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МАГНІТНІ ВЛАСТИВОСТІ МОДЕЛІ ГАББАРДА НА СМУЖКАХ КАГОМЕ

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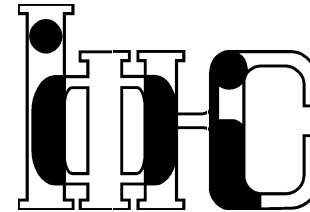
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КОНДЕНСОВАНИХ
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MAGNETIC PROPERTIES OF THE HUBBARD MODEL
ON KAGOME STRIPES

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Магнітні властивості моделі Габбарда на смужках кагоме

О.Держко, М.Максименко, Й.Ріхтер, А.Гонекер, Р.Мьоснер

Анотація. Ми розглядаємо одноорбітальну N -вузлову модель Габбарда з відштовхуванням на двох кагомеподібних ланцюжках, які обидва мають цілком бездисперсійну (плоску) одноелектронну зону. Використовуючи точні багатоелектронні основні стани у підпросторах з числом електронів $n \leq n_{\max}$ ($n_{\max} \propto N$), ми обчислюємо квадрат повного спіну в основному стані для обговорення магнітних властивостей моделей. Ми виявили, що, хоча для $n < n_{\max}$ серед основних станів є повністю поляризовані стани, немає скінченної області електронних густин $n/N < 1$ ($\mathcal{N} = N/3$ чи $\mathcal{N} = N/5$), де б ферромагнетизм в основному станів виживав у границі $\mathcal{N} \rightarrow \infty$.

Ця робота була представлена на 14й чеській і словацькій конференції з магнетизму CSMAG'10 (6–9 липня 2010, Кошіце, Словаччина).

Magnetic properties of the Hubbard model on kagome stripes

O.Derzhko, M.Maksymenko, J.Richter, A.Honecker, R.Moessner

Abstract. We consider the one-orbital N -site repulsive Hubbard model on two kagome-like chains, both of which yield a completely dispersionless (flat) one-electron band. Using exact many-electron ground states in the subspaces with $n \leq n_{\max}$ ($n_{\max} \propto N$) electrons, we calculate the square of the total spin in the ground state to discuss magnetic properties of the models. We have found that although for $n < n_{\max}$ the ground states contain fully polarized states, there is no finite region of electron densities $n/N < 1$ ($\mathcal{N} = N/3$ or $\mathcal{N} = N/5$) where ground-state ferromagnetism survives for $\mathcal{N} \rightarrow \infty$.

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Mechanisms of ferromagnetism in the itinerant electron systems continue to be of great interest [1]. In the early 1990s Mielke and Tasaki proposed several Hubbard models with a unique saturated ferromagnetic ground state [2,3]. This model has an important feature that the lowest-energy one-electron band is completely flat (dispersionless) and, as a result, the corresponding one-electron states can be localized on a small part of the lattice (trapping cell). On the other hand, exact ground states of frustrated quantum spin antiferromagnets have been discovered [4]. These states consist of independent (i.e., isolated) localized magnons located within trapping cells and they dominate the low-temperature properties of the antiferromagnetic Heisenberg model in a strong magnetic field. Interestingly, although the flat-band repulsive Hubbard model far below half filling and the highly frustrated Heisenberg antiferromagnet in a strong magnetic field present different physics, the mathematical structure for their description may be quite similar [4–8].

In this paper we discuss ground-state magnetic properties of Mielke-type flat-band Hubbard ferromagnets focusing for concreteness on two one-dimensional kagome lattices (Fig. 1). The kagome chain I (panel a)

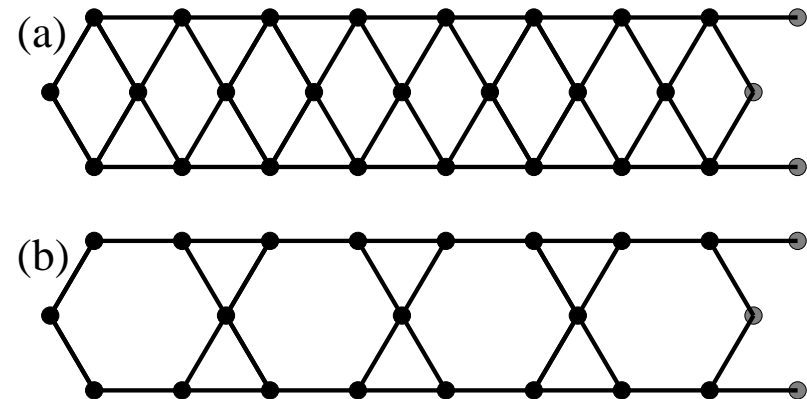


Figure 1. Kagome chain I (a) and kagome chain II (b).

