Effects of geometrical frustration on ferromagnetism in the Hubbard model on the Shastry-Sutherland lattice

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Abstract

The small-cluster exact-diagonalization calculations and the projector quantum Monte Carlo method are used to examine the competing effects of geometrical frustration and interaction on ferromagnetism in the Hubbard model on the Shastry-Sutherland lattice. It is shown that the geometrical frustration stabilizes the ferromagnetic state at high electron concentrations \((n \gtrsim 7/4)\), where strong correlations between ferromagnetism and the shape of the noninteracting density of states are observed. In particular, it is found that ferromagnetism is stabilized only for these values of frustration parameters, which lead to the single peaked noninteracting density of states at the band edge. Once, two or more peaks appear in the noninteracting density of states at the band edge the ferromagnetic state is suppressed. This opens a new route towards the understanding of ferromagnetism in strongly correlated systems.
1 Introduction

Since its introduction in 1963, the Hubbard model \[1\] has become, one of the most popular models of correlated electrons on a lattice. It has been used in the literature to study a great variety of many-body effects in metals, of which ferromagnetism, metal-insulator transitions, charge-density waves and superconductivity are the most common examples. Of all these cooperative phenomena, the problem of ferromagnetism in the Hubbard model has the longest history. Although the model was originally introduced to describe the itinerant ferromagnetism in narrow-band metals like Fe, Co, Ni and others, it soon turned out that the single-band Hubbard model is not the canonical model for ferromagnetism. Indeed, the existence of saturated ferromagnetism has been proven rigorously only for very special limits. The first well-known example is the Nagaoka limit that corresponds to the infinite-$U$ Hubbard model with one hole in a half-filled band \[2\]. Another example, where saturated ferromagnetism has been shown to exist, is the case of the one-dimensional Hubbard model with nearest and next-nearest-neighbor hopping at low electron densities \[3\]. Furthermore, several examples of the fully polarized ground state have been found on special lattices as are the bipartite lattices with sublattices containing a different number of sites \[4\], the fcc-type lattices \[5, 6\], the lattices with long-range electron hopping \[7, 8, 9, 10, 11\], the flat bands \[12, 13, 14, 15\] and the nearly flat-band systems \[16, 17, 18, 19\]. This indicates that the lattice structure, which dictates the shape of the density of states (DOS), plays an important role in stabilizing the ferromagnetic state.

Motivated by these results, in the current paper we focus our attention on the special type of lattice, the so-called Shastry-Sutherland lattice (SSL). The SSL represents one of the simplest systems with geometrical frustration, so that putting the electrons on this lattice one can examine simultaneously both, the ef-
effect of interaction as well as the effect of geometrical frustration on ground-state properties of the Hubbard model. This lattice was first introduced by Shastry and Sutherland [20] as an interesting example of a frustrated quantum spin system with an exact ground state. It can be described as a square lattice with the nearest-neighbor links $t_1$ and the next-nearest neighbors links $t_2$ in every second square (see Fig. 1a). The SSL attracted much attention after its experimental realization in the SrCu$_2$(BO$_3$)$_2$ compound [21]. The observation of a fascinating sequence of magnetization plateaus (at $m/m_s = 1/2, 1/3, 1/4$ and $1/8$ of the saturated magnetization $m_s$) in this material [22] stimulated further theoretical and experimental studies of the SSL. Some time later, many other Shastry-Sutherland magnets have been discovered [23, 24]. In particular, this concerns an entire group of rare-earth metal tetraborides $RB_4$ ($R = La - Lu$). These materials exhibit similar sequences of fractional magnetization plateaus as observed in the SrCu$_2$(BO$_3$)$_2$ compound. For example, for TbB$_4$ the magnetization plateau has been found at $m/m_s = 2/9, 1/3, 4/9, 1/2$ and $7/9$ [23] and for TmB$_4$ at $m/m_s = 1/11, 1/9, 1/7$ and $1/2$ [24].

