The influence of long-range hopping on ferromagnetism in the Hubbard model

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Abstract

The phase diagram of the Hubbard model in an external magnetic field is examined by extrapolation of small-cluster exact-diagonalization calculations. Using a general expression for the hopping matrix elements \( t_{ij} \sim q |i-j| \) the influence of long-range hopping (band asymmetry) on ferromagnetism in this model is studied. It is found that the long-range hopping (nonzero \( q \)) stabilizes ferromagnetism in an external magnetic field for \( n > 1 \). In the opposite limit \( n \leq 1 \) the fully polarized ferromagnetic state is generally suppressed with increasing \( q \). The critical value of magnetic field \( h \) below which the ferromagnetic state becomes unstable is calculated numerically.

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The Hubbard model [1] was originally introduced to describe correlation effects in transition metals, in particular the band ferromagnetism of Fe, Co and Ni. It soon turned out, however, that the single-band Hubbard model is not the canonical model for ferromagnetism. In fact the existence of saturated ferromagnetism has been proven rigorously only for very special limits. The first well-known example is the Nagaoka ferromagnetism that come from the Hubbard model in the limit of infinite repulsion and one hole in a half-filled band [2]. Another example where saturated ferromagnetism has been shown to exist is the case of one dimensional Hubbard model with nearest and next-nearest neighbor hopping at low electron densities [3]. Moreover, several examples of the fully polarized ground state have been found on special lattices (special conduction bands) as are the fcc-type lattices [4], the bipartite lattices with sublattices containing a different number of sites [5], the lattices with unconstrained hopping of electrons [3, 6] and the flat bands [8]. This indicates that the lattice structure and the kinetic energy of electrons (the type of hopping) play the crucial role in stabilizing the ferromagnetic state. The recent results [9] obtained on non-bipartite lattices fully confirm this conjecture. Non–bipartite lattices have an asymmetric density of states (DOS) and it is expected that just this asymmetry which brings more weightage to the one edge of the DOS is the key to understanding of ferromagnetism in the Hubbard model.

In this paper we want to study how sensible ferromagnetism depends on the DOS of the non–interacting electrons, particularly on its asymmetry. To fulfil this program we choose the following general form for the hopping matrix elements in the one dimension (the periodic boundary conditions are used) [10]

\[
t_{ij}(q) = \begin{cases} 
0, & i = j, \\
-tq^{\mid i-j\mid -1}, & 0 < \mid i - j \mid \leq L/2, \\
-tq^{L-\mid i-j\mid -1}, & L/2 < \mid i - j \mid \leq L, 
\end{cases}
\]  

(1)\)

where \(L\) denotes the number of lattice sites and \(0 \leq q \leq 1\).

Such a selection of hopping matrix elements has several advantages. It represents a much more realistic type of electron hopping on a lattice (in comparison to nearest-neighbor hopping), and it allows us to change continuously the type of hopping (band) from nearest-neighbor (\(q = 0\)) to infinite-range (\(q = 1\)) hopping and thus
immediately study the effect of the long-range hopping. Moreover, for non–zero \( q \) the DOS of the non–interacting band corresponding to (1) becomes strongly asymmetric since a more weightage shifts to the upper edge of the band with increasing \( q \). Thus one can study simultaneously (by changing only one parameter \( q \)) the influence of the increasing asymmetry in the DOS and the influence of the long-range hopping on the ground state properties of the model. Here the special attention is devoted to the question whether or not the asymmetry in the DOS (the long-range hopping) can stabilize the ferromagnetic state. As mentioned above the answer to this question could be the key to understanding of ferromagnetism in the Hubbard model.

The Hamiltonian of the Hubbard model in an external magnetic field is given by

\[
H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{h}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow}),
\]

where \( c_{i\sigma}^+ \) and \( c_{i\sigma} \) are the creation and annihilation operators for an electron of spin \( \sigma \) at site \( i \), \( n_{i\sigma} \) is the corresponding number operator (\( n_{\sigma} = \frac{1}{L} \sum_i n_{i\sigma} \)), \( U \) is the on-site Coulomb interaction constant and \( h \) is an external magnetic field.