is a line graph of the two-leg ladder, whereas the kagome chain II (panel b) is a line graph of the decorated two-leg ladder [2,8]. The kagome chain I (II) has an elementary cell with 3 (5) sites. We introduce the number of elementary cells \mathcal{N} and $\mathcal{N} = N/3$ ($\mathcal{N} = N/5$) for the kagome chain I (II). For the even- \mathcal{N} kagome chain I and kagome chain II the parent graphs are bipartite ones, whereas for the odd- \mathcal{N} kagome chain I the

parent graph is nonbipartite (periodic boundary conditions are implied). Furthermore, we consider the usual Hubbard Hamiltonian

$$H = t \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Here the sums run either over the nearest-neighbor pairs $\langle i, j \rangle$ or over N lattice sites i . $t > 0$ is the hopping parameter (then the flat one-electron band is the lowest-energy one) and $U > 0$ is the on-site Coulomb repulsion for electrons with different spins.

We recall here Mielke's results [2] for ground-state ferromagnetism of the Hubbard model on line graphs specifying them for the lattices in question. The repulsive Hubbard model (1) has ferromagnetic ground states with saturated magnetization if the number of electrons satisfies $n \leq n_{\max}$ [$n_{\max} = \mathcal{N} + 1$ (periodic even- \mathcal{N} kagome chain I and periodic kagome chain II) or $n_{\max} = \mathcal{N}$ (periodic odd- \mathcal{N} kagome chain I)] and the ferromagnetic ground state is unique if $n = n_{\max}$. In what follows we illustrate the general statements of A. Mielke and further specify them 1) constructing explicitly the ground states for $n \leq n_{\max}$ electrons and 2) calculating the average of the square of the total spin in these ground states $\langle \mathbf{S}^2 \rangle_n$.

We begin with introducing localized one-electron states. A localized one-electron state can be located on a smallest diamond-shaped (hexagon-shaped) cell of the kagome chain I (II). It is proportional to $\sum_m (-1)^m c_{m\sigma}^\dagger |0\rangle$, where the sum runs over 4 (6) sites of the diamond (hexagon) trapping cell of the kagome chain I (II). The localized electron has the energy $-2t$ and it cannot escape from the trap for the given lattice topology (isosceles triangles with one side belonging to the trap) because of destructive quantum interference. For the even- \mathcal{N} kagome chain I and the kagome chain II there are two more traps for localized states, i.e., the upper and lower legs. Indeed, for periodic boundary conditions imposed each leg is a regular convex polygon with an even number of sides/vertices and $\sum_n (-1)^n c_{n\sigma}^\dagger |0\rangle$, where the sum runs over the sites belonging to the leg, is an eigenstate with the energy $-2t$. Moreover, isosceles triangles with one side belonging to the leg prevent escape of an electron from the leg. The constructed $\mathcal{N} + 2$ one-electron localized states with the energy $-2t$ obey one linear relation and, as a result, we have only $\mathcal{N} + 1$ linearly independent localized states in the subspace with $n = 1$ electron. Thus, we have constructed n_{\max} ($n_{\max} = \mathcal{N}$ for the periodic odd- \mathcal{N} kagome chain I or $n_{\max} = \mathcal{N} + 1$ for the periodic even- \mathcal{N} kagome chain I and kagome chain II) one-electron localized states with the energy $-2t$.

