

Ground-state degeneracy and low-temperature thermodynamics of correlated electrons on highly frustrated lattices

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Abstract

Highly frustrated lattices yield a completely flat lowest single-electron band. Remarkably, exact many-body ground states can be constructed for the repulsive Hubbard model and the $t - J$ model by filling this flat band with localized electron states. This construction leads to a macroscopic ground-state degeneracy. We discuss how to compute these ground-state degeneracies for a certain class of models, including in particular the sawtooth chain. Furthermore, we discuss generic consequences for low-temperature thermodynamic properties, like the appearance of a low-temperature peak in the specific heat. Finally, we present complementary numerical results obtained by exact diagonalization.

Key words: Hubbard and $t - J$ model, flat band, geometric frustration, thermodynamics

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1. Introduction

It is a rare event that one can make exact statements about a strongly correlated electron system, especially in dimensions bigger than one. Competing interactions usually render the problem even more difficult, but sometimes they are also helpful for the analysis. In particular, on highly frustrated lattices it is possible to construct a macroscopic number of ground states (GSs) using localized single-particle excitations as building blocks. On the one hand, such a construction has been applied to the so-called flat-band Hubbard models in order to show that they exhibit fully saturated ferromagnetism for suitable electron fillings (see, e.g., [1–5]). On the other hand, so-called localized magnon states have been found to yield exact many-body GSs for highly frustrated quantum antiferromagnets in high magnetic fields [6–9]. Furthermore, it has been shown that the localized-magnon GSs have important consequences for the low-temperature magneto-thermodynamic properties like an enhanced magnetocaloric effect close to the saturation field [10–16]. Surprisingly, the corresponding thermodynamics of flat-band Hubbard models did not seem to have been investigated despite the long history of these

models [1–3]. This motivated us to start studying the thermodynamic properties of correlated electron systems on highly frustrated lattices [16–20]. Here we summarize some aspects of the construction of localized-electron GSs as well as their consequences for the low-temperature thermodynamics and present some complementary numerical results.

2. Models with localized electron states

We will discuss two classes of models of correlated electrons. Firstly, we consider the N -site Hubbard Hamiltonian

$$H = \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} t_{i,j} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \mu \sum_{i=1}^N n_i, \quad (1)$$

where i denotes the lattice sites, $\langle i, j \rangle$ are pairs of nearest neighbors, the $c_{i,\sigma}^{(\dagger)}$ are the usual fermion operators, $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$. $U \geq 0$ is the on-site Coulomb repulsion. Note that we have chosen [17] non-standard sign conventions for the hopping integrals $t_{i,j}$ and the chemical potential μ in order to emphasize the analogy with the antiferromagnetic Heisenberg model in a magnetic field.

Secondly, we consider the $t - J$ model with Hamiltonian

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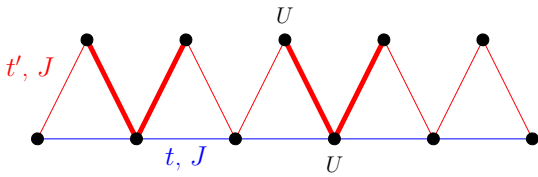


Fig. 1. The sawtooth chain. Filled circles show electron sites. Two trapping cells occupied by localized electron states are indicated by bold lines.

$$\begin{aligned}
 H = & \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} t_{i,j} P \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) P \\
 & + \sum_{\langle i,j \rangle} J_{i,j} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right) + \mu \sum_{i=1}^N n_i. \quad (2)
 \end{aligned}$$

Here P is the projector which eliminates doubly occupied sites and \vec{S}_i are spin-1/2 operators acting on a singly occupied site i . The $t-J$ model (2) arises as the large- U limit of the Hubbard model (1), yielding the relation $J_{i,j} = 4t_{i,j}^2/U$ up to second order in the hopping integrals $t_{i,j}$. However, the implied relation between the $J_{i,j}$ is not important for our purposes. We will therefore ignore it and choose $J_{i,j} = J$. Conversely, one could choose a site-dependent Coulomb repulsion $U_i > 0$ in the Hubbard model (1) without affecting any of our main conclusions.

