

Stability of Ferromagnetism in the Hubbard Model

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(Received 7 April 1994)

Recently certain Hubbard models with flat lowest bands were proved to exhibit ferromagnetism. Here we study perturbed models with nearly flat bands. We prove that the ferromagnetic state is stable against a single-spin flip for sufficiently large Coulomb interaction U , but is unstable for small $U > 0$. This is the first time that the (local) stability of ferromagnetism is proved in nonsingular Hubbard models, in which we must overcome competition between the kinetic energy and the Coulomb interaction.

PACS numbers: 75.10.Lp

It is believed that (spin-independent) Coulomb interaction in some itinerant electron systems can be the origin of ferromagnetism. In spite of considerable interest over the long history, the mechanism of ferromagnetism still remains to be understood [1]. Recently Mielke [2] and Tasaki [3] proved that certain Hubbard models exhibit ferromagnetism when the Coulomb interaction U is finite [4]. The models they treated are special in that, in each model, the lowest band in the single-electron spectrum is completely flat (i.e., dispersionless). It was conjectured that the ferromagnetism in these flat-band models survives if we add small perturbation to the hopping matrices (thus making the lowest band nonflat), provided that U is sufficiently large. Kusakabe and Aoki [5] presented results from numerical experiments and variational calculations, which supported this conjecture.

We stress that this is a very delicate conjecture for the following reasons. (i) When the ground state has a ferromagnetic order, there exist spin-wave (or magnon, or Nambu-Goldstone) excitations whose excitation energies decrease as L^{-2} as the linear size L of the system gets larger. The total energy of the perturbation, on the other hand, increases as L^d , indicating that the perturbation is by no means small. (ii) It is believed that the ground state of the perturbed model is spin singlet for sufficiently small U , so we must have finite U in order to stabilize ferromagnetism. To show the existence of ferromagnetism is a truly "nonperturbative" problem, in which we have to overcome the notorious "competition" between the kinetic energy and the Coulomb interaction.

In the present Letter, we announce the first important step towards the solution of this problem. We treat models with nearly flat bands obtained by adding perturbations to the hopping matrices of the flat-band models. For sufficiently large U , we prove that the ferromagnetic state is stable under a single-spin flip. This result, along with the strong results for the flat-band models, indicates that the ferromagnetic state is the true ground state of the present models for sufficiently large U . We also prove that, in a certain range of U , the spin-wave dispersion relations of the present models behave exactly as those in the Heisenberg ferromagnet, thus confirming the con-

jecture of Kusakabe and Aoki [5]. This indicates that the ferromagnetism in our models is not pathological. As far as we know, this is the first time that the (local) stability of ferromagnetism is proved [6] in truly nonsingular Hubbard models, overcoming the competition between the kinetic energy and the Coulomb interaction. See [3,7] for further discussions about ferromagnetism in the Hubbard model [8].

Definitions and main results.—For simplicity, we describe our results for a class of models on the decorated hypercubic lattice [3]. The results extend to a larger class of perturbed flat-band models [7]. Let $\mathcal{L} (\subset \mathbf{Z}^d)$ be the d -dimensional $L \times \cdots \times L$ hypercubic lattice with periodic boundary conditions, where $d = 1, 2, 3, \dots$. A site $x \in \mathcal{L}$ is written as $x = (x_1, \dots, x_d)$ with each component x_i being an integer with $|x_i| \leq (L-1)/2$. (We assume L is odd.) Let \mathcal{U} be the set of points taken at the center of each bond in \mathcal{L} . We define our Hubbard models on the decorated lattice $\Lambda = \mathcal{L} \cup \mathcal{U}$. As usual, we denote by $c_{x\sigma}^\dagger$, $c_{x\sigma}$, and $n_{x\sigma} = c_{x\sigma}^\dagger c_{x\sigma}$ the creation, annihilation, and number operators, respectively, of an electron at site $x \in \Lambda$ with spin $\sigma = \uparrow, \downarrow$.