The first rigorous criteria for the stability of ferromagnetism in this model (for \( q = 0 \) and \( n = n_{\uparrow} + n_{\downarrow} = 1 \)) have been derived by Strack and Vollhardt [11]. Their results provide the rigorous upper bound on the critical magnetic field above which the fully polarized ferromagnet is the exact ground state. The lower bound on the magnetic field below which the ferromagnetic state becomes locally unstable has been calculated by van Dongen and Janiš [12]. Very recently some exact results about the ground state of the Hubbard model with an infinite-range hopping (\( q = 1 \)) appeared in literature [6, 7]. For the infinite-range hopping and just one electron more than half-filling Pieri [7] proved rigorously that the ground state of the model is the Nagaoka ferromagnetic state for every value of \( U > 0 \). The limit of infinite-range hopping is, however, the least realistic limit of Eq. 1. It is interesting, therefore, to look on the possibility of ferromagnetism in the Hubbard model with a generalized type of hopping for smaller values of \( q \) that describe much more realistic type of electron hopping.

In this paper we extend the calculations to arbitrary \( q \) and arbitrary band fill-
ing \( n \). The ground state properties of the model, and particularly ferromagnetism are studied numerically (using the Lanczos method) for a wide range of parameters \((q, U, h, n)\) and typical examples are then chosen from a large number of available results to represent the most interesting cases. The results obtained are presented in the form of phase diagrams in the \( h-U \) plane. To determine the phase diagram in the \( h-U \) plane (corresponding to some \( q \) and \( n \)) the up-spin (down-spin) electron occupation number \( n^\uparrow (n^\downarrow) \) are calculated point by point as functions of \( h \) and \( U \). Of course, such a procedure demand in practice a considerable amount of CPU time which impose severe restrictions on the size of clusters that can be studied with this method \((L \sim 14)\). However, we will show later that even the study of such small clusters can reveal some general features of the model.

First we have investigated the model for small finite clusters (up to 12 sites) at half-filling. The most important result obtained for the following set of \( q \) values: \( q = 0, 0.2, 0.4, 0.6, 0.8 \) is that the fully polarized ferromagnetic state \((n^\uparrow = 1, n^\downarrow = 0)\) is suppressed with increasing \( q \). Numerical results for the critical magnetic field \( h_c(U) \) above which the ground state is fully polarized ferromagnet are shown in Fig. 1. To determine the finite size effect the critical behavior \( h_c(U) \) has been computed for several values of \( L \) \((L = 6, 8, 10 \text{ and } 12)\), but no significant finite-size effects have been observed over the whole interval of \( U \) plotted. Therefore we suppose that these results can be satisfactory extended to large systems. This conjecture supports also the analytical calculation of \( h_c \) from the well-known single spin-flip ansatz.

The single spin-flip ansatz for the Hamiltonian (2) is \[ \Psi = \sum_{n,m} a_{nm} c^\uparrow_{n^\uparrow} c^\downarrow_{m^\downarrow} |F\rangle, \] where \( |F\rangle = \prod_i c^\uparrow_i |0\rangle \) is the fully polarized ferromagnetic state. Inserting \( |\Psi\rangle \) into the Schrödinger equation yields the consistence relation \[ 1 = \frac{U}{L} \sum_k \frac{1}{\epsilon_k - \epsilon_{K-k} - E + h + U} \] from which the critical magnetic field \( h_c \) can be determined immediately. Since the dispersion relation \( \epsilon_k = \frac{1}{L} \sum_{ij} t_{ij} e^{-i k (R_i - R_j)} \) for the generalized type of electron
hopping (1) is much more complicated than one corresponding to nearest-neighbor hopping we have solved (4) numerically. The results of these numerical calculations (ssf) are compared in Fig. 1 with small-cluster exact-diagonalization calculations. The accordance of results is very good, particularly for \( q \leq 0.5 \), indicating that (i) finite-size effects are small, and (ii) the single spin-flip ansatz is a good approach for the half-filled band case. We have observed the same behavior of the model also for \( n < 1 \) which leads to the conclusion that the long-range hopping of the type (1) does not support ferromagnetism in the Hubbard model at least in the region \( n \leq 1 \).

