Stability of magnetism in the Hubbard model

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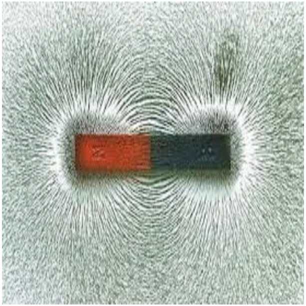
Abstract

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.



Picture: Gakken kidsnet

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Background

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 Λ:

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

- Λ: 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:

$$\mathfrak{E}_N = \bigwedge^N (\ell^2(\Lambda) \oplus \ell^2(\Lambda)).$$

$\bigwedge^n \left(\ell^2(\Lambda) \oplus \ell^2(\Lambda)\right)$ indicates the n-fold antisymmetric tensor product of $\ell^2(\Lambda) \oplus \ell^2(\Lambda)$.

The Holstein-Hubbard model

The Holstein-Hubbard model on Λ

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

- H_{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 $\omega > 0$.

- Hilbert space

$$\mathfrak{E}_N \otimes \mathfrak{P},$$

  $\mathfrak{P} = \bigoplus_{n=0}^{\infty} \otimes_{\mathrm{s}} \ell^2(\Lambda)$, the bosonic Fock space over $\ell^2(\Lambda)$; $\otimes_{\mathrm{s}}^n$ indicates the n-fold symmetric tensor product.
- H_{HH} is self-adjoint on $\mathrm{dom}(N_{\mathrm{b}})$ and bounded from below, where $N_{\mathrm{b}} = \sum_{x\in\Lambda} b_x^* b_x$.

A many-electron system coupled to the quantized radiation field

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

Hamiltonian

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

- Hilbert space

$$\mathfrak{E}_N \otimes \mathfrak{R},$$

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

- $a(k,\lambda)^*$ 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

$$\begin{aligned} &A(r) \\ =&|V|^{-1/2} \sum_{k \in V^*} \sum_{\lambda=1,2} \frac{\chi_\kappa(k)}{\sqrt{2\omega(k)}} \varepsilon(k,\lambda) \Big(e^{ik\cdot r} a(k,\lambda) + e^{-ik\cdot r} a(k,\lambda)^* \Big). \end{aligned}$$

- χ_κ is the indicator function of the ball of radius $0 < \kappa < \infty$, where κ is the ultraviolet cutoff.
- The dispersion relation:

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

  for $k \in V^* \backslash \{0\}$, $\omega(0) = m_0$ 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_{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 Λ be a finite lattice. Let $\{M_{xy}\}$ be a real symmetric $|\Lambda| \times |\Lambda|$ matrix.

(i) We say that Λ 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 Λ is *bipartite in terms of* $\{M_{xy}\}$, if Λ can be divided into two disjoint sets A and B such that $M_{xy} = 0$ whenver $x, y \in A$ or $x, y \in B$. $\diamondsuit$

Lieb's ferrimagnetism

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

$$\tilde{H}_{\mathrm{H}} = H_{\mathrm{H}} \upharpoonright \mathfrak{E}_{N=|\Lambda|}.$$

- Let $S_x^{(+)} = c_{x\uparrow}^* c_{x\downarrow}$ and let $S_x^{(-)} = \big(S_x^{(+)}\big)^*$. 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

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

with eigenvalues $S(S+1)$.

Definition 3.2

If φ is an eigenvector of S_{tot}^2 with $S_{\mathrm{tot}}^2\varphi = S(S+1)\varphi$, then we say that φ has *total spin* S.

Assumptions:

(B. 1) Λ is connected by $\{t_{xy}\}$;

(B. 2) Λ is bipartite in terms of $\{t_{xy}\}$;

(B. 3) $\{U_{xy}\}$ is positive definite.

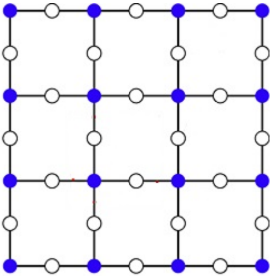
Theorem 3.3 (Lieb's ferrimagnetism)

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

Corollary 3.4

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

Example: copper oxide lattice



Picture: W.Tsai et.al., New Jour. Phys. 17, 2015.

Stability of Lieb's theorem I

- We will study the half-filled case:

$$\tilde{H}_{\mathrm{HH}} = H_{\mathrm{HH}} \restriction \mathfrak{E}_{N=|\Lambda|} \otimes \mathfrak{P}.$$

- 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

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

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

Theorem 3.5 (T.M., 2017)

Assume that $|\Lambda|$ *is even. Assume* **(B. 1)**, **(B. 2)**, **(B. 4)** *and* **(B. 5)**. *Then the ground state of* $\tilde{H}_{\mathrm{HH}}$ *has total spin* $S = \frac{1}{2}\big||A| - |B|\big|$ *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:

$$\tilde{H}_{\mathrm{rad}} = H_{\mathrm{rad}} \restriction \mathfrak{E}_{N=|\Lambda|} \otimes \mathfrak{R}.$$

Theorem 3.6 (T. M.)

Assume that $|\Lambda|$ is even. Assume **(B. 1)**, **(B. 2)** *and* **(B. 3)**. *Then the ground state of $\tilde{H}_{\mathrm{rad}}$ has total spin $S = \frac{1}{2}\big||A| - |B|\big|$ 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) Λ has the *hole-connectivity* associated with $\{t_{xy}\}$.

Remark 4.1

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

(i) Λ 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:

$$H_{\mathrm{H},|\Lambda|-1} = H_{\mathrm{H}} \restriction \mathfrak{E}_{N=|\Lambda|-1}.$$

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 $H_{\mathrm{H}}^{\infty} = P H_{\mathrm{H},|\Lambda|-1}^{U=0} P$, where $H_{\mathrm{H},|\Lambda|-1}^{U=0}$ is the Hubbard Hamiltonian $H_{\mathrm{H},|\Lambda|-1}$ with $U_{xx} = 0$. For all $z \in \mathbb{C} \backslash \mathbb{R}$, we have

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

in the operator norm topology.

- H_{H}^{∞} 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}^{∞} 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:

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

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

Proposition 4.4

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

$$\lim_{U_{xx}\to\infty} \left(H_{\mathrm{HH},|\Lambda|-1} - z\right)^{-1} = \left(H_{\mathrm{HH}}^{\infty} - z\right)^{-1} P$$

in the operator norm topology.

Theorem 4.5 (T. M., 2017)

Assume **(C. 1)** *and* **(C. 2)***. The ground state of* H_{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 $H_{\mathrm{rad},|\Lambda|-1}$ which describes the $N = |\Lambda| - 1$ electron system.

Proposition 4.6

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

$$\lim_{U_{xx}\to\infty} \left(H_{\mathrm{rad},|\Lambda|-1} - z\right)^{-1} = \left(H^{\infty}_{\mathrm{rad}} - z\right)^{-1} P$$

in the operator norm topology.

Theorem 4.7 (T. M., 2017)

Assume **(C. 1)** *and* **(C. 2)**. *The ground state of $H^{\infty}_{\mathrm{rad}}$ 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-Hubbad model.
- Construction of the ferromagnetic ground states in the Hubbard model and Holstein-Hubbard model.
- Existence of long range orders in the *square lattice*.

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