To describe some of the above mentioned plateaus correctly, it was necessary to generalize the Shastry-Sutherland model by including couplings between the third

Figure 1: (a) The original SSL with the first ($t_1$) and second ($t_2$) nearest-neighbor couplings. (b) The generalized SSL with the first ($t_1$), second ($t_2$) and third ($t_3$) nearest-neighbor couplings.
and even between the fourth nearest neighbors\cite{25}. The SSL with the first, second and third nearest-neighbor links is shown in Fig. 1b and this is just the lattice that will be used in our next numerical calculations.

Thus our starting Hamiltonian, corresponding to the one band Hubbard model on the SSL, can be written as

\[ H = -t_1 \sum_{\langle ij \rangle_1, \sigma} c_{i\sigma}^+ c_{j\sigma} - t_2 \sum_{\langle ij \rangle_2, \sigma} c_{i\sigma}^+ c_{j\sigma} - t_3 \sum_{\langle ij \rangle_3, \sigma} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1} \]

where \( c_{i\sigma}^+ \) and \( c_{i\sigma} \) are the creation and annihilation operators for an electron of spin \( \sigma \) at site \( i \) and \( n_{i\sigma} \) is the corresponding number operator \( (N = N_{\uparrow} + N_{\downarrow} = \sum_{i\sigma} n_{i\sigma}) \). The first three terms of (1) are the kinetic energies corresponding to the quantum-mechanical hopping of electrons between the first, second and third nearest neighbors and the last term is the Hubbard on-site repulsion between two electrons with opposite spins. We set \( t_1 = 1 \) as the energy unit and thus \( t_2 \) (\( t_3 \)) can be seen as a measure of the frustration strength.

To identify the nature of the ground state of the Hubbard model on the SSL we have used the small-cluster-exact-diagonalization (Lanczos) method\cite{26} and the projector quantum Monte-Carlo method\cite{27}. In both cases the numerical calculations proceed in the following steps. Firstly, the ground-state energy of the model \( E_g(S_z) \) is calculated in all different spin sectors \( S_z = N_{\uparrow} - N_{\downarrow} \) as a function of model parameters \( t_2, t_3 \) and \( U \). Then the resulting behaviors of \( E_g(S_z) \) are used directly to identify the regions in the parametric space of the model, where the fully polarized state has the lowest energy.

2 Results and discussion

To reveal possible stability regions of the ferromagnetic state in the Hubbard model on the SSL, let us first examine the effects of the geometrical frustration, represented by nonzero values of \( t_2 \) and \( t_3 \), on the behavior of the non-interacting DOS.
The previous numerical studies of the standard one and two-dimensional Hubbard model with next-nearest \[3\] as well as long-range \[9, 10, 11\] hopping showed that just this quantity could be used as a good indicator for the emergence of ferromagnetism in the interacting systems. Indeed, in both models the strong correlation between ferromagnetism and the anomalies in the noninteracting DOS are observed. In the first model the ferromagnetic state is found at low electron concentrations and the noninteracting DOS is strongly enhanced at the low-energy band edge, while in the second one the ferromagnetic phase is stabilized at the high electron concentrations and the spectral weight is enhanced at the high-energy band edge. This leads to the scenario according to which the large spectral weight in the noninteracting DOS that appears at the low (high) energy band edges allows for a small kinetic-energy loss for a state with total spin \(S \neq 0\) in reference to one with \(S = 0\). At some finite value of interaction \(U\), the Coulomb repulsion paid for the low-spin states overcomes this energy loss and the high-spin state becomes energetically favored. The key point in this picture is the assumption that the shape of the DOS is only weakly modified as the interaction \(U\) is switched on, at least within its low (high) energy sector.

