Enhanced low-temperature entropy and flat-band ferromagnetism in the $t - J$ model on the sawtooth lattice

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Abstract

Using the example of the sawtooth chain, we argue that the $t - J$ model shares important features with the Hubbard model on highly frustrated lattices. The lowest single-fermion band is completely flat (for a specific choice of the hopping parameters $t_{i,j}$ in the case of the sawtooth chain), giving rise to single-particle excitations which can be localized in real space. These localized excitations do not interact for sufficient spatial separations such that exact many-electron states can also be constructed. Furthermore, all these excitations acquire zero energy for a suitable choice of the chemical potential $\mu$. This leads to: (i) a jump in the particle density at zero temperature, (ii) a finite zero-temperature entropy, (iii) a ferromagnetic ground state with a charge gap when the flat band is fully occupied and (iv) unusually large temperature variations when $\mu$ is varied adiabatically at finite temperature.

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During the past years, it has been noted that exact ground states can be constructed for the antiferromagnetic $X X Z$ model at high fields on a large class of highly frustrated lattices (see [1,2,3] and references therein). This leads to a finite zero-temperature entropy exactly at the saturation field and an enhanced magnetocaloric effect [4,7], suggesting potential applications for efficient low-temperature magnetic refrigeration [4,7]. Recently, we have pointed out [8] analogies to flat-band ferromagnetism in the Hubbard model on the same lattices (see e.g. [9,10,11,12,13]).

Here we will illustrate some of the issues with exact diagonalization results for the $t - J$ model. The $t - J$ model arises as the large-$U$ limit of the Hubbard model and is defined by the Hamiltonian

$$
H = \sum_{\langle i,j \rangle} t_{i,j} \left( c_{i,\sigma}^+ c_{j,\sigma} + c_{j,\sigma}^+ c_{i,\sigma} \right) P + \sum_{\langle i,j \rangle} J_{i,j} \left( S_i \cdot S_j - \frac{1}{4} n_i n_j \right) + \mu \sum_{i=1}^{N} n_i.
$$

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Here we will concentrate on the sawtooth chain model sketched in the inset of Fig. 1. The lower of the two branches of the single-electron dispersion becomes completely flat for \( t' = \sqrt{2} t \). For this choice one can construct first localized single-electron excitations living in one of the valleys of the sawtooth chain (bold dashed line in the inset of Fig. 1), and then excitations with \( N_{el} \) electrons which are non-interacting for sufficient spatial separations and thus have energy \( E = (−2 t + \mu) N_{el} \), in exactly the same manner as for the Hubbard model [8]. So far, the magnetic exchanges \( J_{i,j} \) are arbitrary. However, it will turn out that they should be chosen sufficiently weak in order to ensure that the non-interacting localized many-electron states are the ground states in their respective particle number subspaces. At half filling \( n = \langle n_{i} \rangle = 1 \) only the magnetic part of the \( t − J \) model survives such that it reduces to the previously studied antiferromagnetic spin-1/2 Heisenberg model (see [1,3,4,5,6] for the sawtooth chain).

The main panel of Fig. 1 shows finite-system results for \( n_{h} = 1 − n \) at \( T = 0 \) versus \( \mu \) for \( t' = \sqrt{2} t \) (these curves are the electronic counterpart of the magnetization curves [3]). For small magnetic exchange (like \( J' = J = 0.2 t \)), there is a jump of height \( \delta n = 1/2 \) exactly at \( \mu = 2 t \). At this point, all localized many-electron excitations collapse to \( E = 0 \). Furthermore, for \( N = 12 \) the number of ground states is 1, 12, 54, 112, 105, 36, 7 in the sectors with \( N_{el} = 0 \), 1, 2, 3, 4, 5, 6, respectively. This leads to a ground-state entropy per site \( \ln(327)/12 = 0.48 \ldots \) at \( \mu = 2 t \) for \( N = 12 \). The ground-state degeneracies are exactly the same as for the Hubbard model [14] consistent with the ground states of the \( t − J \) model for small \( J_{i,j} \) and \( N_{el} \leq N/2 \) being projections of those of the Hubbard model. General theorems for the Hubbard model imply a saturated ferromagnetic ground state for \( N_{el} = N/2 \) (see e.g. [11,12,13] for the sawtooth chain). Numerically, we find a fully saturated ferromagnet for the \( t − J \) model in the sectors with \( N_{el} = N/2 \) and \( N/2 − 1 \). The plateau at \( n = N_{el}/N = 1/2 \) in the \( n(\mu) \)-curve in Fig. 1 shows that the ground state is a saturated ferromagnet for \( 0 < \mu < 2 t \), corresponding to an appreciable charge gap.

The situation changes for larger antiferromagnetic \( J_{i,j} \), as illustrated for \( J' = J = 2 t \) in Fig. 1. In this case the localized states are no longer the lowest-energy states. This is signalled by a shift of the jump between \( n = 1/2 \) and \( n = 0 \) to \( \mu > 2 t \) which now corresponds to a true first-order transition. The charge gap, i.e., the plateau at \( n = 1/2 \) is also present in this case.

The ground-state degeneracies are reflected by thermodynamic properties, as illustrated for the entropy \( S \) in Fig. 2 (the curves of constant \( S \) correspond to the adiabatic demagnetization curves of the magnetic counterpart [4]). In particular, the finite \( T = 0 \) entropy at \( \mu = 2 t \) leads to large temperature changes during adiabatic variations of \( \mu \), even cooling to \( T = 0 \) as \( \mu = 2 t \) at low temperatures. The low-temperature properties for \( \mu \) close to \( 2 t \) are controlled by the localized states and are independent of the details of the microscopic model \( (J_{i,j} \text{ in the } t − J \text{ model and } U \text{ in the Hubbard model [14]); finite-size effects are also small in this region. By contrast, the behavior for \( \mu < 0 \) in Fig. 2 exhibits strong finite-size effects at low temperatures and depends on details of the model: for example, in this region the presence of doubly occupied sites leads to qualitatively different behavior of the Hubbard model [14].

We have focussed on the sawtooth chain, but it should share important features with a large class of highly frustrated lattices such as the kagomé lattice [1,6,9] which do not require any fine-tuning. We expect that the \( t − J \) model with weak \( J_{i,j} \) has the same localized excitations as the repulsive Hubbard model such that it shares in particular the same properties with respect to flat-band ferromagnetism [9,10,11,12,13]. The main advantage of the \( t − J \) model is a substantially reduced Hilbert space dimension close to \( n = 1 \) which simplifies a full diagonalization and thus the exact determination of finite-temperature properties of a finite system.

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