Ferromagnetism in a Hubbard model for an atomic quantum wire: 
a realization of flat-band magnetism from even-membered rings

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We have examined a Hubbard model on a chain of squares, which was proposed by Yajima et al. as a model of an atomic quantum wire As/Si(100), to show that the flat-band ferromagnetism according to a kind of Mielke-Tasaki mechanism should be realized for an appropriate band filling in such a non-frustrated lattice. Reflecting the fact that the flat band is not a bottom one, the ferromagnetism vanishes, rather than intensified, as the Hubbard $U$ is increased. The exact diagonalization method is used to show that the critical value of $U$ is in a realistic range. We also discussed the robustness of the magnetism against the degradation of the flatness of the band.

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Recent progress in atom manipulation on solid surfaces using scanning tunneling microscope has opened up an unprecedented possibilities for designed structures on atomic scales. Specifically, Hashizume et al. has fabricated atomic wires from Ga adatoms bound to a row of dangling bonds on a hydrogen-terminated Si(100) 2×1 surface. Watanabe et al. have obtained its band structure with the first-principles calculation. Interestingly, they have found that a partially flat band appears in the dispersion and suggested a possibility of the ferromagnetism arising from the flat band. Some of the present authors have then extended the electronic-structure calculation by going from a group III adatom (Ga) to a group V adatom (As). Unexpectedly, a flat (dispersionless) band appears for some atomic configurations for the As wire as well, which again suggests a possibility of ferromagnetism. As a possible origin of the flat band, Yajima et al. have proposed a tight-binding model, which is thought to capture the essential feature of the arrangement of the arsenic atoms on the wire as a chain of connected squares. (fig.1)

Possibility of ferromagnetism due to the electron-electron repulsion on flat one-electron bands, or a macroscopic degeneracy in the one-electron states, was first shown rigorously for the Hubbard model by Lieb. While Lieb considered the models on bipartite lattices that have different numbers of sublattice sites ($N_A - N_B \propto$ the magnetization), Mielke and Tasaki have later considered line-graph theoretical (non-bipartite) models in which flat bands appear from interferences between the nearest-neighbor transfer $t$ and more distant transfer $t'$. The interference in each plaquette (which is triangular) is in fact a key to their rigorous reasoning why the flat band, when half-filled, leads to the ferromagnetism in the presence of the Hubbard repulsion $U$. One remarkable feature of the Mielke-Tasaki theorem is that an infinitesimal $U$ is enough to make the ground state fully spin-polarized despite the fact that the magnetism appear from the electron correlation.

Now, Yajima’s model for the atomic wire is bipartite, so that Lieb’s theorem is applicable if the site energies are all identical. Since the model is a chain of squares with $N_A = N_B$, the ground state is spin-singlet at half-filling (number of electrons = number of sites). Hence, a kind of Mielke-Tasaki mechanism has to somehow work to realize ferromagnetism in this model.

Usually Mielke’s models (as exemplified by Kagomé lattice) and Tasaki’s models are conceived as the graphs comprising triangles. Penc et al. have actually shown that a chain of connected triangles is favorable for ferromagnetism. One is then tempted to interpret the interference mentioned above as an outcome of a frustration in odd-membered rings. So the challenge here is that: is it possible to have ferromagnetism à la Mielke-Tasaki for non-frustrated (e.g., a chain of even-membered rings as in the model proposed by Yajima et al). This is a doubly nontrivial question, since, even when one has a flat band from even-membered rings, it is by no means a sufficient condition for ferromagnetism and the applicability of the Mielke-Tasaki mechanism has to be examined. In this paper, we address to this question to conclude that, unexpectedly, a ferromagnetism à la Mielke-Tasaki does indeed exist for the non-frustrated model for the atomic-scale wire structure.

We consider the Hamiltonian, which consists of the one-electron tight-binding part, $\mathcal{H}_0$, and the Hubbard repulsion, $\mathcal{H}_U$, where
have a notable property that each eigenfunction cannot be accommodated within a unit cell of the structure (a shaded area in fig.1). This feature is favorable for a realization of the connectivity condition conceived by Mielke and Tasaki.

We first apply the reasoning employed by Mielke and Tasaki to the flat band here, while the effect of other bands is examined later. For this we can use the subspace spanned by \{\psi_{i\sigma}\} for the number of electrons fixed to L (i.e., the half-filled flat band). Any states in this subspace are represented as

\[
\Phi = \sum_{|L_t|+|L_\downarrow|=L} f(L_t, L_\downarrow) \prod_{i \in L_t} \phi^\dagger_{i\uparrow} \prod_{j \in L_\downarrow} \phi^\dagger_{j\downarrow}|0]\]

where \(L_t, L_\downarrow\) are arbitrary subsets of \{1 \cdots L\} with \(|L_t|\) and \(|L_\downarrow|\) being the number of elements, respectively.

