Ferromagnetism in Hubbard models with nearest-neighbor Coulomb repulsion

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Abstract

We propose a mechanism which leads to ferromagnetism in extended Hubbard models on lattices composed of triangles. We show that the ferromagnetic ground state is stabilized in the quarter filling case through a third-order electron exchange process around a triangle when both on-site repulsive interaction and nearest-neighbor one are much larger than the hopping terms. Numerical calculations for a one-dimensional lattice consisting of triangles give the evidence that the ground state is ferromagnetic not only in the quarter-filling case but also away from quarter-filling.

Key words: Hubbard model; nearest-neighbor Coulomb repulsion; groundstate; ferromagnetism

Much effort has been invested in studying the Hubbard model, the tight binding model with the on-site repulsive interaction, to understand ferromagnetism in itinerant electron systems. Through a number of analytical and numerical works and a few rigorous works [1-4], it is now known that the model exhibits ferromagnetism in certain cases, although a true theoretical understanding of itinerant electron ferromagnetism is far away.

The Coulomb interaction is a long range interaction, so that it is important to clarify effects of long distance electron-electron interactions on ferromagnetism in real materials. The extended Hubbard model which includes nearest-neighbor electron-electron interactions is usually used to study the problem. So far the importance of the direct exchange interaction in stabilizing ferromagnetism has been reported [5, 6], but literature concerning effects of nearest-neighbor Coulomb repulsion, which can be the largest among nearest-neighbor electron-electron interactions, is still limited.

The purpose of the present paper is to examine the effect of the nearest-neighbor Coulomb repulsion. It is noted that the nearest-neighbor Coulomb repulsion is independent of spin, unlike the direct exchange interaction, and how ferromagnetism is affected by it is a non-trivial problem [7]. We consider the following extended Hubbard model on a one-dimensional trestle lattice (Fig.1),

$$H = \sum_{j,\sigma}(-t\ c^{\dagger}_{j,\sigma}c_{j+1,\sigma} + t'\ c^{\dagger}_{j,\sigma}c_{j+2,\sigma} + \mathrm{H.c.}) + U\sum_{j} n_{j,\uparrow}n_{j,\downarrow} + V\sum_{j,\sigma,\tau} n_{j,\sigma}n_{j+1,\tau}, \tag{1}$$

where $c^{\dagger}_{j,\sigma}$, $c_{j,\sigma}$ and $n_{j,\sigma}$ are the creation, annihilation and number operators for an electron with spin σ at the j th site, respectively. The density of electrons is defined by $n = N_{\mathrm{e}}/L$, where N_{e} is the number of electrons, and L is the total number of sites. We show that the ferromagnetic phase exists in the ground state of Hamiltonian (1) at the quarter-filling by a perturba-

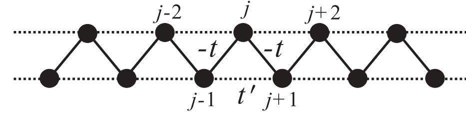

Fig. 1. A one-dimensional trestle lattice

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tion theory and away from quarter-filling by numerical calculations.

First, we consider the case of $U \to \infty$ and $V \to \infty$ at the quarter-filling ($n = 1/2$). In this limit, the states in which each even site is occupied by just one electron are the ground states. There is no spin-spin correlation in these states, i.e., the ground states are paramagnetic.

Next, relaxing the condition as $t, t' \ll V$, we derive the effective Hamiltonian. The first-order perturbation theory in $1/V$ is vanishing and the second-order one only shifts the energy by a constant, but through the third-order perturbation process (Fig.2) we obtain the following effective Hamiltonian:

$$H_{\rm eff} = -4t'\left(\frac{t}{V}\right)^2 \sum_j \left(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+2} - \frac{1}{4}\right) + \text{const}, \qquad (2)$$

where $\boldsymbol{S}_j$ is an operator of a spin-1/2 at site j. This is just a ferromagnetic Heisenberg model.

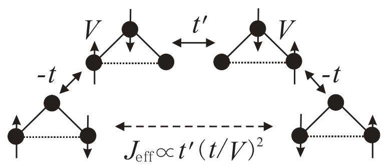

Fig. 2. The third-order process leading to ferromagnetic effective exchange $J_{\rm eff} = -4t'(t/V)^2$.

Furthermore, assuming $t, t' \ll U$, we take into account the lowest term in $1/U$. The term which should be added to the effective Hamiltonian (2) is $4[(t')^2/U]\sum_j(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+2} - \frac{1}{4})$, i.e., a kinetic exchange one. Therefore, whether the effective Hamiltonian for large values of U and V favors ferromagnetism or not will be decided by the competition between a ferromagnetic term and an antiferromagnetic one, in other words, whether $U \geq U_c \sim t'(V/t)^2$ or not.

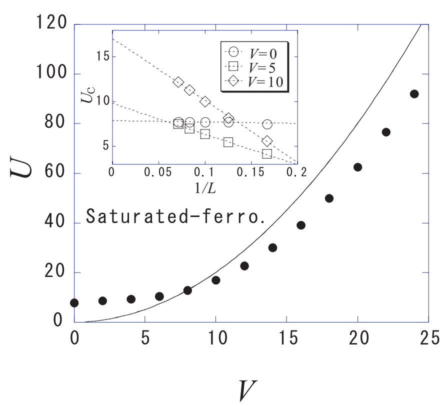

Fig. 3. The phase diagram for $n = 1/2$, $t = 1.0$ and $t' = 0.2$. The solid line is $U = t'(V/t)^2$, and U_c which is represented by solid circles are estimated by a sample-size scaling of numerical calculations. In the inset we display the sample-size scaling for some values of V.

Figure 3 is a result of exact numerical diagonalizations with open boundary conditions. The result supports the mechanism for ferromagnetism by the third-order process for $t, t' \ll U, V$. Our numerical calculations also indicate that the ground states are ferromagnetic for sufficiently large values of U even if the value of V is small, in which the perturbation theory breaks down.

Finally, we discuss the case of $n < 1/2$. Figure 4 is a result of exact numerical diagonalizations with open boundary conditions. This result shows that for sufficiently large values of U and V the ground states are saturated ferromagnetic over a wide range of $n < 1/2$. In particular, we find that ferromagnetism is most stabilized in a certain density ($n \sim 0.4$) of electrons away from the quarter-filling. This indicates that greater mobility of electrons in addition to the ferromagnetic exchange interaction arising from the third-order electron exchange process in $1/V$ generates ferromagnetism successfully.

In this paper we investigated the one-dimensional trestle lattice, and it is expected that the present mechanism for ferromagnetism can work for other lattices composed of triangles, such as bcc and fcc, provided U and V are much larger than hopping terms.

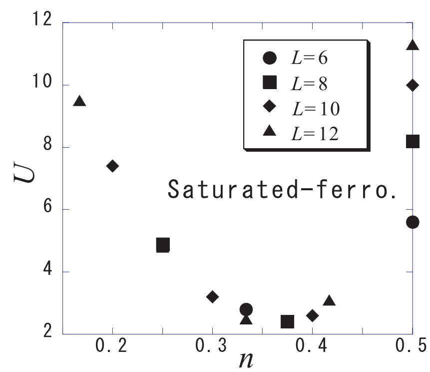

Fig. 4. The phase diagram for $t = 1.0$, $t' = 0.2$ and $V = 10$.

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