positive definite. If $||A| - |B|| = \text{const.} |\Lambda|$, then

$$m(Q) \geq m(0) = O(|\Lambda|).$$

(14)

Thus, the antiferromagnetic and ferrimagnetic long range order coexist in the ground state.
Finally, we present a theorem on the charge susceptibility. Suppose that that \( \Lambda, g_{xy} \) and \( U_{xy} \) are given in Remark 5. Let \( q_x = n_x - 1 \). The charge susceptibility (at \( \beta = \infty \)) with the wave vector \( k \) is given by

\[
\chi_k = \langle \hat{q}_k (H - E)^{-1} \hat{q}_{-k} \rangle, \tag{15}
\]

where \( \hat{q}_k = L^{-d/2} \sum_{x \in \Lambda} e^{-ik \cdot x} q_x \) and \( E \) is the ground state energy of \( H \).

**Theorem 7** Assume that \(|\Lambda|\) is even. Assume that \( \{ U_{\text{eff},xy} \} \) is positive semidefinite\(^4\), that is, \( U(k) \geq \frac{2}{\omega} G(k)^2 \) for all \( k \in T_d \). Then we have

\[
\chi(k) \leq \frac{1}{U_{\text{eff}}(k)}, \tag{16}
\]

where \( U_{\text{eff}}(k) = U(k) - \frac{2}{\omega} G(k)^2 \). Thus, if there exists a constant \( c_0 > 0 \) such that \( U_{\text{eff}}(k) \geq c_0 \) for all \( k \in T_d \), then there is no long range charge order.

**Remark 8** Theorems 6 and 7 suggest that coexistence of the ferrimagnetic and charge long range orders would be impossible. For instance, consider the model on the Lieb lattice with \( U_{xy} = U_0 \delta_{xy} \) and \( g_{xy} = g_0 \delta_{xy} \). Suppose that \( |g_0| < \sqrt{\omega U_0/2} \). By Theorem 6, we have

\[
\chi(k) \leq (U_0 - 2g_0^2/\omega)^{-1}, \tag{17}
\]

which implies the absence of the long range charge order. On the other hand, Theorem 6 claims the coexistence of the ferrimagnetic and antiferromagnetic long range orders. 

\[\Diamond\]

### 2 Proofs

#### 2.1 Preliminaries: An extension of Lieb’s theorem

We denote the spectrum of \( S^{(3)} \) by \( \text{spec}(S^{(3)}) \). Remark that \( \text{spec}(S^{(3)}) = \{-|\Lambda|/2, -|\Lambda|/2 + 1, \ldots, |\Lambda|/2\} \). For each \( M \in \text{spec}(S^{(3)}) \), we set

\[
\mathcal{H}_M := (\mathcal{E}_{n=|\Lambda|} \otimes \mathcal{P}) \cap \ker (S^{(3)} - M). \tag{18}
\]

We call \( \mathcal{H}_M \) the \( S^{(3)} = M \) subspace.

The following theorem is a basic input in the present paper.

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\(^4\) A matrix \( \{ M_{xy} \} \) will be called positive semidefinite if, for all \( \{ \xi_x \}_{x \in \Lambda} \in \mathbb{C}^{|\Lambda|}, \sum_{x,y \in \Lambda} \xi_x \xi_y M_{xy} \geq 0 \) holds.
Theorem 9 \cite{13} Assume that $|\Lambda|$ is even. Assume (A. 1)–(A. 3). Assume that $\{U_{\text{eff},xy}\}$ is positive definite. For each $M \in \{-|\Lambda|/2, -|\Lambda|/2 + 1, \ldots, |\Lambda|/2\}$, the ground state of $H$ is unique in each $S^{(3)} = M$ subspace. Let $\varphi_M$ be the unique ground state of $H$ in the $S^{(3)} = M$ subspace. Then the following holds:

$$
\langle \varphi_M | S_x^+ S_y^- | \varphi_M \rangle \begin{cases} > 0 & \text{if } x, y \in A \text{ or } x, y \in B \\ < 0 & \text{otherwise} \end{cases} \quad (19)
$$