If there is a state that satisfies \(\mathcal{H}_U \Phi_{GS} = 0\), then \(\Phi_{GS}\) is the ground state in this subspace and, following the argument by Mielke and Tasaki, we can show for any \(U > 0\) that such states exist, non-degenerate apart from the trivial spin degeneracy as follows. First we require that \(n_i^{\uparrow} n_i^{\downarrow} \Phi_{GS} \equiv 0\) or \(n_i^{\uparrow} n_i^{\downarrow} \Phi_{GS} \equiv 0\) for any \(i\). To satisfy this condition, we must choose \(L_t\) and \(L_\downarrow\) so that \(L_t \cap L_\downarrow = \emptyset\). Hence, we can represent any ground state as

\[
\Phi_{GS} = \sum_{\tilde{\sigma}} g(\tilde{\sigma}) \prod_{i} \phi^\dagger_{i\tilde{\sigma}(i)}|0]\]

where \(\tilde{\sigma}\) represents the spin configuration.

For \(\mathcal{H}_U \Phi_{GS} = 0\) to be fulfilled we require \(n_i^{\uparrow} n_i^{\downarrow} \Phi_{GS} \equiv 0\) or \(n_i^{\uparrow} n_i^{\downarrow} \Phi_{GS} \equiv 0\) for any \(i\). This requirement amounts to

\[
0 = b_i^{\uparrow} b_i^{\downarrow} \Phi_{GS} = \sum_{\tilde{\sigma}} [g(\tilde{\sigma}) - g(\tilde{\sigma}_{i\uparrow\downarrow})] \prod_{j,j \neq i} \phi^\dagger_{j\tilde{\sigma}(j)}|0],
\]

where \(\sum\) stands for a summation over \(\tilde{\sigma}\) that satisfies \(\tilde{\sigma}(i-1) = \downarrow\) and \(\tilde{\sigma}(i) = \uparrow\). From this we can see that \(g(\tilde{\sigma}) = g(\tilde{\sigma}_{x\cdots y})\) for any \(x, y \in \{1 \cdots L\}\), where \(\tilde{\sigma}_{x\cdots y}\) denotes the spin configuration obtained by exchanging \(\tilde{\sigma}(x)\) and \(\tilde{\sigma}(y)\). The lowest energy state \((\mathcal{H}_U \Phi_{GS} = 0)\) with a given total \(S_z(= \frac{1}{2}(L_t - L_\downarrow))\) is unique because all the \(g(\tilde{\sigma})\)'s for each \(S_z\) sector take the same value and factor out. This is exactly the ferromagnetic ground states, since the fully polarized state does not experience \(U\), and this concludes the proof of the above statement.

In the present model a dispersive band lies below the flat one unlike the Mielke’s or Tasaki’s model. We can expect that a small enough \(U\) does not mix the bands since they are separated with a finite gap, but this has to be examined. For that purpose we take account of the one-electron states \{\psi_{i\sigma}\}_{i=1 \cdots L_\downarrow} on the dispersive band as well (where the number of states \(L_\downarrow\) is just \(L\) here, since we have only one dispersive band below the flat one). As Mielke discussed, sufficiently small \(U\) can be
treated with a degenerate perturbation theory, and we can show that the ground state of $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_U$ with $L + 2L_c$ electrons still has the total spin $S = L/2$ for a small $U$.

By contrast, this approach becomes invalid for a large $U$, so that it is necessary to determine the total spin of the ground state from other methods. We have determined this numerically with the exact diagonalization. First, let us consider the case of $\Delta \varepsilon = 0$. In fig.5 we show the result for the case of 6 electrons in 8 sites ($L = 2$) or 12 electrons in 16 sites ($L = 4$), for which the band filling is $n = 3/4$ with the flat band being half-filled. We denote the lowest energy among the states having a given total $S_z$ by $E_{\text{min}}(S_z)$, and plot $\Delta \equiv E_{\text{min}}(S_{\text{max}}) - E_{\text{min}}(0)$, where $S_{\text{max}} = L/2$ is the $S_z$ when the flat band is fully spin polarized ($S_{\text{max}} = 1$ for the 8-site case, $S_{\text{max}} = 2$ for the 16-site case), as a function of $U$. In agreement with the above analysis, the ground state has indeed the polarized flat band from an infinitesimal $U$.

Our second new finding is that the ferromagnetism is destroyed when the interaction is too large ($U > U_C$). The critical value $U_C$ at which the ground state becomes unpolarized is seen to be $U_C = 2.3 \sim 2.4$, where the sample-size dependence is small. To the best of our knowledge this is the first example of the ferromagnetism that is unstable for large interactions.