The noninteracting DOS of the \(U = 0\) Hubbard model on the SSL of size \(L = 200 \times 200\), obtained by exact diagonalization of \(H\) (for \(U = 0\)) is shown in Fig. 2. The left panels correspond to the situation when \(t_2 > 0\) and \(t_3 = 0\), while the right panels correspond to the situation when both \(t_2\) and \(t_3\) are finite. One can see that once the frustration parameter \(t_2\) is nonzero, the spectral weight starts to shift to the upper band edge and the noninteracting DOS becomes strongly asymmetric. Thus taking into account the above mentioned scenario, there is a real chance that the interacting system could be ferromagnetic in the limit of high electron concentrations. To verify this conjecture we have performed exhaustive numerical
Figure 2: Non-interacting DOS calculated numerically for different values of $t_2$ and $t_3$ on the finite cluster of $L = 200 \times 200$ sites.

studies of the model Hamiltonian (1) for a wide range of the model parameters $U, t_2$ and $n$ at $t_3 = 0$. Typical results of our PQMC calculations obtained on finite cluster of $L = 6 \times 6$ sites, in two different concentration limits ($n \leq 1$ and $n > 1$) are shown in Fig. 3. There is plotted the difference $\Delta E = E_f - E_{\text{min}}$ between the ferromagnetic state $E_f$, which can be calculated exactly and the lowest ground-state energy from $E_g(S_z)$ as a function of the frustration parameter $t_2$. According
Figure 3: The difference $\Delta E = E_f - E_{\text{min}}$ between the ferromagnetic state $E_f$ and the lowest ground-state energy from $E_g(S_z)$ as a function of the frustration parameter $t_2$ calculated for $n \leq 1$ (a) and $n > 1$ (b) on the finite cluster of $L = 6 \times 6$ sites ($U = 1, t_3 = 0$). The inset shows $\Delta E$, calculated for two different electron densities on clusters of $L = 6 \times 6$ and $L = 8 \times 8$ sites.

to this definition the ferromagnetic state corresponds to $\Delta E = 0$. It is seen that for electron concentrations below the half filled band case $n = 1$, $\Delta E$ is the increasing function of $t_2$, and thus there is no sign of stabilization of the ferromagnetic state for $n \leq 1$, in accordance with the above mentioned scenario. The situation looks more promising in the opposite limit $n > 1$. In this case, $\Delta E$ is considerably reduced with increasing $t_2$, however, this reduction is still insufficient to reach the ferromagnetic state $\Delta E = 0$ for physically reasonable values of $t_2$ ($t_2 < 1.6$) that correspond to the situation in the real materials. To exclude the finite-size effect, we have also performed the same calculations on the larger cluster of $L = 8 \times 8$ sites, but again no signs of stabilization the ferromagnetic state have been observed (see inset to Fig. 4b).

For this reason we have turned our attention to the case $t_2 > 0$ and $t_3 > 0$. The noninteracting DOS corresponding to this case is displayed in Fig. 1 (the right panels). These panels clearly demonstrate that with the increasing value of the frustration parameter $t_3$, still a more spectral weight is shifted to the upper band edge. A special situation arises at $t_3 = 0.6$, when the spectral weight is strongly peaked
at the upper band edge. In this case the noninteracting DOS is practically identical with one corresponding to noninteracting electrons with long-range hopping [9]. Since the long-range hopping supports ferromagnetism in the standard Hubbard model for electron concentrations above the half-filled band case [9, 10, 11], we expect that this could be true also for the Hubbard model on the SSL, at least for some values of frustration parameters $t_2$ and $t_3$. Therefore, we have decided to perform numerical studies of the model for a wide range of $t_3$ values at fixed $t_2, U$ and $n$ ($t_2 = 1, U = 1, n = 7/4$). To minimize the finite-size effects, the numerical calculations have been done on two different finite clusters of $L = 6 \times 6$ and $L = 8 \times 8$ sites. The results of our calculations for $\Delta E$ as a function of $t_3$ are displayed in Fig. 4a. In accordance with the above mentioned assumptions we find a relatively wide region of $t_3$ values around $t_3 = 0.6$, where the ferromagnetic state is stable. It is seen that the finite-size effects on the stability region of the ferromagnetic phase are negligible and thus these results can be satisfactorily extrapolated to the thermodynamic limit $L \to \infty$. Moreover, the same calculations performed for different values of the Hubbard interaction $U$ showed that correlation effects

