Flat-band ferromagnetism induced by off-site repulsions

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Density matrix renormalization group method is used to analyze how the nearest-neighbor repulsion \( V \) added to the Hubbard model on 1D triangular lattice and a railway trestle \((t-t')\) model will affect the electron-correlation dominated ferromagnetism arising from the interference (frustration). Obtained phase diagram shows that there is a region in smaller-\( t' \) side where the critical on-site repulsion above which the system becomes ferromagnetic is reduced when the off-site repulsion is introduced.

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The itinerant-electron ferromagnetism arising from electron correlations has a long history, dating back to the works by Hubbard, Kanamori and Gutzwiller for the Hubbard model. It has become increasingly clear that the criterion for the ferromagnetism is a formidable question when the correlation effect is fully taken into account. There is a rigorous work by Nagaoka in the limit of infinite repulsion and infinitesimal doping, but the ferromagnetism is there singular in that the spin stiffness vanishes as an inverse system size.

Recently, a new light has been shed on the problem, when Lieb and later Mielke and Tasaki, have shown that flat (dispersionless) bands in the one-electron band structure are good news for the ferromagnetism. Remarkably, we can show that the correlation rigorously guarantees the ferromagnetism for arbitrary strength of the repulsion \( U \) when the flat band is half-filled.

Occurrence of flat bands requires two classes of special lattice structures. Lieb’s model exploits the lattices that have different numbers of sublattice sites, while Mielke’s and Tasaki’s model provide the flat bands from interferences between the nearest-neighbor transfer \( t \) and more distant transfers \( t' \), which are assumed to have sizeable magnitude \( (t' \approx t) \). Kusalabe and Aoki have shown that the ferromagnetism is indeed stable, since, first, the spin stiffness is finite both in \( U/t \to 0 \) and \( U/t \to \infty \) limits despite an apparent lack of relevant energy scales, and second, the magnetism survives for finite dispersions. Tasaki has shown exactly that the magnetism is not destroyed for some class of dispersive bands for sufficiently large \( U \).

These systems should be regarded as insulators because half-filled flat bands are considered there. Whether a ferromagnetic ground state persists in metallic phases, i.e., for non-half-filled bands, is of great interest, since this will imply an itinerant ferromagnetism. Penc et al. studied one dimensional (1D) models such as triangles connected linearly, which may be thought of as a strip cut out from Kagomé lattice, a realization of Mielke’s model. Intuitively, a single triangle alone has a frustration in spin configurations, which results in an effectively ferromagnetic exchange interaction. Penc et al have shown, using an effective Hamiltonian in some limit \( (U/t \to \infty, \text{etc}) \), that the 1D triangular lattice (Fig.1b) also has a ferromagnetic effective coupling between spins. The system is then expected to show ferromagnetism for general electron density in this limit. Sakamoto and Kubo studied with the density matrix renormalization group (DMRG) whether the ferromagnetic ground state survives finite dispersions when hole is doped to the nearly flat band.

On the other hand, Daul and Noack numerically determined the phase diagram of a 1D Hubbard model having both nearest- and next-nearest-neighbor transfers \((t-t' \text{ Hubbard model})\), which is topologically equivalent to a railway trestle (Fig.1c). They have found a large ferromagnetic region for finite densities and finite on-site interactions. While a 1D triangular lattice is a two-band system with the lower band being flat, the trestle has a single band, but its bottom can be nearly flat depending on the value of \( t' \). Hence we may include this ferromagnetism in the flat-band ferromagnetism in a broader context.

In the studies mentioned above, only the on-site repulsion \( (U) \) is considered. In real materials, however, there are additional terms of appreciable strengths such as nearest-neighbor charge-charge interaction \( (V) \), bond-charge interaction \( (X) \), exchange interaction \( (F) \), or on-site pair-hopping \( (P') \), which have been investigated for itinerant ferromagnetism, Kollar, Strack and Vollhardt have derived sufficient conditions for realizing a ferromagnetic ground state for general lattices with one hole in a half-filled band (generalized Nagaoka’s case). They conclude that \( F \) is important in stabilizing ferromagnetism for finite \( U \), while for the special case of \( X = t \)
the ferromagnetism is stable for $F = 0$.

The purpose of the present paper is to study the effect of the nearest-neighbor repulsion $V$ for the flat-band ferromagnetism as exemplified by the 1D triangular lattice or trestle. The reason why we focus on the effect of $V$ is that it usually takes the largest value among $V, X, F, F'$, playing an important role in such materials as organic compounds. Physically, the repulsion $V$, despite being a charge-charge interaction, can affect the magnetism through Pauli’s exclusion that makes the interaction effectively spin-dependent, but how the effect is exerted is a non-trivial question. Here we have employed DMRG, a powerful method for investigating strongly correlated 1D systems, to obtain the phase diagram against $U$ and $t'$. We have found that the ferromagnetic region shifts to the smaller-$t'$ side when $V$ is switched on.