It should be noted that our findings are fully consistent with results of Salerno [6] and Pieri [7]. They found no ferromagnetic ground state in the Hubbard model with infinite-range hopping \((q = 1)\) for \( n \leq 1 \) and \( h = 0 \). Therefore we have turned our attention to the case \( n > 1 \).

The results of small-cluster exact-diagonalization calculations obtained for \( n = 3/2 \) and different values of \( q \) are shown in Fig. 2 and Fig. 3. To reveal the finite-size effects we have displayed results for two finite clusters of \( L = 8 \) and \( L = 14 \) sites. It is seen that the finite-size effects are now non-zero, but in spite of this fact some general features of the model are obvious. The most important result is that the ferromagnetic state is stabilized with increasing asymmetry of the DOS. The influence of asymmetry is so strong that for \( q \) sufficiently large the transition to the ferromagnetic state can be induced even at \( h = 0 \). This result confirms the conjecture that the asymmetry of the DOS (the long-range hopping) plays the crucial role in stabilizing the ferromagnetic state at \( h = 0 \), at least on finite clusters. Unfortunately, the size of clusters that can be studied with the Lanczos method is too small to show satisfactory whether or not this important result persists also in the thermodynamic limit \( L \to \infty \). To resolve this problem some other methods that allow to work with larger clusters (e.g. the density-matrix renormalization group) should be used. Work in this direction is currently in progress.

Another important result that can be found using small-cluster exact-diagonalization calculations is shown in Fig. 3. There are compared small-cluster exact-diagonalization results with numerical results obtained from the single spin-flip ansatz. It is seen that the results strongly differ, particularly for \( U \) sufficiently large. This
indicates that the transition to the ferromagnetic state is probably discontinuous at least in the strong coupling limit. At the same time this result explains why the critical interaction strength $U_c(h = 0)$ obtained from the single spin-flip ansatz lies usually much lower than the exact $U_c$ [13]. For $n > 1$ the single spin-flip ansatz is not a good approach to determine the ferromagnetic region.

In summary, the numerical study of the Hubbard model in an external magnetic field shows that the long-range hopping (band asymmetry) stabilizes ferromagnetism in this model for $n > 1$. In the opposite limit $n \leq 1$ the fully polarized ferromagnetic state is generally suppressed with increasing band asymmetry. In addition, small-cluster exact-diagonalization calculations indicate that the transition to the ferromagnetic state (for $n > 1$) is probably discontinuous at least in the strong coupling limit.

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Figure Captions

Fig. 1. The critical magnetic field $h_c$ as a function of $U$ calculated from the single spin-flip ansatz (ssf) and exactly (exact) for $n = 1$. Curves (from down to up) correspond to $q = 0, q = 0.2, q = 0.4$, and $q = 0.6$. For $L = 10$ ssf and exact-diagonalization results are identical.

Fig. 2. The critical magnetic field $h_c$ as a function of $U$ calculated exactly for $L = 8$ and $n = 3/2$. Curves (from up to down) correspond to $q = 0, q = 0.2$, $q = 0.4, q = 0.6$ and $q = 0.8$.

Fig. 3. The critical magnetic field $h_c$ as a function of $U$ calculated from the single spin-flip ansatz (ssf) and exactly (exact) for $L = 14$ and $n = 3/2$. Curves (from up to down) correspond to $q = 0, q = 0.2, q = 0.4$, and $q = 0.6$. 
$L=14$
$n=3/2$

$h_c$

U

- - - - ssf

--- exact