![Figure 4](image-url)
(nonzero $U$) further stabilize the ferromagnetic state and lead to the emergence of macroscopic ferromagnetic domain in the $t_3$-$U$ phase diagram (see inset to Fig. 4a). This confirms the crucial role of the Hubbard interaction $U$ in the mechanism of stabilization of ferromagnetism on the geometrically frustrated lattice. In Fig. 4b we have also plotted the comprehensive phase diagrams of the model in the $t_3$-$n$ as well as $t_3$-$t_2$ plane, which clearly demonstrate that the ferromagnetic state is robust with respect to doping ($n \gtrsim 7/4$) and frustration.

To check the convergence of PQMC results we have performed the same calculations by the Lanczos exact diagonalization method. Of course, on such a large cluster, consisting of $L = 6 \times 6$ sites, we were able to examine (due to high memory requirements) only several electron fillings near the fully occupied band ($N = 2L$). The exact diagonalization and PQMC results for the width of the ferromagnetic phase obtained on finite cluster of $L = 6 \times 6$ sites, for three different electron fillings from the high concentration limit ($N = 66, 67, 68$), are displayed in the inset to Fig. 4b and they show a nice convergence of PQMC results.

Let us finally turn our attention to the question of possible connection between ferromagnetism and the noninteracting DOS that has been discussed at the beginning of the paper. Figs. 4a and 4b show, that for each finite $U$ and $n$ sufficiently large ($n \gtrsim 7/4$), there exists a finite interval of $t_3$ values, around $t_3 \sim 0.6$, where the ferromagnetic state is the ground state of the model. To examine a possible connection between ferromagnetism and the noninteracting DOS, we have calculated numerically the noninteracting DOS for several different values of $t_3$ from this interval and its vicinity. The results obtained for $U = 1, n = 7/4$ and $t_2 = 1$ are displayed in Fig. 5. Comparing these results with the ones presented in Fig. 4a for the stability region of the ferromagnetic phase at the same values of $U, n$ and $t_3$, one can see that there is an obvious correlation between the shape of the noninter-
acting DOS and ferromagnetism. Indeed, the ferromagnetic state is stabilized only for these values of frustration parameters $t_2, t_3$, which lead to the single peaked noninteracting DOS at the band edge. Once, two or more peaks appear in the noninteracting DOS at the band edge (by changing $t_2$ or $t_3$), ferromagnetism is suppressed.

In summary, the small-cluster exact-diagonalization calculations and the PQMC
method were used to examine possible mechanisms leading to the stabilization of ferromagnetism in strongly correlated systems with geometrical frustration. Modelling such systems by the Hubbard model on the SSL, we have found that the combined effects of geometrical frustration and interaction strongly support the formation of the ferromagnetic phase at high electron densities. The effects of geometrical frustration transform to the mechanism of stabilization of ferromagnetism via the behaviour of the noninteracting DOS, the shape of which is determined uniquely by the values of frustration parameters $t_2$ and $t_3$. We have found that it is just the shape of the noninteracting DOS near the band edge (the single peaked DOS) that plays the central role in the stabilization of the ferromagnetic state. Since the same signs have been observed also in some other works (e.g., the Hubbard model with nearest and next-nearest neighbor hopping, or the Hubbard model with long range hopping), it seems that such a behaviour of the noninteracting DOS near the band edge should be used like the universal indicator for the emergence of ferromagnetism in the interacting systems.

This work was supported by the Slovak Research and Development Agency (APVV) under Grant APVV-0097-12 and ERDF EU Grant under the contract No. ITMS26210120002 and ITMS26220120005.
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