We study the standard Hubbard Hamiltonian

$$H = \sum_{\sigma=\uparrow,\downarrow} \sum_{x,y \in \Lambda} t_{xy} c_{x\sigma}^\dagger c_{y\sigma} + U \sum_{x \in \Lambda} n_x \uparrow n_x \downarrow, \quad (1)$$

where $U > 0$ is the on-site Coulomb repulsion energy [9], and the hopping matrix elements are written as $t_{xy} = t_{xy}^{(0)} + \kappa t'_{xy}$. Here $t_{xy}^{(0)} = t_{yx}^{(0)}$ are the hopping matrix elements of the flat-band model of [3]. There are nonvanishing nearest and next-nearest neighbor hoppings which are written in terms of two parameters $t > 0$ and $\lambda > 0$ as (i) $t_{xx}^{(0)} = 2dt$ if $x \in \mathcal{L}$, (ii) $t_{xx}^{(0)} = \lambda^2 t$ if $x \in \mathcal{U}$, (iii) $t_{xy}^{(0)} = t$ if $x, y \in \mathcal{L}$ and $|x-y|=1$, (iv) $t_{xy}^{(0)} = \lambda t$ if $|x-y|=1/2$, and (v) $t_{xy}^{(0)} = 0$ otherwise (Fig. 1). The parameter $\kappa \geq 0$ determines the magnitude of perturbation to the hopping matrix. The perturbation $\{t'_{xy}\}$ is arbitrary, except for the requirements that (i) $t'_{xy} = t'_{yx}$ for any $x, y \in \Lambda$, (ii) $t'_{x+z, y+z} = t'_{xy}$ for any $x, y \in \Lambda$ and any $z \in \mathbf{Z}^d$, (iii) $\sum_y |t'_{xy}| \leq t$ for any x , and (iv) $t'_{xy} = 0$ for any x, y with $|x-y| \geq R$, where R is a finite constant.

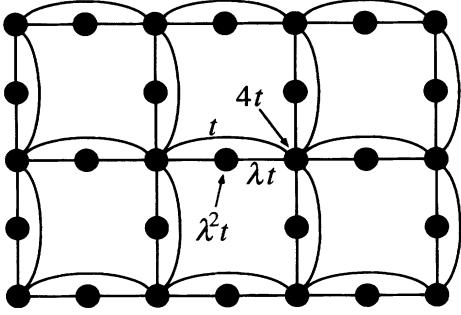


FIG. 1. The two dimensional lattice, and the hopping matrix elements of the flat-band model. We add arbitrary small hoppings as a perturbation, thus making the lowest band nonflat.

The single-electron Schrödinger equation corresponding to (1) is

$$\sum_{y \in \Lambda} t_{xy} \varphi_y = \varepsilon \varphi_x, \quad (2)$$

where $\varphi = (\varphi_x)_{x \in \Lambda}$ is a wave function [i.e., a $(d+1)L^d$ -dimensional vector] and ε is the energy eigenvalue. When $\kappa = 0$ (i.e., $t_{xy} = t_{xy}^{(0)}$), the ground states of the Schrödinger equation (2) are L^d -fold degenerate, and form a flat band. Remaining dL^d eigenvalues of (2) form upper bands, which are separated from the flat lowest band by a band gap $\lambda^2 t$. For $\kappa > 0$, the degeneracy in the lowest band is lifted for a generic choice of $\{t'_{xy}\}$, and we get a nonflat band.

Throughout the present Letter, we only consider many-electron states in which the total electron number [i.e., eigenvalue of $\sum_{x \in \Lambda} (n_{x\uparrow} + n_{x\downarrow})$] is fixed to L^d . This corresponds to the $\{2(d+1)\}^{-1}$ filling of the whole bands, or the half filling of the lowest band [10].

As usual, we define the total spin operators by $S_{\text{tot}}^{(3)} = \sum_{x \in \Lambda} (n_{x\uparrow} - n_{x\downarrow})/2$, and $(S_{\text{tot}})^2 = \sum_{x,y \in \Lambda} (S_x^+ S_y^- + S_x^- S_y^+)/2 + (S_{\text{tot}}^{(3)})^2$, where $S_x^+ = c_{x\uparrow}^\dagger c_{x\downarrow}$ and $S_x^- = (S_x^+)^{\dagger}$. We denote an eigenvalue of $(S_{\text{tot}})^2$ as $S_{\text{tot}}(S_{\text{tot}} + 1)$. We write $S_{\text{max}} = L^d/2$, which is the maximum possible value of S_{tot} . The following theorem of [3] establishes the existence of ferromagnetism in the flat-band model.

