Stability of magnetism in the Hubbard model

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Abstract

I will report the stabilities of the Nagaoka theorem and Lieb theorem in the Hubbard model, even if the influence of phonons and photons is taken into account.

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Background

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A brief history

- Magnets have a long history, e.g., Chinese writing dating back to 4000 B.C. mention magnetite, ancient Greeks knew magnetite, etc.
- The origin of ferromagnetism in material has been a mystery.
- Modern approach was initiated by Kanamori, Gutzwiller, and Hubbard.
  They studied a simple tight-binding model, called the **Hubbard model**.
- **Nagaoka’s ferromagnetism** (1965):
  A first rigorous result about ferromagnetism in the Hubbard model. (Cf. D. J. Thouless, 1965)
- **Lieb’s ferrimagnetism** (1989):
  A rigorous example of ferrimagnetism in the Hubbard model.
- Mielke, Tasaki’s ferromagnetism (1991–):
  Construction of flat-band ferromagnetism
Motivation

- Electrons always interact with phonons (or photons) in actual metals.
- On the other hand, ferromagnetism is experimentally observed in various metals and has a wide range of uses in daily life.

Motivation

If Nagaoka’s and Lieb’s theorems contain an essence of real ferromagnetism, their theorems should be stable under the influence of the electron-phonon (or electron-photon) interaction.
The Hubbard model

The Hubbard model on \( \Lambda \):

\[
H_H = \sum_{x,y \in \Lambda} \sum_{\sigma = \uparrow, \downarrow} t_{xy} c_{x\sigma}^* c_{y\sigma} + \sum_{x,y \in \Lambda} \frac{U_{xy}}{2} (n_x - 1)(n_y - 1)
\]

- \( \Lambda \): finite lattice
- \( c_{x\sigma} \): the electron annihilation operator at site \( x \);
  \[ \{ c_{x\sigma}, c_{y\sigma'}^* \} = \delta_{xy} \delta_{\sigma\sigma'} \]
- \( n_x \): the electron number operator at site \( x \in \Lambda \) given by \( n_x = \sum_{\sigma = \uparrow, \downarrow} n_{x\sigma} \), \( n_{x\sigma} = c_{x\sigma}^* c_{x\sigma} \).
- \( t_{xy} \): the hopping matrix.
- \( U_{xy} \): the energy of the Coulomb interaction.
\( \{ t_{xy} \} \) and \( \{ U_{xy} \} \) are real symmetric \(|\Lambda| \times |\Lambda|\) matrices.

- \( N \)-electron Hilbert space:

\[
\mathcal{E}_N = \bigwedge^N (\ell^2(\Lambda) \oplus \ell^2(\Lambda)).
\]

\( \bigwedge^n (\ell^2(\Lambda) \oplus \ell^2(\Lambda)) \) indicates the \( n \)-fold antisymmetric tensor product of \( \ell^2(\Lambda) \oplus \ell^2(\Lambda) \).
The Holstein-Hubbard model

The Holstein-Hubbard model on $\Lambda$

$$H_{\text{HH}} = H_{\text{H}} + \sum_{x,y \in \Lambda} g_{xy} n_x (b_x^* + b_y) + \sum_{x \in \Lambda} \omega b_x^* b_x$$

- $H_{\text{H}}$ is the Hubbard Hamiltonian.
- $b_x^*$ and $b_x$ are phonon creation- and annihilation operators at site $x \in \Lambda$, respectively:
  $$[b_x, b_y^*] = \delta_{xy}, \quad [b_x, b_y] = 0.$$  
- $g_{xy}$ is the strength of the electron-phonon interaction. We assume that $\{g_{xy}\}$ is a real symmetric matrix.
- The phonons are assumed to be dispersionless with energy $\omega > 0$. 

$\text{HH}$
- Hilbert space

\[ \mathcal{E}_N \otimes \mathcal{F}, \]

\[ \mathcal{F} = \bigoplus_{n=0}^{\infty} \otimes_s \ell^2(\Lambda), \] the bosonic Fock space over \( \ell^2(\Lambda); \)
\( \otimes^n_s \) indicates the \( n \)-fold symmetric tensor product.