In order to check whether the transition to the unpolarized state is abrupt, we plot in the inset of fig.3 $\Delta = E_{\text{min}}(2) - E_{\text{min}}(1)$ along with $\Delta = E_{\text{min}}(2) - E_{\text{min}}(0)$ against $U$ for the 16-site system. We can see that the transition from the state with $S = L/2$ directly into the $S = 0$ state.

So far we have considered the case of half-filled flat band. In the As/Si system this would require a doping with e.g., alkali metal atoms. The ferromagnetism is expected to be degraded when the flat band is pushed away from the half filling. It is believed that one-dimensional Tasaki’s model is ferromagnetic only when the flat band is half-filled, while paramagnetic for lower electron densities. In order to see if this is also the case in the present model, we calculate $\Delta = E_{\text{min}}(1) - E_{\text{min}}(0)$ as a function of $U$ for the number of electrons decreased from 12 to 10 (quarter-filled flat band) in the 16-site system. For the parameter region we have investigated, the ground state is paramagnetic, i.e., the model shares the instability against the hole doping with the one dimensional Tasaki’s model.

We must also look into how the ferromagnetism proposed here is robust against the degradation of the flatness of the band. For Tasaki’s model, Kusakabe and Aoki have shown that ferromagnetic ground state survives small perturbations that make the flat band dispersive. Here we look at the stability of the ferromagnetism against the perturbation, $\mathcal{H}' = \delta t \sum_{i, \sigma} (c_i^\dagger b_{i+1} + \text{h.c.})$.

There are two reasons why we consider such an extra transfer. First, in real atomic wires, there should be a finite transfer between the adjacent As clusters, and secondly, the ferromagnetism on the ladder system is subject to recent investigations, so that the effect of a perturbation toward the ladder is of interest. In fig.6 we plot $\Delta = E_{\text{min}}(S_{\text{max}}) - E_{\text{min}}(0)$ as a function of $U$ for $\delta t = 0.1, 0.2$ for 6 electrons in 8 sites. We can see that the ferromagnetism survives $\delta t = 0.1$, while destroyed for $\delta t = 0.2$.

Next, we look at the robustness of the ferromagnetism for the general value of $\Delta \varepsilon \neq 0$ ($\theta \neq -\pi/6$). We can start from an observation that the ferromagnetism will be lost for $\theta = 0$ or $-\pi/2$, since $\{ \phi_{i,\sigma} \}$ fails to satisfy the connectivity condition for $\theta = 0$ invalidating Mielke-Tasaki’s argument, or the lattice becomes disconnected with $t_3 = 0$ for $\theta = -\pi/2$. We have numerically obtained $U_C$ as a function of $\Delta \varepsilon$ for 8 sites in fig.7. We can see that $U_C$ is finite between $\theta = 0$ and $-\pi/2$, taking its maximum at $\Delta \varepsilon \sim 0.5$ ($\theta \sim -\pi/4$), or, equivalently, $\Delta \varepsilon \sim -0.5$ with $t_1, t_2 < 0$.

Finally let us make a brief comment. If we change $t_2$ from positive to negative, the flat band becomes the lowest band, where the ferromagnetic ground state is realized for arbitrary $U > 0$ when the flat band is half-filled as in Tasaki’s model or Mielke’s model.

To summarize, we have proposed that the flat-band ferromagnetism can occur in a non-frustrated structure that can model atomic-scale quantum wires. Further investigations with the density matrix renormalization group method will be published elsewhere. Also, the fabrication of the As/Si(100) wire is experimentally under way. R.A. is grateful to K. Kusakabe for illuminating discussions. Numerical computations were done on FACOM VPP 500/40 at the Supercomputer Center, Institute of Solid State Physics, University of Tokyo.

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FIG. 1. A tight binding model proposed by Yajima et al. We have indicated the eigenstate on the flat band. Open circles represent As atoms, while filled circles Si. Shaded area depicts a ‘Wannier’ state.

FIG. 2. The dispersion relation for the tight-binding model on the connected square lattice for a general value of θ (a) and for θ = −π/6 (∆ε = 0) (b).

FIG. 3. The difference in energy, ∆ ≡ E_{\text{min}}(S_{\text{max}}) − E_{\text{min}}(0) for 6 electrons in 8 sites (squares), and for 12 electrons in 16 sites (circles). In the inset, we plot the difference in energy, E_{\text{min}}(1) − E_{\text{min}}(0) (squares) and E_{\text{min}}(2) − E_{\text{min}}(0) (circles) for 12 electrons in 16 sites.

FIG. 4. A similar plot as in Fig. 3 for ∆ = E_{\text{min}}(S_{\text{max}}) − E_{\text{min}}(0) when an extra transfer δt (= 0.1:circles or 0.2:squares) is introduced (as in the inset) for 6 electrons in 8 sites.

FIG. 5. U_{\text{C}} as a function of ∆ε for 6 electrons in 8 sites.
Fig. 1

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Fig. 2

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Fig. 3

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Fig. 5

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