From Theorem 9, we can derive an extension of Lieb’s theorem \cite{7}. Let $H_\text{H}$ be the extended Hubbard model defined by

$$
H_\text{H} = \sum_{x,y \in \Lambda} \sum_{\sigma \in \{\uparrow, \downarrow\}} t_{xy} c_{x\sigma}^* c_{y\sigma} + \sum_{x,y \in \Lambda} \frac{U_{xy}}{2} (n_x - 1)(n_y - 1). \quad (20)
$$

Theorem 10 Assume that $|\Lambda|$ is even. Assume (A. 1)–(A. 3). Assume that $\{U_{xy}\}$ is positive definite. Then the ground state of $H_\text{H}$ has total spin $S = \frac{1}{2}|B| - |A|$ and is unique apart from the trivial $(2S + 1)$-degeneracy.

Proof. We provide a sketch of the proof only. We apply Lieb’s argument in \cite{7}.

Since $S^{(3)}$ and $S^2_\text{tot}$ are conserved, we work in the $S^{(3)} = 0$ subspace. By putting $g_{xy} = 0$ in Theorem 9 we know that the ground state of $H_\text{H}$ in the $S^{(3)} = 0$ subspace is unique. For each $U_0 \geq 0$, let $H_\text{H}(U_0) = H_\text{H} + \sum_{x \in \Lambda} U_0(n_x - 1)^2$. Since $\{U_{xy}\}$ is positive definite, so is $\{U_{xy} + 2U_0 \delta_{xy}\}$. Thus, the ground state of $H_\text{H}(U_0)$ in the $S^{(3)} = 0$ subspace is unique for all $U_0 \geq 0$. By the continuity, the value of $S$ of the ground state of $H_\text{H}(U_0)$ in the $S^{(3)} = 0$ subspace is independent of $U_0$.

Let $P = \prod_{x \in \Lambda} (n_x^\uparrow - n_x^\downarrow)^2$. Then it is known that

$$
\| \{ \mathcal{W} U_0 H_\text{H}(U_0) \mathcal{W}^{-1} - h \} P \| \rightarrow 0 \quad \text{as } U_0 \rightarrow \infty, \quad (21)
$$

where $h$ is the antiferromagnetic Heisenberg model defined by

$$
h = \sum_{x,y \in \Lambda} J_{xy}(S_x \cdot S_y - \frac{1}{4}) \quad (22)
$$

with $J_{xy} = 2t_{xy}^2$ and $\mathcal{W}$ is the Schrieffer-Wolff transformation. By Marshall-Lieb-Mattis theorem \cite{6}, the ground state of $hP$ is unique and this state has total spin $S = \frac{1}{2}|A| - |B|$. Since the ground state of $\mathcal{W} U_0 H_\text{H}(U_0) \mathcal{W}^{-1}$ converges to that of $hP$, the value $S$ of the ground state of $H_\text{H}(U_0)$ must be identical to that of $hP$. \hfill \Box
2.2 Proof of Theorem 3

In this proof, we work in the $S^{(3)} = 0$ subspace, because $S^{(3)}$ and $S_{\text{tot}}^2$ are conserved. Because the boson operators are unbounded, the proof has to be addressed carefully.

Our proof is an extension of Lieb’s argument in [7]. For each $\theta \in [1, \infty)$, let $H_\theta$ be the Hamiltonian $H$ with $\omega$ replaced by $\theta \omega$. Of course, $H_{\theta=1} = H$.

**Lemma 11** The ground state of $H_\theta$ in the $S^{(3)} = 0$ subspace is unique for all $\theta \geq 1$.

**Proof.** By Theorem 9, it suffices to show that $\{U_{xy} - \frac{2}{\theta \omega} \sum_{z \in \Lambda} g_{xz} g_{yz}\}_{x,y}$ is positive definite for all $\theta \geq 1$.

First, we claim that the matrix $\{\frac{2}{\omega} \sum_{z \in \Lambda} g_{xz} g_{yz}\}_{x,y}$ is positive semidefinite. To see this, let

$$M_{xy} = \frac{2}{\omega} \sum_{z \in \Lambda} g_{xz} g_{yz}. \quad (23)$$

Clearly,

$$\sum_{x,y \in \Lambda} \xi_x \xi_y M_{xy} = \frac{2}{\omega} \sum_{z \in \Lambda} \left| \sum_{x \in \Lambda} \xi_x g_{zx} \right|^2 \geq 0 \quad (24)$$

for all $\{\xi_x\} \in \mathbb{C}^{\Lambda}$. Hence, $\{M_{xy}\}$ is positive semidefinite.