- \( H_{HH} \) is self-adjoint on \( \text{dom}(N_b) \) and bounded from below, where
\[ N_b = \sum_{x \in \Lambda} b_x^* b_x. \]
A many-electron system coupled to the quantized radiation field

We suppose that $\Lambda$ is embedded into the region $V = [-L/2, L/2]^3 \subset \mathbb{R}^3$ with $L > 0$.

Hamiltonian

\[
H_{\text{rad}} = \sum_{x,y \in \Lambda} \sum_{\sigma = \uparrow, \downarrow} t_{xy} \exp \left\{ i \int_{C_{xy}} dr \cdot A(r) \right\} c_{x\sigma}^* c_{y\sigma} + \sum_{x,y \in \Lambda} \frac{U_{xy}}{2} (n_x - 1)(n_y - 1) + \sum_{k \in V^*} \sum_{\lambda = 1,2} \omega(k) a(k, \lambda)^* a(k, \lambda).
\]
Hilbert space

\[ \mathcal{E}_N \otimes \mathcal{R}, \]

where \( \mathcal{R} \) is the bosonic Fock space over \( \ell^2(V^* \times \{1, 2\}) \) with \( V^* = \left( \frac{2\pi}{L} \mathbb{Z} \right)^3 \).

- \( a(k, \lambda)^* \) and \( a(k, \lambda) \) are photon creation- and annihilation operators, respectively:

\[
[a(k, \lambda), a(k', \lambda')^*] = \delta_{\lambda\lambda'} \delta_{kk'}, \quad [a(k, \lambda), a(k', \lambda')] = 0.
\]

- \( A(r) \) (\( r \in V \)) is the quantized vector potential given by

\[
A(r) = |V|^{-1/2} \sum_{k \in V^*} \sum_{\lambda=1,2} \frac{\chi_{\lambda}(k)}{\sqrt{2\omega(k)}} \varepsilon(k, \lambda) \left( e^{ik \cdot r} a(k, \lambda) + e^{-ik \cdot r} a(k, \lambda)^* \right).
\]
- $\chi_\kappa$ is the indicator function of the ball of radius $0 < \kappa < \infty$, where $\kappa$ is the ultraviolet cutoff.

- The dispersion relation:

$$\omega(k) = |k|$$

for $k \in V^* \setminus \{0\}$, $\omega(0) = m_0$ with $0 < m_0 < \infty$.

- $C_{xy}$ is a piecewise smooth curve from $x$ to $y$.

- For concreteness, the polarization vectors are chosen as

$$\varepsilon(k, 1) = \frac{(k_2, -k_1, 0)}{\sqrt{k_1^2 + k_2^2}}, \quad \varepsilon(k, 2) = \frac{k}{|k|} \wedge \varepsilon(k, 1).$$

(To avoid ambiguity, we set $\varepsilon(k, \lambda) = 0$ if $k_1 = k_2 = 0$.)

- $H_{\text{rad}}$ is essentially self-adjoint and bounded from below. We denote its closure by the same symbol.

- This model was introduced by Giuliani et al. in [GMP].
Stability of Lieb’s ferrimagnetism
Basic definitions

Definition 3.1
Let \( \Lambda \) be a finite lattice. Let \( \{ M_{xy} \} \) be a real symmetric \( |\Lambda| \times |\Lambda| \) matrix.

(i) We say that \( \Lambda \) is connected by \( \{ M_{xy} \} \), if, for every \( x, y \in \Lambda \), there are \( x_1, \ldots, x_n \in \Lambda \) such that
\[
M_{xx_1} M_{x_1 x_2} \cdots M_{x_n y} \neq 0.
\]

(ii) We say that \( \Lambda \) is bipartite in terms of \( \{ M_{xy} \} \), if \( \Lambda \) can be divided into two disjoint sets \( A \) and \( B \) such that \( M_{xy} = 0 \) whenever \( x, y \in A \) or \( x, y \in B \). \( \diamond \)
Lieb’s ferrimagnetism

- Since we are interested in the half-filled system, we will study the Hamiltonian

\[ \tilde{H}_H = H_H \upharpoonright \mathcal{E}_{N=|\Lambda|}. \]

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

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

- The total spin operator is defined by

\[
S_{\text{tot}}^2 = (S^{(3)})^2 + \frac{1}{2} S^{(+)} S^{(-)} + \frac{1}{2} S^{(-)} S^{(+)}
\]

with eigenvalues \( S(S + 1). \)
Definition 3.2

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 \( S \).

