Ferromagnetism in one-dimensional Hubbard model induced by the next-nearest-neighbor hopping at electron density 3/2*

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Ferromagnetism in the one-dimensional Hubbard model with the next-nearest-neighbor hopping is explored by using the exact-diagonalization method in a small cluster and the equation-of-motion method in the thermodynamic limit with electron density $n = 3/2$. With these two complementary methods, it is found that an intermediate value of the next-nearest-neighbor hopping amplitude t_1 tends to stabilize the fully polarized ferromagnetic state under the condition that the on-site coulomb interaction U is sufficiently large in our model. The ground-state phase diagram of the model is presented in the t_1–U plane.

Keywords: ferromagnetism, frustration effect, random phase approximation

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1. Introduction

Since its introduction in 1963, the Hubbard model has become one of the most popular models that describe a strongly correlated electron system with short-range interactions. A great variety of many-body phenomena in metals have been investigated using this model, including ferromagnetism, metal–insulator transitions, charge-density waves, and superconductivity. Originally, the model was expected to describe the behavior of metallic ferromagnetism. However, it was soon realized that the single-band Hubbard model is more convenient to explain the antiferromagnetism for a half-filled band. In fact, only in a few very special cases is the existence of ferromagnetism proven rigorously.

The first well-known realization of ferromagnetism is the Nagaoka state, which originates from the Hubbard model when the on-site coulomb interaction is infinitely large with one hole in a half-filled band.[1] Later, the result was generalized to an infinite number of holes in a half-filled band, but the density of the holes is still in the limit of zero.[2,3] Some special lattices have also been proposed to have a ground state with ferromagnetism.[4,5] Moreover, when the next-nearest-neighbor hopping is introduced in the Hubbard model, it has been shown that the ferromagnetism can exist for the one-dimensional Hubbard model at low electron densities.[6] This discovery implies that the hopping term plays an important role in stabilizing the ferromagnetic state. By following this direction, the generalized long-range and unconstrained hopping of electrons has been introduced to realize ferromagnetism ground states.[7–10] In order to achieve ferromagnetism in a realistic material, the frustration effect was considered in a small cluster doped with electrons. We found that the ferromagnetic ground state is stable as long as the Coulomb repulsion interaction between electrons is sufficiently strong.[11] However, the result is valid only for a finite size. The exploration of ferromagnetism for an actual material in the thermodynamic limit is still an open question.

In this paper, we investigate a possible mechanism, which is based on the frustration effect induced by the next-nearest-neighbor electron hopping, to stabilize ferromagnetism in the one-dimensional Hubbard model in the thermodynamic limit and the region with overdoped electrons in a half-filled band. To understand why such a frustration effect is important in the system, let us recall first some basic facts. As is well known, the spontaneous magnetization of solids is caused by the correlation effect of electrons, whose hopping among different ionic orbitals is greatly hindered by the strong on-site Coulomb repulsion. On the other hand, the hopping amplitude t_{ij} of the electrons decays rapidly as the distance between two sites i and j increases. Therefore, for a bulk material with a crystalline structure, one can simply assume that the electron hopping takes place between the nearest-neighbor lattice sites. In this case, the frustration effect is less important and the antiferromagnetic superexchange interaction caused by the electron virtual hopping process is dominant.[12] However, when the next-nearest-neighbor electron hopping is introduced, the frustration effect might suppress the antiferromagnetic superexchange. As we shall show in the following, such an effect indeed plays an essential role in stabilizing ferromagnetism in our proposed system.

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2. Model and method

The Hamiltonian of the one-dimensional Hubbard model with the next-nearest-neighbor electron hopping reads

$$H = \sum_{i,\sigma} -(tc^{\dagger}_{i,\sigma}c_{i+1,\sigma} + t_1 c^{\dagger}_{i,\sigma}c_{i+2,\sigma} + \text{H.c.}) + \sum_i U n_{i\uparrow}n_{i\downarrow}, \quad (1)$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator that creates (annihilates) an itinerant electron of spin σ at lattice site i, t_{ij} represents the hopping of electrons between sites i and j, and parameter $U > 0$ is the on-site Coulomb interaction between two itinerant electrons.