Since $\{U_{\text{eff},xy}\}$ is positive definite, we have $\sum_{x,y \in \Lambda} \xi_x \xi_y U_{\text{eff},xy} > 0$ for all $\{\xi_x\}_{x \in \Lambda} \in \mathbb{C}^{\Lambda} \setminus \{0\}$. Therefore, we obtain

$$\sum_{x,y \in \Lambda} \xi_x \xi_y (U_{xy} - \theta^{-1} M_{xy}) = \sum_{x,y \in \Lambda} \xi_x \xi_y U_{\text{eff},xy} + (1 - \theta^{-1}) \sum_{z,y \in \Lambda} \xi_x \xi_y M_{xy} > 0 \quad (25)$$

for all $\{\xi_x\}_{x \in \Lambda} \in \mathbb{C}^{\Lambda} \setminus \{0\}$. Accordingly, $\{U_{xy} - \theta^{-1} M_{xy}\}$ is positive definite for all $\theta \geq 1$. □

The Lang-Firsov transformation [5] is defined by $e^L$ with

$$L = (\theta \omega)^{-1} \sum_{x,y \in \Lambda} g_{xy} n_x (b^*_y - b_y). \quad (26)$$
Set $H'_\theta = e^{L} H_\theta e^{-L}$. We have

$$H'_\theta = \sum_{x,y \in \Lambda} \sum_{\sigma} t_{xy} e^{i \Phi_{xy}} c_{x\sigma} c_{y\sigma} + \theta \omega N_b +$$

$$+ \sum_{x,y \in \Lambda} \left( U_{xy} - \frac{2}{\theta \omega} \sum_{z \in \Lambda} g_{xz} g_{yz} \right) (n_x - 1)(n_y - 1), \quad (27)$$

where $\Phi_{xy} = -i(\theta \omega)^{-1} \sum_{z \in \Lambda} (g_{xz} - g_{yz})(b^*_z - b_z)$.

We rewrite $H'_\theta$ as $H'_\theta = H_H + \Delta_\theta + \theta \omega N_b$, where

$$\Delta_\theta = \sum_{x,y \in \Lambda} \sum_{\sigma \in \{\uparrow, \downarrow\}} t_{xy} (e^{i \Phi_{xy}} - 1) c_{x\sigma}^* c_{y\sigma} - \sum_{x,y \in \Lambda} \theta^{-1} M_{xy} (n_x - 1)(n_y - 1), \quad (28)$$

where $M_{xy}$ is given by (23)

**Lemma 12** Let $K_\theta = H_H + \theta \omega N_b$. We have

$$\| \Delta_\theta (K_\theta - z)^{-1} \| \leq C \theta^{-1} \left( 1 + \frac{1 + |z|}{|\text{Im} z|} \right) \quad (29)$$

for all $z \in \mathbb{C} \setminus \mathbb{R}$, where $C$ is a positive constant independent of $\theta$ and $z$.

**Proof.** Let

$$T = \sum_{x,y \in \Lambda} \sum_{\sigma \in \{\uparrow, \downarrow\}} t_{xy} (e^{i \Phi_{xy}} - 1) c_{x\sigma}^* c_{y\sigma}. \quad (30)$$

Since $\|(e^{i A} - 1) \phi\| \leq \|A \phi\|$ for any self-adjoint operator $A$, we have

$$\|T \phi\| \leq C_1 \sum_{x,y \in \Lambda} \| \Phi_{xy} \phi \|, \quad \phi \in \text{dom}(N_b) \quad (31)$$

where $C_1$ is independent of $\theta$. Using the well-known bounds $^5$: $\|b_x \phi\| \leq \|(N_b + 1) \phi\|$ and $\|b_x^* \phi\| \leq \|(N_b + 1) \phi\|$, we have

$$\|\Phi_{xy} \phi\| \leq C_2 \theta^{-1} \|(N_b + 1) \phi\|, \quad (34)$$

$^5$ Proof of the bounds. Observe that

$$\|b_x \phi\|^2 = \langle \phi | b_x^* b_x \phi \rangle \leq \langle \phi | N_b \phi \rangle \leq \|N_b \phi\|^2. \quad (32)$$