Assumptions:

(B. 1) \( \Lambda \) is connected by \( \{t_{xy}\} \);
(B. 2) \( \Lambda \) is bipartite in terms of \( \{t_{xy}\} \);
(B. 3) \( \{U_{xy}\} \) is positive definite.

Theorem 3.3 (Lieb's ferrimagnetism)

Assume that \( |\Lambda| \) is even. Assume (B. 1), (B. 2) and (B. 3). The ground state of \( \tilde{H}_H \) has total spin \( S = \frac{1}{2}||A| - |B|| \) and is unique apart from the trivial \( (2S+1) \)-degeneracy.
Corollary 3.4

If $|A| - |B| = c|\Lambda|$, then the ground state of $\tilde{H}_H$ exhibits ferrimagnetism.

Example: copper oxide lattice

Stability of Lieb’s theorem I

- We will study the half-filled case:

\[ \tilde{H}_{HH} = H_{HH} \upharpoonright \mathcal{E}_{N=|\Lambda|} \otimes \mathcal{Y}. \]

- We continue to assume (B. 1) and (B. 2).

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

(B. 4) \[ \sum_{x \in \Lambda} g_{xy} \] is a constant independent of \( y \in \Lambda \).
The effective Coulomb interaction is defined by

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

\((\text{B. 5})\) \(\{U_{\text{eff},xy}\}\) is positive definite.

**Theorem 3.5 (T.M., 2017)**

Assume that \(|\Lambda|\) is even. Assume \((\text{B. 1}), (\text{B. 2}), (\text{B. 4})\) and \((\text{B. 5})\). Then the ground state of \(\tilde{H}_{\text{HH}}\) has total spin \(S = \frac{1}{2} ||A| - |B||\) and is unique apart from the trivial \((2S + 1)\)-degeneracy.
Stability of Lieb’s ferrimagnetism II

- Consider a many-electron system coupled to the quantized radiation field.
- We will study the Hamiltonian at half-filling:

\[
\tilde{H}_{\text{rad}} = H_{\text{rad}} \upharpoonright \mathcal{E}_N = |\Lambda| \otimes \mathcal{N}.
\]

**Theorem 3.6 (T. M.)**

Assume that $|\Lambda|$ is even. Assume (B. 1), (B. 2) and (B. 3).

Then the ground state of $\tilde{H}_{\text{rad}}$ has total spin $S = \frac{1}{2} |A| - |B|$ and is unique apart from the trivial $(2S + 1)$-degeneracy.
Stability of Nagaoka’s ferromagnetism
Nagaoka’s ferromagnetism

Let us consider the *Hubbard model* $H_H$. We assume the following:

(C. 1) $t_{xy} \geq 0$ for all $x, y \in \Lambda$.

(C. 2) $\Lambda$ has the *hole-connectivity* associated with $\{t_{xy}\}$.

**Remark 4.1**

The following (i) and (ii) satisfy the hole-connectivity condition:

(i) $\Lambda$ is a triangular, square cubic, fcc, or bcc lattice;
(ii) $t_{xy}$ is nonvanishing between nearest neighbor sites.

We are interested in the $N = |\Lambda| - 1$ electron system. Thus, we will study the restricted Hamiltonian:

$$H_{H,|\Lambda|-1} = H_H \upharpoonright \mathcal{E}_{N=|\Lambda|-1}.$$
The effective Hamiltonian describing the system with \(U_{xx} = \infty\)

- The Gutzwiller projection by

\[
P = \prod_{x \in \Lambda} (\mathbb{1} - n_x \uparrow n_x \downarrow).
\]

- \(P\) is the orthogonal projection onto the subspace with no doubly occupied sites.