Theorem I.—When $\kappa = 0$, the ground state of the Hamiltonian (1) has $S_{\text{tot}} = S_{\text{max}}$, and is nondegenerate apart from the trivial $(2S_{\text{max}} + 1)$ -fold degeneracy.

The purpose of the present Letter is to discuss the cases with $\kappa \neq 0$, where the lowest band is no longer flat. We shall assume that the (dimensionless) parameters κ and λ satisfy $\kappa \leq \kappa_0$ and $\lambda \geq \lambda_0$, where the constants κ_0 and λ_0 (which are determined in the proof) depend only on the dimension d and the range R of the hopping.

Let us denote by $E(S_{\text{tot}})$ the lowest energy among the (L^d -electron) states which have the total spin equal to S_{tot} . It is easy to see that the state which gives the lowest energy $E(S_{\text{max}})$ in the sector with $S_{\text{tot}} = S_{\text{max}}$ is unique (apart from the spin degeneracy), and is obtained by completely filling the lowest band by spin-up electrons.

For convenience, we call this state the “ferromagnetic ground state” although it may not be the true ground state. The following theorem establishes the stability and instability of the ferromagnetic ground state against a single-spin flip.

Theorem II.—Suppose that $C_1 \lambda^2 t \kappa \leq U$, where C_1 is a positive finite constant which depends only on d and R . Then the ferromagnetic ground state is stable under a single-spin flip in the sense that $E(S_{\text{max}}) < E(S_{\text{max}} - 1)$. On the other hand, when we have $0 \leq U \leq C_2$, the ferromagnetic ground state is unstable as $E(S_{\text{max}}) > E(S_{\text{max}} - 1)$. Here C_2 is a non-negative (generically strictly positive) constant proportional to the bandwidth of the lowest band.

By τ_x we denote the translation operator by a lattice vector $x \in \mathbf{Z}^d$. Let $E(k)$ be the energy of the elementary spin-wave excitation with the wave number vector k , which is defined as the lowest energy among the states that satisfy $S_{\text{tot}}^{(3)} \Phi = (S_{\text{max}} - 1) \Phi$, and $\tau_x[\Phi] = e^{ik \cdot x} \Phi$ for any $x \in \mathcal{L}$. Here the wave number vector is $k = (2\pi n_1/L, \dots, 2\pi n_d/L)$ with n_i being an integer with $|n_i| \leq (L-1)/2$. (We denote the space of all such k by \mathcal{K} .) The following theorem determines the behavior of $E(k)$ almost completely, and establishes that the spin-wave excitation of the present model behaves exactly as those in the ferromagnetic Heisenberg model with the exchange interaction $J = U\lambda^{-4}$.

Theorem III.—Suppose that $C_1 \lambda^2 t \kappa \leq U \leq C_3 \lambda^2 t$, where C_3 is a positive finite constant which depends only on d and R . Then we have

$$F_1 U \lambda^{-4} G(k) \leq E(k) - E(S_{\text{max}}) \leq F_2 U \lambda^{-4} G(k) \quad (3)$$

for any $k \in \mathcal{K}$, where $G(k) = \sum_{j=1}^d 4\{\sin(k_j/2)\}^2$. The prefactors are written as $F_1(\lambda, \kappa, U) = 1 - C_4/\lambda - C_5\kappa - C_6\lambda^2 t \kappa/U$ and $F_2(\lambda) = 1 + C_7/\lambda$, where the positive finite constants C_i ($i = 4, \dots, 7$) depend only on d and R . We thus have $F_1 \approx F_2 \approx 1$ for λ large and κ small.

Sketch of the proof.—We now sketch the basic ideas of the proofs, leaving details to [7]. We first briefly discuss easier parts. The latter half of Theorem II, which states the instability of the ferromagnetic ground state, is easily proved by appropriately choosing a trial state with $S_{\text{tot}} = S_{\text{max}} - 1$, and using the variational argument. The upper bound in (3) of Theorem III is also easily proved by the variational argument as in [3].