To investigate the stability of ferromagnetism of this system in the thermodynamic limit, the retarded Green function G^{r}_{σ} will be calculated by using the equation of motion (EOM) method and the random phase approximation (RPA). In this section, we discuss the EOM in brief.

Following the standard procedure,[13,14] we take the derivative of $G^{\mathrm{r}}_{\sigma}(t-t')$ with respect to t first. By setting $\hbar = 1$, we obtain

$$\mathrm{i}\frac{\partial}{\partial t}G^{\sigma}_{ij}(t-t') = \delta(t-t') + \langle\langle [c_{i\sigma}(t), H]; c^{\dagger}_{j\sigma}(t')\rangle\rangle, \quad (2)$$

with

$$\langle\langle A(t); B(t')\rangle\rangle = -\mathrm{i}\theta(t-t')\langle\{A(t); B(t')\}\rangle, \quad (3)$$

where $\{A;B\}$ is the anticommutator of the operators. Therefore, we have the identity $G^{\mathrm{r}}_{\sigma}(t-t') \equiv \langle\langle c_{\sigma}(t); c^{\dagger}_{\sigma}(t')\rangle\rangle$. By using the Fourier transformation, the above equation can be simplified to

$$\omega\langle\langle c_{i\sigma}; c^{\dagger}_{j\sigma}\rangle\rangle_{\omega} = \langle [c_{i\sigma}, c^{\dagger}_{j\sigma}]\rangle + \langle\langle [c_{i\sigma}, H]; c^{\dagger}_{j\sigma}\rangle\rangle_{\omega}, \quad (4)$$

where

$$[c_{i\sigma}, H] = \sum_j t_{ij}c_{j\sigma} + U n_{i\bar{\sigma}}c_{i\sigma}, \quad (5)$$

$$[n_{i\bar{\sigma}}c_{i\sigma}, H] = U n_{i\bar{\sigma}}c_{i\sigma} + \sum_j t_{ij}n_{i\bar{\sigma}}c_{j\sigma} + \sum_j t_{ij}(c^{\dagger}_{i\bar{\sigma}}c_{j\bar{\sigma}} - c^{\dagger}_{j\bar{\sigma}}c_{i\bar{\sigma}})c_{i\sigma}. \quad (6)$$

Obviously, equation (4) is not closed. To make Eq. (4) closed, we can use the Hartree–Fock decoupling approximation. However, if we carry out the procedure at this stage, we can not obtain a convincing result for the phase transition from the non-ferromagnetic phase (NFM) to the ferromagnetic phase (FM). Therefore, we need to further calculate the higher-order Green functions on the right-hand side of Eq. (4). To decouple Eq. (4), the random phase approximation is introduced:

$$\sum_j t_{ij}(c^{\dagger}_{i\bar{\sigma}}c_{j\bar{\sigma}} - c^{\dagger}_{j\bar{\sigma}}c_{i\bar{\sigma}}) = 0. \quad (7)$$

$\hat{n}_{i\sigma}$ will be substituted by its expectation value $\langle n_{\sigma}\rangle$.

The closed equation group is derived as follows:

$$\omega G^{\sigma}_{ij}(\omega) = \delta_{ij} + \sum_k t_{ik}G^{\sigma}_{kj}(\omega) + U\Gamma^{\sigma}_{ij}(\omega), \quad (8)$$

$$\omega\Gamma^{\sigma}_{ij}(\omega) = \langle n_{\sigma}\rangle\delta_{ij} + \langle n_{\bar{\sigma}}\rangle\sum_k t_{ik}G^{\sigma}_{kj}(\omega) + U\Gamma^{\sigma}_{ij}(\omega), \quad (9)$$

where $\Gamma^{\sigma}_{ij}(\omega) = \langle\langle n_{i\bar{\sigma}}c_{i\sigma}; c^{\dagger}_{j\sigma}\rangle\rangle_{\omega}$.