**Proposition 4.2**

We define the effective Hamiltonian by \(H_H^\infty = P H_{H,|\Lambda| - 1}^{U=0} P\), where \(H_{H,|\Lambda| - 1}^{U=0}\) is the Hubbard Hamiltonian \(H_{H,|\Lambda| - 1}\) with \(U_{xx} = 0\). For all \(z \in \mathbb{C} \setminus \mathbb{R}\), we have

\[
\lim_{U_{xx} \to \infty} \left( H_{H,|\Lambda| - 1} - z \right)^{-1} = \left( H_H^\infty - z \right)^{-1} P
\]

in the operator norm topology.
$H_{H}^\infty$ describes a situation with $U_{xx} = \infty$ and a single hole.

In [Tasaki1], Tasaki extended Nagaoka’s theorem as follows.

**Theorem 4.3 (Generalized Nagaoka’s theorem)**

Assume (C. 1) and (C. 2). The ground state of $H_{H}^\infty$ has total spin $S = (|\Lambda| - 1)/2$ and is unique apart from the trivial $(2S + 1)$-degeneracy.
Stability of Nagaoka’s theorem I

- Let us consider the Holstein-Hubbard Hamiltonian $H_{HH}$.
- We will study the $N = |\Lambda| - 1$ electron system:

$$H_{HH,|\Lambda| - 1} = H_{HH} \upharpoonright \mathcal{E}_{N=|\Lambda| - 1} \otimes \mathcal{P}.$$  

- As before, we can derive an effective Hamiltonian describing the system with $U_{xx} = \infty$. 

**Proposition 4.4**

We define the effective Hamiltonian by

\[ H^\infty_H = PH_{HH,U=0}^0 H_{HH,|\Lambda|-1} P, \]

where \( H_{HH,U=0}^0 H_{HH,|\Lambda|-1} \) is \( H_{HH,|\Lambda|-1} \) with \( U_{xx} = 0 \). For all \( z \in \mathbb{C} \setminus \mathbb{R} \), we have

\[
\lim_{U_{xx} \to \infty} \left( H_{HH,|\Lambda|-1} - z \right)^{-1} = \left( H^\infty_{HH} - z \right)^{-1} P
\]

in the operator norm topology.

**Theorem 4.5 (T. M., 2017)**

Assume (C. 1) and (C. 2). The ground state of \( H^\infty_{HH} \) has total spin \( S = (|\Lambda| - 1)/2 \) and is unique apart from the trivial \( (2S + 1) \)-degeneracy.
Stability of Nagaoka’s theorem II

- Consider a many-electron system coupled to the quantized radiation field.
- We will study the Hamiltonian $H_{\text{rad},|\Lambda|-1}$ which describes the $N = |\Lambda| - 1$ electron system.

**Proposition 4.6**

*We define the effective Hamiltonian by* $H_{\text{rad}}^\infty = PH_{\text{rad},|\Lambda|-1}^U=0 P$, *where* $H_{\text{rad},|\Lambda|-1}^U=0$ *is* $H_{\text{rad},|\Lambda|-1}$ *with* $U_{xx} = 0$. *For all* $z \in \mathbb{C} \setminus \mathbb{R}$, *we have*

$$\lim_{U_{xx} \to \infty} (H_{\text{rad},|\Lambda|-1} - z)^{-1} = (H_{\text{rad}}^\infty - z)^{-1} P$$

*in the operator norm topology.*
Theorem 4.7 (T. M., 2017)

Assume (C. 1) and (C. 2). The ground state of \( H_{\text{rad}}^{\infty} \) has total spin \( S = (|\Lambda| - 1)/2 \) and is unique apart from the trivial \( (2S + 1) \)-degeneracy.
Summary

- Lieb’s ferrimagnetism is stable, even if the influence of phonons and photons is taken into account.
- Nagaoka’s ferromagnetism is stable, even if the influence of phonons and photons is taken into account;
- Proofs of these stabilities rely on the operator theoretic correlation inequalities.
Open problems

- Stabilities of phase diagram in the Holstein-Hubbard model.
- Construction of the ferromagnetic ground states in the Hubbard model and Holstein-Hubbard model.
- Existence of long range orders in the *square lattice*. 
Background
Stability of Lieb’s ferrimagnetism
Stability of Nagaoka’s ferromagnetism

References


Miyao3 T. Miyao, arXiv:1610.09039