We move onto the harder parts. The basic strategy is simple. For each $k \in \mathcal{K}$, we construct a complete basis \mathcal{B}_k of the L^d -electron states with the given wave number k and $S_{\text{tot}}^{(3)} = S_{\text{max}} - 1$. For $\Phi \in \mathcal{B}_k$, we define

$$D[\Phi] = h[\Phi, \Phi] - \sum_{\Psi \in \mathcal{B}_k, \Psi \neq \Phi} |h[\Phi, \Psi]|, \quad (4)$$

where $h[\Phi, \Psi]$ is the matrix element [11] of the Hamiltonian (1). It is easily found that [12]

$$E(k) \geq \min_{\Phi \in \mathcal{B}_k} D[\Phi]. \quad (5)$$

Being a very crude bound, (5) may yield physically significant results only when we chose bases \mathcal{B}_k which "almost diagonalize" the low-energy part of H .

In what follows, we restrict ourselves to the case with $d = 1$ in order to simplify the discussion. The generalizations to higher dimensions turn out to be straightforward in principle [7]. We first construct a nonorthogonal but highly localized basis for the single-electron Hilbert space. For each $u \in \Lambda$, we take a state $\varphi^{(u)} = (\varphi_x^{(u)})_{x \in \Lambda}$, so that the set $\{\varphi^{(u)}\}_{u \in \mathcal{L}}$ spans the lower band [13], and the set $\{\varphi^{(u)}\}_{u \in \mathcal{U}}$ spans the upper band. The state $\varphi_x^{(u)}$ is localized at the reference site u as $\varphi_u^{(u)} \approx 1$, $|\varphi_x^{(u)}| \approx \lambda^{-1}$ for $|x - u| = 1/2$, and $\varphi_x^{(u)} \approx C\kappa\lambda^{-2}$ for $|x - u| = 1$, where C is a constant. $\varphi_x^{(u)}$ is much smaller for $|x - u| > 1$, and decays exponentially in $|x - u|$.

We denote by $\tilde{\varphi}^{(u)} = (\tilde{\varphi}_x^{(u)})_{x \in \Lambda}$ the states in the corresponding dual basis. They are related to the basis states by $\sum_{x \in \Lambda} \tilde{\varphi}_x^{(u)} \tilde{\varphi}_x^{(v)} = \delta_{u,v}$ and $\sum_{u \in \Lambda} \tilde{\varphi}_x^{(u)} \varphi_y^{(u)} = \delta_{x,y}$. The dual state satisfies $\tilde{\varphi}_u^{(u)} \approx 1$, $|\tilde{\varphi}_x^{(u)}| \approx \lambda^{-1}$ for $|x - u| = 1/2$, $\tilde{\varphi}_x^{(u)} \approx -\lambda^{-2}$ for $|x - u| = 1$, and decays exponentially in $|x - u|$. Note that the basis state $\varphi^{(u)}$ is strictly localized in the flat-band limit $\kappa = 0$, while the dual basis state $\tilde{\varphi}^{(u)}$ is only moderately localized.

Let us define the creation and annihilation operators by $a_{u\sigma}^\dagger = \sum_{x \in \Lambda} \varphi_x^{(u)} c_{x\sigma}^\dagger$ and $b_{u\sigma} = \sum_{x \in \Lambda} \tilde{\varphi}_x^{(u)} c_{x\sigma}$. They satisfy the standard anticommutation relations $\{a_{u\sigma}^\dagger, b_{v\tau}\} = \delta_{u,v} \delta_{\sigma,\tau}$. By using the inversion formulas $c_{x\sigma}^\dagger = \sum_{u \in \Lambda} \tilde{\varphi}_x^{(u)} a_{u\sigma}^\dagger$, $c_{x\sigma} = \sum_{u \in \Lambda} \varphi_x^{(u)} b_{u\sigma}$, we can rewrite the Hamiltonian (1) as