It is heuristic to start with a single triangle consisting of sites 1, 2, 3 (Fig. 3). The Hamiltonian is given by

$$
\mathcal{H} = -t \sum_{i=1}^{2} \sum_{\sigma} (c_{i\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) + t' \sum_{\sigma} (c_{j-1,\sigma}^\dagger c_{j+1,\sigma} + \text{H.c.}) + U \sum_{k=1}^{3} n_{k\uparrow} n_{k\downarrow} + V \sum_{i=1}^{2} n_{i\uparrow} n_{i+1}
$$

in standard notations, where $t$ is the transfer between 1, 2 and 2, 3, $t'$ the transfer between 1, 3 with $j = 1$, and $U$ the on-site repulsion. The nearest-neighbor repulsion $V$ is assumed to act between 1, 2 and 2, 3 only. Hereafter we take $t = 1$ as a unit of energy and consider the case of $t' > 0$, which favors the occurrence of flat bands.

In Fig. 2, we show for two electrons on a triangle the difference in energy, $\Delta \equiv E_t - E_s$, between the lowest spin-triplet state ($E_t$) and the lowest spin-singlet state ($E_s$) as a function of $V$ for $U = 10$ with $t'$ varied from 0.15 to 0.25. Unexpectedly, the curves can be non-monotonic: For $t' = 0.2$ the ground state, which is a spin-singlet at $V = 0$, becomes a triplet around $V = 5$, then re-enters into a singlet for $V > 7$.

The curious behavior can be understood intuitively as follows. Let us assume that the effect of the repulsion $V$ can be taken into account by reducing $t$ to a smaller $t_{\text{eff}}$, because $V$ reduces the amplitude of an electron residing on the top site 1. This is reminiscent of the approximation often adopted in the $t$-$J$ model, where the effect of the infinite on-site repulsion is taken into account by a reduction in $t$. When we vary $t'$ in the absence of $V$, the high-spin state becomes most stable ($\Delta$ takes its minimum) at $t' = t$ as shown in Fig. 3 for $U = 10$. In the above argument $V = 5$ should then correspond to the case where $t$ is reduced to $t_{\text{eff}} \simeq t'$ (= 0.2 here).

Now, an obvious question is: can this ferromagnetism induced by a repulsion survive when we connect the triangles into a 1D chain? So we have applied the DMRG method to the Hubbard model on a 1D triangular chain and to the trestle to look into such a possibility.

The phase boundary between the ferromagnetic and paramagnetic phases can be determined in finite size systems as follows. For $V \neq 0$, we first calculate the ground-state energy ($E_{\text{FP}}$) for fully spin-polarized state with DMRG. There the Hilbert space is much smaller than that of spinful electrons and the energy can be obtained very accurately. For $V = 0$, the ground state energy can be readily obtained, since spinless fermions do not feel $U$. Next we calculate with DMRG the ground-state energy ($E_{\text{G}}$) of a system having equal numbers of up-spins and down-spins (with $S_z = 0$) to compare with $E_{\text{FP}}$. Alternatively we can directly calculate the total spin from

$$
S_{\text{tot}}^2 = \sum_{i,j} \langle S_i \cdot S_j \rangle.
$$

From these independent methods we can determine whether the ground state is ferromagnetic. In our calculation the two methods gave the same result.

The calculation has been performed mainly for the number of atoms $L = 39$ with an open boundary condition, and the convergence with respect to the system size has been confirmed by extending $L$ to 90. We have kept up to 120 states per block at each step. Using the finite-size algorithm, we swept the system about ten times. We stored the density matrix at each step to construct a good initial vector for each superblock diagonalization.

We have obtained accurate wave functions with inverse iteration and conjugate-gradient optimization after each diagonalization.

Let us first look at the 1D triangular chain, for which the one-electron energy band has a perfectly flat branch when $t' = t/\sqrt{2}$. The Hamiltonian is given as before, where we have now $1 \leq i \leq L - 1$, $1 \leq j \leq (L - 1)/2$, $1 \leq k \leq L$. We have found that the value of $U$ required for the ferromagnetic ground state can indeed be reduced for nonzero $V$ for appropriate values of parameters, i.e., the band filling $n = \text{(number of electrons)/(number of sites)} < 0.4$ and $t' < 0.5$. A typical result is displayed in Fig. 2 where we plot $\Delta = E_{\text{FP}} - E_{\text{G}}$ as a function of $U$ for $n = 0.2$ and $t' = 0.31$. The one-electron band structures are depicted in the inset of the figure. We can see that the ground state becomes ferromagnetic for $U > 5$ for $V = 0$, while the onset of the ferromagnetism is reduced to $U = 4$ for $V = 2$. Thus there is a parameter region in which the ferromagnetism is realized only when the on-site repulsion exists, as in the case of a single triangle.