On the other hand, by the commutation relation $[b_x, b_x^*] = 1$, we have

$$\|b_x^* \phi\|^2 = \|\phi\|^2 + \|b_x \phi\|^2 \leq \|\phi\|^2 + \|N_b \phi\|^2. \quad (33)$$

Since $\|N_b \phi\| \leq \|(N_b + 1) \phi\|$ and $\|\phi\|^2 + \|N_b \phi\|^2 \leq \|(N_b + 1) \phi\|^2$, we obtain the desired bounds.
where $C_2$ is a positive constant independent of $\theta$. Combining (31) and (34), we have

$$
\|T\phi\| \leq C_3 \theta^{-1} \|(N_b + 1)\phi\|, \quad (35)
$$

where $C_3$ is a positive constant independent of $\theta$.

Since

$$
N_b = (\omega \theta)^{-1} \{ (K_\theta - z) - (H_H - z) \}, \quad (36)
$$

we have

$$
\|(N_b + 1)\phi\| \leq (\theta \omega)^{-1} \{ \|(K_\theta - z)\phi\| + (\|H_H\| + 1 + |z|)\|\phi\| \}. \quad (37)
$$

Hence,

$$
\|T\phi\| \leq C_3 \omega^{-1} \theta^{-2} \{ \|(K_\theta - z)\phi\| + (\|H_H\| + 1 + |z|)\|\phi\| \}. \quad (38)
$$

Because $\|\sum_{x,y \in \Lambda} \theta^{-1} M_{xy} (n_x - 1)(n_y - 1)\| \leq C_4 \theta^{-1}$ with $C_4$, a positive constant independent of $\theta$, we have

$$
\|\Delta_\theta \phi\| \leq \theta^{-1} C \left\{ \|(K_\theta - z)\phi\| + (\|H_H\| + 1 + |z|)\|\phi\| \right\}. \quad (39)
$$

Using $\|(K_\theta - z)^{-1}\| \leq |\Im z|^{-1}$, we obtain the desired bound. $\Box$

**Lemma 13** For all $z \in \mathbb{C} \backslash \mathbb{R}$, we have

$$
\lim_{\theta \to \infty} \|(H_H - z)^{-1} \otimes P_\Omega - (H_\theta' - z)^{-1}\| = 0, \quad (40)
$$

where $P_\Omega = |\Omega\rangle \langle \Omega|$ with $\Omega$, the bosonic Fock vacuum.

**Proof.** By Lemma 12 and the fact $\|(H_\theta' - z)^{-1}\| \leq |\Im z|^{-1}$, we have

$$
\|(H_\theta' - z)^{-1} - (K_\theta - z)^{-1}\| = \|(H_\theta' - z)^{-1} \Delta_\theta(K_\theta - z)^{-1}\|
\leq C \theta^{-1} |\Im z|^{-1} \left( 1 + \frac{1 + |z|}{|\Im z|} \right) \to 0 \quad (41)
$$

as $\theta \to \infty$ for every $z \in \mathbb{C} \backslash \mathbb{R}$.

On the other hand, we obtain that

$$
\|(K_\theta - z)^{-1} - (H_H - z)^{-1} \otimes P_\Omega\| \to 0 \quad (42)
$$
as \( \theta \to \infty \). To see this, we decompose the \( S^{(3)} = 0 \) subspace as

\[
\mathcal{H}_{M=0} = \bigoplus_{n=0}^{\infty} \mathcal{K}_n, \quad \mathcal{K}_n = \mathcal{H}_{M=0} \cap \ker(N_b - n).
\]  

(43)

\( \mathcal{K}_n \) is called the \( n \) phonon subspace. Corresponding to (43), we have

\[
\mathcal{K}_\theta = \bigoplus_{n=0}^{\infty} \left( H_H + \theta \omega n \right),
\]

(44)

which implies

\[
(K_\theta - z)^{-1} = \bigoplus_{n=0}^{\infty} (H_H + \theta \omega n - z)^{-1}
\]