$$H = \sum_{\substack{\sigma=\uparrow,\downarrow \\ u,v \in \Lambda}} \tilde{t}_{uv} a_{u\sigma}^\dagger b_{v\sigma} + \sum_{u,v,w,z \in \Lambda} \tilde{U}_{u,v,w,z} a_{u\uparrow}^\dagger a_{v\downarrow}^\dagger b_w b_z, \quad (6)$$

where $\tilde{t}_{uv} = \tilde{t}_{vu} = \sum_{x,y \in \Lambda} t_{xy} \tilde{\varphi}_x^{(u)} \varphi_y^{(v)}$, and $\tilde{U}_{u,v,w,z} = U \sum_{x \in \Lambda} \tilde{\varphi}_x^{(u)} \tilde{\varphi}_x^{(v)} \varphi_x^{(w)} \varphi_x^{(z)}$. It can be shown that the effective hoppings satisfy $\tilde{t}_{uv} = 0$ for any $u \in \mathcal{L}$ and $v \in \mathcal{U}$. For $u \in \mathcal{L}$, \tilde{t}_{uu} is equal to the average of the single-electron energies in the lower band, which we assume to be vanishing for simplicity.

Rather than constructing the whole basis \mathcal{B}_k , we here introduce its elements, which play essential roles in getting the desired lower bounds [14]. Let Φ_{vac} be the state with no electrons, and $\Phi_\uparrow = \prod_{u \in \mathcal{L}} a_{u\uparrow}^\dagger \Phi_{\text{vac}}$ be the ferromagnetic ground state. The state

$$\Phi_0(k) = [\alpha(k)]^{-1} \sum_{x \in \mathcal{L}} e^{ikx} a_{x\uparrow}^\dagger b_{x\uparrow} \Phi_\uparrow \quad (7)$$

should be a good approximation to the elementary spin-wave excitation, where the constant $\alpha(k)$ will be determined later. The states

$$\Phi_\pm(k) = \sum_{x \in \mathcal{L}} e^{ikx} a_{x \pm 1\uparrow}^\dagger b_{x\uparrow} \Phi_\uparrow, \quad (8)$$

$$\Psi(k) = \sum_{x \in \mathcal{L}} e^{ikx} a_{x+(1/2)\uparrow}^\dagger b_{x+1\uparrow} \Phi_\uparrow \quad (9)$$

play crucial roles in instabilization against paramagnetism.

By using the representation (6), we write down the dominant parts of matrix elements between these states as

$$h[\Phi_0(k), \Phi_0(k)] \approx 4\tilde{U}_{0,1,0,1} \{\sin(k/2)\}^2, \quad (10)$$

$$h[\Phi_0(k), \Phi_\pm(k)] \approx \alpha(k) (1 - e^{\mp ik}) (\tilde{t}_{01} + \tilde{U}_{0,1,1,1}), \quad (11)$$

$$h[\Phi_0(k), \Psi(k)] \approx \alpha(k) (e^{-ik} - 1) \tilde{U}_{0,1;1/2,1/2}, \quad (12)$$

$$h[\Phi_\pm(k), \Phi_\pm(k)] \approx U_{0,0;0,0}, \quad (13)$$

and

$$h[\Phi_\pm(k), \Phi_0(k)] \approx [\alpha(k)]^{-1} (1 - e^{\pm ik}) (\tilde{t}_{01} + \tilde{U}_{1,1,0,1}). \quad (14)$$

From the properties of the basis states $\varphi_x^{(u)}$, $\tilde{\varphi}_x^{(u)}$, we can estimate the coupling constants as $\tilde{U}_{0,1,0,1} \approx U\lambda^{-4}$, $\tilde{U}_{0,1,1,1} \approx -U\lambda^{-2}$, $\tilde{U}_{1,1,0,1} \approx (C\kappa + \lambda^{-2})U\lambda^{-2}$, $\tilde{U}_{0,1;1/2,1/2} \approx U\lambda^{-2}$, and $\tilde{U}_{0,0;0,0} \approx U$. Note that $\tilde{U}_{0,1,1,1}$ is different from $\tilde{U}_{1,1,0,1}$, reflecting the nonorthogonality of the basis states. This asymmetry plays the most important role in our proof. We also note that $|\tilde{t}_{01}| \leq \kappa t$.