The result that this phenomenon occurs only for smaller band fillings ($n < 0.5$) may be understood as follows. In the above argument for a single triangle, we have assumed two electrons. If we envisage that we require at least one hole per triangle (i.e., one hole per unit cell that consists of two sites) for the triangle lattice in a similar manner, this precisely amounts to $n < 0.5$.

Let us next consider the $t$-$t'$ Hubbard model (fig. 2c). The Hamiltonian is given as
\[ \mathcal{H} = -t \sum_{i,\sigma}(c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}) + t' \sum_{i,\sigma}(c_{i\sigma}^\dagger c_{i+2\sigma} + \text{H.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{i} n_{i\uparrow} n_{i+1}. \]

In Fig. 3, we again plot \( \Delta = E_{FP} - E_{G} \) as a function of \( U \) for \( t' = 0.16, n = 0.4, \) and \( V = 0 \) or 4. It can be seen that the critical value, \( U_c \), above which the ferromagnetism appears is reduced from \( U_c = 7 \) down to \( U_c = 5 \) for \( V = 4 \). When we make the off-site repulsion too large \((V = 20)\), the ferromagnetic ground state is washed away at least for \( U < 8 \). Thus, as in a triangle and in a one-dimensional chain, an intermediate value of \( V \) makes the ground state to be ferromagnetic for appropriate values of \( t', n \) and \( U \).

Figure 3 is the full phase diagram on the \( U - t' \) plane. From this we can see that the ferromagnetic region, which has a concave boundary for \( V = 0 \), shifts to the lower side of \( t' \) when \( V \) is introduced. The reduction of \( U_c \) found above is one manifestation of this. Intuitively, the reason why we have a concave ferromagnetic boundary with a minimum around \( t' \approx 0.36t \) for \( V = 0 \) is that the ferromagnetism becomes most favorable when the one-electron band, displayed in the accompanied panels in the figure, approaches a flat band. Namely, the band in the \( t - t' \) model cannot become exactly flat, but can become nearly so for \( t' \approx 0.36t \), which is in between the single-minimum band and the double-minimum band. The shift of this concave curve with \( V \) may be understood qualitatively from the above argument that \( V \) effectively reduces 0.36t into 0.36\text{eff}.

For the generalized Nagaoka’s ferromagnetism, a sufficient condition for a reduction of \( U_c \) has been shown by Kollar et al. \cite{Kollar}, where for \( F \neq 0 \) or \( X = t \) the condition on \( U \) is relaxed when we take an appropriate value of \( V \). The present result implies that for small \( t' \), off-site repulsion can stabilize the flat-band ferromagnetism as well.

To summarize, we have found for (nearly) flat bands arising from frustration (1D t-t’ model and triangular lattice) a region in the phase diagram where the critical on-site repulsion for ferromagnetism is reduced when we introduce an off-site repulsion. Recently, ferromagnetism in three-dimensional lattice structures (bcc, fcc, etc) has received attention. \cite{Vollhardt, Hanisch} Since network formed by the transfers in bcc and fcc lattices are also frustrated in that they comprise triangles, it may be interesting to analyze the effect of \( V \) in these systems.

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\[ \text{FIG. 1. A single triangle (a), 1D triangular lattice(b), and the railway trestle (or t-t') model(c).} \]

\[ \text{FIG. 2. The difference in energy, } E_1 - E_2, \text{ between the lowest triplet state and the lowest singlet state for a single triangle plotted as a function } V \text{ with } U = 10 \text{ for } t' \text{ varied from 0.15 to 0.25.} \]

\[ \text{FIG. 3. The difference in energy, } E_1 - E_2, \text{ between the lowest triplet state and the lowest singlet state for a single triangle plotted as a function } t' \text{ for } U = 10 \text{ with } V = 0. \]
FIG. 4. The difference in energy ($\Delta$) between the lowest ferromagnetic state and the ground-state for a 1D triangular lattice plotted as a function of $U$ for $t' = 0.31$, $n = 0.2$ with $V = 0$ or 2. Solid circles represent the result for 39 sites, diamonds for 59 sites, while the arrows indicate $U_c$. Inset shows one-electron band structures, where the horizontal dashed line indicates the Fermi level.

FIG. 5. A similar plot as in the previous figure for the $t$-$t'$ Hubbard model for $t' = 0.16$, $n = 0.4$ with $V = 0$ or 4.

FIG. 6. The phase diagram (P: paramagnetic, F: ferromagnetic) against $U$ and $t'$ for the $t$-$t'$ Hubbard model for $n = 0.4$ with $V = 0$ or 4. One-electron band structures are displayed in the accompanied panels for three typical values of $t'$ labeled with (a),(b),(c), where the horizontal dashed lines indicate the Fermi level.
Fig. 1

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Fig. 2

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Fig. 3

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$1D$ triangular lattice
t' = 0.31, n = 0.2

Fig. 4

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Fig. 5

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Fig. 6

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