(45)

for all \( z \in \mathbb{C} \setminus \mathbb{R} \). Let \( e \) be the lowest energy of \( H_H \) in the \( S^{(3)} = 0 \) subspace. If \( \theta \) is large enough such that \( e + \theta \omega - |\text{Re} z| > 0 \), we obtain

\[
\| (H_H + \theta \omega N_b - z)^{-1} \| \leq (e + \theta \omega - |\text{Re} z|)^{-1}
\]

(46)

for all \( n \geq 1 \). Therefore,

\[
\| (K_\theta - z)^{-1} - (H_H - z)^{-1} \otimes P_\Omega \| = \sup_{n \geq 1} \| (H_H + \theta \omega n - z)^{-1} \|
\]

\[
\leq (e + \theta \omega - |\text{Re} z|)^{-1} \to 0
\]

(47)

as \( \theta \to \infty \) for \( z \in \mathbb{C} \setminus \mathbb{R} \).

By (41) and (42), we obtain (40). \( \square \)

**Lemma 14** Let \( E_0(\theta) \) and \( E_1(\theta) \) be the ground state energy and the first excited energy of \( H_\theta \) in the \( S^{(3)} = 0 \) subspace, respectively. In addition, let \( E_0 \) and \( E_1 \) be the ground state energy and the first excited energy of \( H_H \) in the \( S^{(3)} = 0 \) subspace, respectively.

(i) \( E_0(\theta) \) converges to \( E_0 \), and \( E_1(\theta) \) converges to \( E_1 \) as \( \theta \to \infty \), respectively.

(ii) \( E_0(\theta) \) and \( E_1(\theta) \) are continuous in \( \theta \).

**Proof.** (i) follows from Lemma 13.

(ii) Note that dom(\( H_\theta \)) = dom(\( N_b \)) for all \( \theta \). In addition, \( H_\theta \phi \) is a vector-valued analytic function of \( \theta \) for all \( \phi \in \text{dom}(N_b) \). Thus, \( H_\theta \) is an analytic family of type (A) \cite{17} in a neighborhood of \([1, \infty) \subset \mathbb{C} \). By \cite{17} Theorem XII. 13, \( E_0(\theta) \) and \( E_1(\theta) \) are analytic, in particular, continuous in \( \theta \). \( \square \)
Lemma 15 Set $\delta := \inf_{\theta \geq 1} |E_1(\theta) - E_0(\theta)|$. We have $\delta > 0$.

Proof. We claim that $E_0(\theta) \neq E_1(\theta)$ for all $\theta \geq 1$. Indeed, assume that there exists a $\theta_0 \geq 1$ such that $E_0(\theta_0) = E_1(\theta_0)$. Then the uniqueness of the ground states is broken at $\theta = \theta_0$, which contradicts with Lemma 11. Because $E_1 - E_0 > 0$, we get $\delta > 0$ by Lemma 14. □

Let $\psi_\theta$ be the ground state of $H'_\theta$ and let $\psi$ be the ground state of $H_H$ in the $S^{(3)} = 0$ subspace. Remark that these are unique ground states of $H'_\theta$ and $H_H$ by Lemma 11.

Lemma 16 Let $S_\theta$ be the total spin of $\psi_\theta$: $S_{\text{tot}}^2 \psi_\theta = S_\theta(S_\theta + 1) \psi_\theta$. The value of $S_\theta$ is independent of $\theta \geq 1$.

Proof. First, we claim that $\psi_\theta$ is continuous in $\theta$, namely,

$$\lim_{\theta' \to \theta} \|\psi_\theta - \psi_{\theta'}\| = 0. \quad (48)$$

Indeed, since $H_\theta \phi$ is continuous in $\theta$ for all $\phi \in \text{dom}(N_h)$, $(H_\theta - z)^{-1} \phi$ is continuous in $\theta$ for all $\phi \in \text{dom}(N_h)$ by [16, Theorem VIII 25]. Here, we used the fact that $\text{dom}(H_\theta) = \text{dom}(N_h)$ for all $\theta \geq 1$. Thus, applying [16, Theorem VIII 24], we conclude (48).