Combining these estimates, we can roughly evaluate [15] the quantity $D[\Phi]$ for small enough k as

$$D[\Phi_\pm(k)] \approx h[\Phi_\pm(k), \Phi_\pm(k)] - |h[\Phi_\pm(k), \Phi_0(k)]| \approx U - [\alpha(k)]^{-1} k(\beta + \kappa C + \lambda^{-2})U\lambda^{-2} = U/2, \quad (15)$$

where we wrote $\beta = \lambda^2 t \kappa / U$, and set $\alpha(k) = 2k(\beta + \kappa C + \lambda^{-2})\lambda^{-2}$. Then we have

$$\begin{aligned} D[\Phi_0(k)] &\approx h[\Phi_0(k), \Phi_0(k)] - \sum_{\pm} |h[\Phi_0(k), \Phi_\pm(k)]| - |h[\Phi_0(k), \Psi(k)]| \\ &\approx U\lambda^{-4} G(k) - \alpha(k) k(2\beta + 3)U\lambda^{-2} \approx U\lambda^{-4} \{1 - (4\beta + 6)(\beta + \kappa C + \lambda^{-2})\} G(k), \end{aligned} \quad (16)$$

where we used $G(k) \approx k^2$. The right-hand side is the desired lower bound for $E(k)$ in (3). It becomes strictly positive if we take β , κ , and λ^{-2} sufficiently small. We stress that the above mentioned asymmetry in the matrix elements of H played an essential role in making the right-hand side of (16) positive. If we used, for example, the Wannier functions as our basis (which would yield symmetric matrix elements) and followed the present strategy, this quantity would always be negative. For other states Φ in \mathcal{B}_k , it is easy to show that $D[\Phi] \geq U/2$. These estimates for $D[\Phi]$, with the inequality (5), essentially prove the harder half of Theorem III. The lower bound in Theorem II has also been proved except for the sector with $k = (0, \dots, 0)$.

To prove the remainder of Theorem II, we note that $\Phi_0(0, \dots, 0)$ has $S_{\text{tot}} = S_{\text{max}}$, and is nothing but [an SU(2) rotation of] the ferromagnetic ground state Φ_{\uparrow} . In order to get a lower bound for $E(S_{\text{max}} - 1)$ in the sector with $k = (0, \dots, 0)$, we repeat the previous argument but without including Φ_0 . Then we easily find that the excitation energy in this subspace is bounded from below by $U/2$. Finally we remove the upper bound for U (as required in Theorem III) by noting that $E(S_{\text{max}} - 1)$ is nonincreasing in U while $E(S_{\text{max}})$ is independent of U .

I wish to thank Tohru Koma and Andreas Mielke for useful discussions and suggestions, as well as Hideo Aoki and Koichi Kusakabe for stimulating discussions.

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- [1] For a review of the early history, see C. Herring, in *Magnetism IV*, edited by G.T. Rado and H. Schul (Academic Press, New York, 1966). The two standard heuristic explanations of ferromagnetism is Heisenberg's exchange interaction and the Hartree-Fock theory for band electrons. It is interesting that the ferromagnetism in the models discussed in the present Letter may be understood in terms of either of these two pictures, which are sometimes considered incompatible with each other.
- [2] A. Mielke, J. Phys. A **24**, L73 (1991); **24**, 3311 (1991); **25**, 4335 (1992); Phys. Lett. A **174**, 443 (1993).
- [3] H. Tasaki, Phys. Rev. Lett. **69**, 1608 (1992); A. Mielke and H. Tasaki, Commun. Math. Phys. **158**, 341 (1993).
- [4] There are also rigorous examples of ferromagnetism in the Hubbard model due to Nagaoka and Thouless [Y. Nagaoka, Phys. Rev. **147**, 392 (1966); D.J. Thouless, Proc. Phys. Soc. London **86**, 893 (1965)], and due to Lieb [E.H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989)]. For a recent survey of rigorous results in the Hubbard model, see E.H. Lieb, in Proceedings of Advances in Dynamical Systems and Quantum Physics (World Scientific, Singapore, to be published) and in Proceedings of 1993 NATO ASW "The Physics and Mathematical Physics of the Hubbard Model" (Plenum, New York, to be published).