We pass to subspaces with $1 < n \leq n_{\max}$ electrons. Since the localized one-electron states are located within a restricted part of the lattice only, we can construct many-electron eigenstates placing localized electrons sufficiently far from each other. Moreover, the Hubbard repulsion is a positive semidefinite operator which can only increase the energy. As a result, the isolated localized electron states which are the ground states for $U = 0$ remain the ground states for $U > 0$. Furthermore, electrons obviously can be localized within neighboring trapping cells if they all have the same spin polarization, since in such a case the on-site Hubbard repulsion is irrelevant. Starting from such a spin-polarized state and using the global SU(2) invariance of the Hubbard model (1) more ground states can be trivially constructed. Denote by $g_{\mathcal{N}}(n)$ the number of the ground states in the subspace with $n \leq n_{\max}$ electrons. The ground states for the odd- \mathcal{N} kagome chains I are constructed from the one-electron states trapped by diamonds only. Repeating the arguments elaborated for the sawtooth Hubbard chain (see Ref. [7]a) we arrive at the following result: $g_{\mathcal{N}}(n) = D_{\mathcal{N}}(n)$, $D_{\mathcal{N}}(n) = \mathcal{Z}(n, \mathcal{N}) + (\mathcal{N} - 1)\delta_{n, \mathcal{N}}$, where $\mathcal{Z}(n, \mathcal{N})$ is the canonical partition function of n classical hard dimers on an auxiliary (periodic) chain of $2\mathcal{N}$ sites. For the even- \mathcal{N} kagome chains I and kagome chains II the states which are constructed also from the one-electron leg states are among the ground states for $n = 1, \dots, \mathcal{N} + 1$ and, as a result, $g_{\mathcal{N}}(n) = D_{\mathcal{N}}(n)(1 - \delta_{n, \mathcal{N}+1}) + L_{\mathcal{N}}(n)(1 - \delta_{n, 0})$ with $L_{\mathcal{N}}(n) = (n + 1) \binom{\mathcal{N}}{n-1} + \delta_{n, 2}$. Further details can be found in Ref. [8].

To reveal the ferromagnetic ground states we consider the equal-weight average over all $g_{\mathcal{N}}(n)$ ground states for a given number of electrons n of the total spin, $\langle \mathbf{S}^2 \rangle_n = 3 \langle S^z{}^2 \rangle_n$. Since each of the $D_{\mathcal{N}}(n)$ states can be encoded by a certain configuration of n hard dimers on the chain of $2\mathcal{N}$ sites [7, 8], $\langle S^z{}^2 \rangle_n$ is related to density-density correlation functions of the hard-dimer system. For the even- \mathcal{N} kagome chain I or kagome chain II we have to take into account in addition the ground states involving the leg states all of which are ferromagnetic (except one state for $n = 2$ electrons). In Table 1 we report $\langle \mathbf{S}^2 \rangle_n$ for the two kagome chains with 7 cells. Using a MAPLE code we have computed $\langle \mathbf{S}^2 \rangle_n$, $n = 1, \dots, n_{\max}$ for essentially longer chains with several hundred cells [8]. Examining $\langle \mathbf{S}^2 \rangle_n / \mathcal{N}^2$ vs n / \mathcal{N} as \mathcal{N} increases we have found that there is no finite region of electron density $n / \mathcal{N} < 1$ for which $\langle \mathbf{S}^2 \rangle_n / \mathcal{N}^2$ remains finite for both kagome chains as $\mathcal{N} \rightarrow \infty$ (in this limit $\langle \mathbf{S}^2 \rangle_n \rightarrow 3n/4$) [8].

Finally, one can add to the Hamiltonian (1) the Zeeman term $-h \sum_i (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) / 2$, which removes the degeneracy of SU(2) multiplets. We have also calculated the localized-electron contribution to the

Table 1. $\langle S^2 \rangle_n$, $n = 1, \dots, n_{\max}$ for the kagome chains I and II with $\mathcal{N} = 7$ cells. Localized-state predictions coincide with exact diagonalization data for the Hubbard model.

	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$
I	$\frac{3}{4}$	$\frac{18}{11}$	$\frac{11}{4}$	$\frac{30}{7}$	$\frac{27}{4}$	12	$\frac{63}{4}$	
II	$\frac{3}{4}$	$\frac{83}{49}$	$\frac{85}{28}$	$\frac{330}{67}$	$\frac{903}{116}$	12	$\frac{63}{4}$	20

partition function in the presence of the Zeeman term and determined the magnetization and susceptibility, confirming in an alternative way the results of the preceding paragraph.

In summary, we have illustrated in detail Mielke's results about ground-state ferromagnetism of the Hubbard model on line graphs for the two kagome stripes. An ambitious task is to extend such an analysis for the (two-dimensional) kagome lattice.

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