Since $S_{\text{tot}}^2$ is bounded, we have

$$\left| S_\theta(S_\theta + 1) - S_{\theta'}(S_{\theta'} + 1) \right| \leq \left\| S_{\text{tot}}^2 \psi_\theta - S_{\text{tot}}^2 \psi_{\theta'} \right\|$$

$$\leq \left\| S_{\text{tot}}^2 (\psi_\theta - \psi_{\theta'}) \right\|$$

$$\leq \left\| S_{\text{tot}}^2 \right\| \|\psi_\theta - \psi_{\theta'}\| \to 0 \quad (49)$$

as $\theta \to \theta'$. Thus, $S_\theta$ is continuous in $\theta$. On the other hand, because $S_\theta$ takes discrete values, it must be independent of $\theta \geq 1$. □

Completion of proof of Theorem 3

First, we remark the following formula:

$$|\psi_\theta \rangle \langle \psi_\theta| = \frac{i}{2\pi} \oint_{|E - E_0| = \delta/2} (H'_\theta - E)^{-1} dE \quad \text{for all } \theta \geq 1, \quad (50)$$

$$|\psi \rangle \langle \psi| \otimes P_N = \frac{i}{2\pi} \oint_{|E - E_0| = \delta/2} (H_H - E)^{-1} \otimes P_N dE, \quad (51)$$
where \( \delta \) is given in Lemma 15. By (40), (50) and (51), we have \( \| \psi_\theta - \psi \otimes \Omega \| \to 0 \) as \( \theta \to \infty \). Recall that the value of \( S \) of \( \psi_\theta \) must be independent of \( \theta \) by Lemma 16. Since the ground state \( \psi \otimes \Omega \) has spin \( S = \frac{1}{2} |B| - |A| \) by Theorem 10, so does \( \psi_\theta \) due to the continuity. To see this, suppose that \( \psi_\theta \) has total spin \( S' \) for all \( \theta \geq 1 \). By Lemma 16, \( S' \) is independent of \( \theta \). We have
\[
|S(S + 1) - S'(S' + 1)| \leq \| S_{tot}^2(\psi_\theta - \psi \otimes \Omega) \| \\
\leq \| S_{tot}^2\| \| \psi_\theta - \psi \otimes \Omega \| \\
\to 0
\]
(52)
as \( \theta \to \infty \). Hence, \( S' = S \). \( \square \)

### 2.3 Proof of Theorem 6

We follow [18]. By Theorem 9, we obtain that
\[
m(0) = |\Lambda|^{-1} \sum_{x,y} \langle S_x^+ S_y^- \rangle \\
\leq |\Lambda|^{-1} \sum_{x,y} \gamma(x) \gamma(y) \langle S_x^+ S_y^- \rangle \\
= m(Q).
\]
Since \( m(0) = O(\Lambda) \) by Theorem 3, we conclude the assertions in Theorem 6. \( \square \)

### 2.4 Proof of Theorem 7

We provide a sketch only. We apply Kubo-Kishi argument [4], which originates from [1], see also [3]. For each \( h = \{ h_x \}_{x \in \Lambda} \in \mathbb{R}^\Lambda \), let \( H'(h) \) be the Hamiltonian \( H'_{y=1} \) with \( U_{eff} = \frac{1}{2} \sum_{x,y \in \Lambda} U_{eff,xy}(n_{x\uparrow} - n_{x\downarrow})(n_{y\uparrow} - n_{y\downarrow}) \) replaced by \( U_{eff}(h) = \frac{1}{2} \sum_{x,y \in \Lambda} U_{eff,xy}(n_{x\uparrow} - n_{x\downarrow} + h_x)(n_{y\uparrow} - n_{y\downarrow} + h_y) \). Clearly, we have \( H'(0) = H'_{y=1} \). We denote by \( \mathcal{H} \) the \( S(3) = 0 \) subspace. Let \( Z_\beta(h) = \text{Tr}_\mathcal{H}[e^{-\beta H'(h)}] \). Then we can show that \( Z_\beta(h) \leq Z_\beta(0) \), see [13] for details. This implies \( E(0) \leq E(h) \), where \( E(h) \) is the ground state energy of \( H'(h) \) in the \( S(3) = 0 \) subspace. Thus, we get \( d^2E(\lambda h)/d\lambda^2|_{\lambda=0} \leq 0 \), which implies Theorem 7. \( \square \)

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