- [5] K. Kusakabe and H. Aoki, Physica (Amsterdam) **194-196B**, 215 (1994); Phys. Rev. Lett. **72**, 144 (1994); K. Kusakabe, thesis, University of Tokyo (1994).
- [6] There are many works based on variational calculations which discuss "stability" of ferromagnetism. It should be noted, however, that a variational calculation is only useful in proving instability. The absence of instability for artificially chosen trial states does not necessarily imply stability.
- [7] H. Tasaki (to be published).
- [8] We can formulate an interesting problem in one dimension, which is suitable for numerical experiments. Consider a Hubbard model on the chain with $2L$ sites with L electrons (which makes it quarter filled). The Hamiltonian $H = t_1 \sum_{\sigma} \sum_{i=1}^{2L} (c_{i/2\sigma}^{\dagger} c_{(i+1)/2\sigma} + \text{H.c.}) + t_2 \sum_{\sigma} \sum_{j=1}^L (c_{j-(1/2),\sigma}^{\dagger} c_{(j+1/2),\sigma} + \text{H.c.}) + V \sum_{j=1}^L (n_{j\uparrow} + n_{j\downarrow}) + U \sum_{i=1}^{2L} n_{i/2\uparrow} n_{i/2\downarrow}$ defines simple two-band models. The flat-band models are obtained by setting $t_1 = \lambda t_2$ and $V = (\lambda^2 - 2)t_2$ with $\lambda > 0$, $t_2 > 0$, in which case the existence of ferromagnetism is proved for any $U > 0$. We expect the ferromagnetism to survive for the parameters close to these values. To find out precise conditions for the occurrence of ferromagnetism in the above class of models, however, is still wide open and would be very illuminating.
- [9] It is straightforward to extend the present results to models with site-dependent U .
- [10] If the ground state is completely ferromagnetic (as we expect for sufficiently large U), the lower band is filled, and the system should be insulating. We expect metallic ferromagnetism from models with smaller filling factor, but the problem becomes much more difficult. See [3] for such results in the flat-band models.
- [11] The matrix elements are defined by the unique expansion $H\Phi = \sum_{\Psi \in \mathcal{B}_k} h[\Psi, \Phi]\Psi$ for $\Phi \in \mathcal{B}_k$.
- [12] To see this, fix $k \in \mathcal{K}$, and denote the matrix elements simply as h_{ij} , where $i, j \in \mathcal{B}_k$. An eigenvalue E of the matrix (h_{ij}) satisfies $Ev_i = \sum_j h_{ij} v_j$ for any i . Let ℓ be such that $|v_j/v_\ell| \leq 1$ for any j . Then it follows that $|E - h_{\ell\ell}| \leq \sum_{j \neq \ell} |h_{\ell j}|$, and hence $E \geq h_{\ell\ell} - \sum_{j \neq \ell} |h_{\ell j}|$. Thus the desired bound holds for the lowest eigenvalue.
- [13] Let $\psi^{(k)} = (\psi_x^{(k)})_{x \in \Lambda}$ denote an eigenstate of (2) in the lower band with the wave number k . A state localized at $u \in \mathcal{L}$ is constructed as $\varphi_x^{(u)} = (2\pi)^{-1} \int dk e^{-iku} \psi_x^{(k)}$. If we normalized $\psi^{(k)}$, this would yield the standard Wannier functions which form orthonormal basis. In our case, we leave $\psi^{(k)}$ unnormalized but chose it to be less singular (as a function of k) as much as is possible [7].
- [14] Take $x \in \Lambda$ and $A \subset \Lambda$ with $L - 1$ sites. A general element Φ in \mathcal{B}_k is constructed as $\sum_{y \in \mathcal{L}} e^{iky} \tau_y [a_{x1}^{\dagger} (\prod_{z \in A} a_{z1}^{\dagger}) \Phi_{\text{vac}}]$.
- [15] In the actual proof, we have to deal with various summations over lattice sites. It turns out, however, that relevant quantities exhibit exponential decay, and the control of summations is not difficult in principle.