We are able to solve the above equations and obtain

$$\omega G^{\sigma}_{ij}(\omega) = \frac{1 + U\langle n_{\bar{\sigma}}\rangle}{\omega - U}\left[\delta_{ij} + \sum_k t_{ik}G^{\sigma}_{kj}(\omega)\right]. \quad (10)$$

The above equation can be transformed to its momentum representation by the following Fourier transformation:

$$G^{\sigma}_{ij}(\omega) = \frac{1}{N}\sum_k \mathrm{e}^{\mathrm{i}\bar{k}(\bar{R}_i - \bar{R}_j)}G^{\sigma}_k(\omega). \quad (11)$$

So we have

$$\omega G^{\sigma}_k(\omega) = \frac{1 + U\langle n_{\bar{\sigma}}\rangle}{\omega - U}[1 + \varepsilon(k)G^{\sigma}_k(\omega)]. \quad (12)$$

Here $\varepsilon(k)$ is the dispersion with expression $-2t\cos k - 2t_1\cos(2k)$ in our model. The final explicit expression of $G^{\sigma}_k(\omega)$ is derived as

$$G^{\sigma}_k(\omega) = \frac{\omega - U(1 - \langle n_{\bar{\sigma}}\rangle)}{(\omega - \varepsilon(k))(\omega - U) - \langle n\sigma\rangle U\varepsilon(k)}. \quad (13)$$

Consequently, under the RPA approximation, the energy state density ρ_{σ} can be written as

$$\rho_{\sigma}(\omega) = \frac{\mathrm{i}}{2\pi}\sum_k [G^{\sigma}_k(\omega + \mathrm{i}\eta) - G^{\sigma}_k(\omega - \mathrm{i}\eta)], \quad (14)$$

where $\eta = 0^+$.

To determine $\langle n_{\sigma}\rangle$ and chemical potential μ, we use the following self-consistent equation:

$$\langle n_{\sigma}\rangle = \frac{1}{N}\int_{\infty}^{\mu}\rho_{\sigma}(\omega)\mathrm{d}\omega, \quad (15)$$

under the constraint

$$\langle n\rangle = \langle n_{\uparrow}\rangle + \langle n_{\downarrow}\rangle = \frac{3}{2}. \quad (16)$$

By solving the above equations self-consistently, we obtain NFM when $\langle n_{\uparrow}\rangle = \langle n_{\downarrow}\rangle$ and FM when $\delta = (\langle n_{\uparrow}\rangle - \langle n_{\downarrow}\rangle) \neq 0$.

To decide which phase is more stable, the ground energy of the system is calculated as

$$E = \sum_{\sigma}\int_{-\infty}^{\mu}\omega\rho_{\sigma}(\omega)\mathrm{d}\omega. \quad (17)$$

3. Results and discussion

To begin with, we study first an idealized model for a finite one-dimensional cluster with $N = 12$ identical atoms (molecules) and density of electrons $n = 3/2$. With the exact-diagonalization method, we investigate the stability of various ordered phases in the ground state of the model. As discussed above, our main concern is whether the ferromagnetism survives when considering the next-nearest-neighbor electron hopping t_1. We expect to observe a fully polarized ground state at a finite t_1 with large on-site Coulomb interaction U. The total spin and the two-site von Neumann entropy (the local entanglement as we will call it hereafter) of the ground state will be calculated to study the quantum phase transition. The local entanglement is defined as[15]

$$\text{Entanglement} = -\text{tr}\rho_{i,i+1}\ln\rho_{i,i+1}, \tag{18}$$

where i and $i+1$ denote two nearest-neighbor sites in our model, and $\rho_{i,i+1}$ is the reduced density matrix of this two-site subsystem, which be read out from the ground state wave function.

We study the phases of the model at temperature $T = 0$ with Coulomb interaction $U = 10$. From Fig. 1, we find three phase transition points at $t_1 = 0.56$, 0.78, and 0.84. The fully polarized ferromagnetic phase is stable in the region $0.56 < t_1 < 0.78$ and a partially polarized phase survives in the region $0.78 < t_1 < 0.84$. To understand this phenomenon, let us first consider a half-filled band. The electrons tend to localize at each site and the antiferromagnetic interaction between the adjacent electrons arises under the condition that U is sufficiently large and only the nearest-neighbor hopping term is allowed. When an extra electron with spin up (down) is introduced into the system, it will cause an effective ferromagnetic interaction when the electron jumps between sites i and $i+1$; the spins of the localized electrons at the two sites will be forced to point down (up) due to Pauli's exclusion principle. However, the ferromagnetic long-range order will not survive in this one-dimensional system insured by the Lieb–Mattis theorem. When the next-nearest-neighbor hopping t_1 exists and has an appropriate value, the antiferromagnetic superexchange interaction caused by the nearest electron virtual hopping process is depressed, and the system will favor ferromagnetism. Under the condition that the density of overdoped electrons has a suitable value (0.5 for our model), a long range order of ferromagnetism emerges. Therefore, the speculations proposed before, which stimulate us to carry out the present work, are supported. Furthermore, the local entanglement is calculated. Interestingly, we obtain one more phase transition point at $t_1 = 0.15$ in Fig. 2. This point reflects a level crossing between the lowest energy level and the first excited energy level.

Next we study the role played by the Coulomb interaction. The phase transition of the model with Coulomb interaction U is calculated at $t_1 = 0.6$. Our results are shown in Figs. 3 and 4. Both the total spin and the two-site entropy of the ground state reflect the phase identically. The large U always stabilizes ferromagnetism when t_1 has an appropriate value.

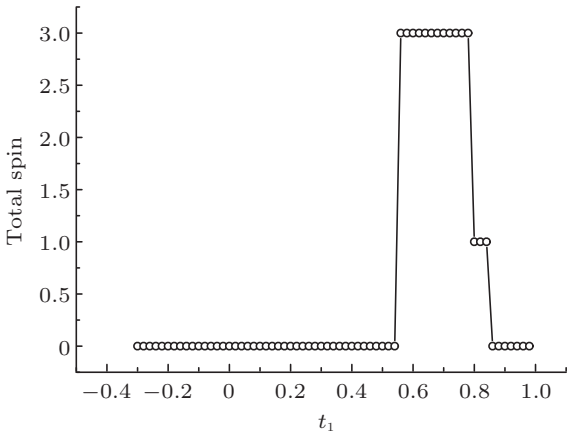


Fig. 1. The total spin versus t_1 with $t = 1$ and $U = 10$.

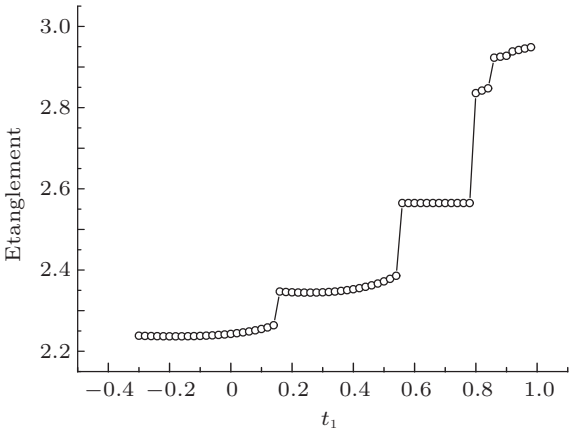


Fig. 2. Entanglement versus t_1 with $t = 1$ and $U = 10$.

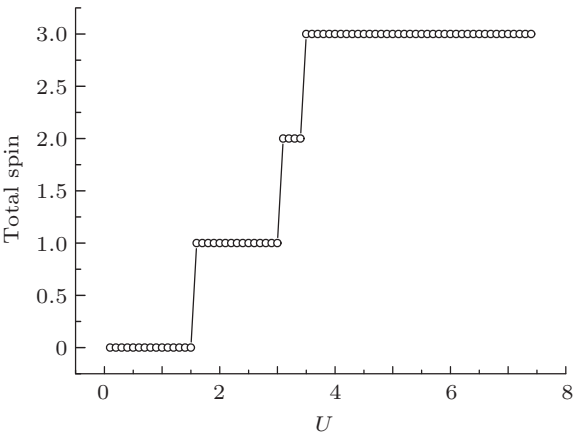


Fig. 3. The total spin versus U with $t = 1$ and $t_1 = 0.6$.

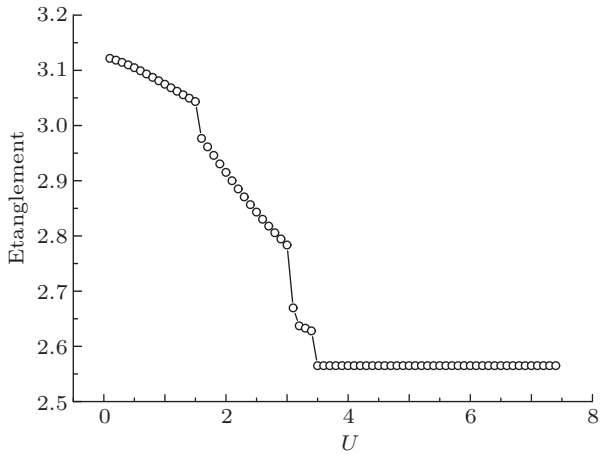


Fig. 4. Entanglement versus U with $t = 1$ and $t_1 = 0.6$.

Last, we investigate the stability of ferromagnetism in the thermodynamic limit. We investigate the stability of the two phases FM and NFM in the ground state of the model at $n = 3/2$. As discussed above, our main concern is whether the ferromagnetism survives when t_1 is introduced. We expect to observe a nonzero δ at large U when the next-nearest-neighbor hopping amplitude is at an intermediate value if our proposal is correct. The ground energies of FM and NFM are calculated self-consistently by using the equation-of-motion method with the random phase approximation. The results are shown in Fig. 5. Pleasingly, we find that FM survives at a moderate region of t_1 when U is sufficiently large. Noticeably, the phase transition point of t_1 decreases for fixed Coulomb interactions U, which probably originates from the size effect.

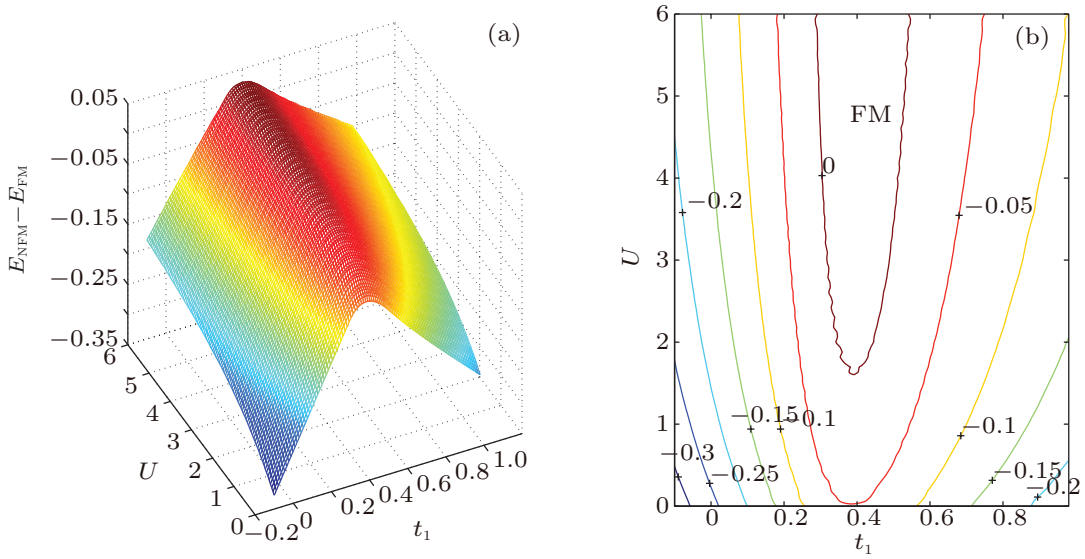


Fig. 5. (a) Relative energy $E_{\rm NFM} - E_{\rm FM}$ versus U and t_1 with $t = 1$. (b) The corresponding contour plot.

4. Summary

We establish a new model for realizing ferromagnetism by introducing the next-nearest-neighbor hopping in the one-dimensional Hubbard model at $n = 3/2$. The small cluster is explored by the exact-diagonalization method in detail, and the thermodynamic limit is studied by using the equation-of-motion method with RPA. Ferromagnetism is found to survive in an intermediate region of t_1 when U is sufficiently large. The critical value of the next-nearest-neighbor hopping t_1 decreases in the thermodynamic limit compared to the small cluster.

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