We would like to emphasize that our main conclusions apply to any highly frustrated lattice. However, for the sake of concreteness, we will focus on the sawtooth chain sketched in Fig. 1. The hopping integrals $t_{i,j}$ are t along the base line and t' along the zigzag-line, respectively. Periodic boundary conditions are imposed along the chain direction.

The single-electron problem is solved as usually by introducing a momentum k . On the sawtooth lattice one finds two branches whose dispersions read

$$\varepsilon_{\pm}(k) = t \cos k \pm \sqrt{t^2 \cos^2 k + 2t'^2 \cos k + 2t'^2} + \mu. \quad (3)$$

Remarkably, the lower branch $\varepsilon_{-}(k)$ becomes completely flat, *i.e.*, k -independent for $t' = \sqrt{2}t$. The sawtooth Hubbard model (1) with this choice of hopping integrals is a particular case of Tasaki's model which exhibits saturated ferromagnetism for a half-filled flat band, *i.e.*, when the number of electrons is $n = N/2$ [2,3]. It is common practice to introduce on-site energies for Tasaki's model [2,3] such that the flat-band condition $t' = \sqrt{2}t$ can be replaced by a condition for the on-site energies (see also [4,5]). However, since this generalization does not change any of the fundamental physics, we will not pursue this either here.

There are many frustrated lattices which yield a lowest completely flat single-electron band, including popular lattices like the kagome and pyrochlore lattices in two and three dimensions, respectively. In fact, a completely flat lowest single-electron band can be taken as the defining property of a highly frustrated lattice.

Given such a flat band of excitations, one can transform back to real space and localize the excitations in a finite region. Such 'localized electron excitations' live in trapping

cells which for the sawtooth chain are the valleys formed by three neighboring sites (see bold lines in Fig. 1). Typically, each site adjacent to a trapping cell is connected to several sites of the trapping cell such that destructive quantum interference between the different paths prevents escape of the electron. Now one can occupy each trapping cell independently by electrons with the two different spin projections. For $U = 0$, this yields many-electron GSs of the Hubbard model (1) by construction. For $U > 0$, double occupancy of a trapping cell is forbidden, but a subset of these states remain exact eigenstates: completely spin-polarized states or states consisting of spatially sufficiently separated localized electron excitations (like the two bold valleys in Fig. 1) remain exact eigenstates also for $U > 0$. Positivity of the Coulomb term in the Hubbard model (1) implies that such states remain in fact *ground states* for $U > 0$. In fact, the same class of states are also exact eigenstates of the $t-J$ model (2). However, in this case the magnetic interaction term is no longer a positive operator. Thus, for sufficiently strong $J > 0$ other states may acquire lower energy, as has been observed for the sawtooth chain with $J = 2t$, $t' = \sqrt{2}t$ [18]. Therefore, the exact eigenstates under discussion are ground states of the $t-J$ model (2) generally only for sufficiently small J .

One can tune the energy of the flat band to zero by setting $\mu = \mu_0$ with a suitable μ_0 . For the sawtooth chain with $t' = \sqrt{2}t$, Eq. (3) shows that $\varepsilon_{-}(k) = 0$ for $\mu = \mu_0 = 2t$. All localized-electron GSs have zero energy for $\mu = \mu_0$. It was argued in [17] that the GS degeneracy is always macroscopic by giving an explicit lower bound. An alternative lower bound can be derived along the lines of section 2.6.4 of [8]: take a unit cell of the lattice with l sites such that it contains at least one trapping cell which does not overlap with the corresponding trapping cell in the neighboring unit cells (for the sawtooth chain one can use a unit cell of two valleys, *i.e.*, $l = 4$). Then each of these trapping cells can be either empty or independently occupied by a spin-up or -down electron. This yields $3^{N/l}$ GSs, *i.e.*, a lower bound for the GS entropy per site $S/N \geq \ln 3/l$.

Two cases should be distinguished for the further analysis. If all trapping cells are non-overlapping, spatial separation is automatically ensured and each trapping cell can be independently occupied by up to one electron in the presence of repulsive interactions. It is straightforward to count the localized-electron GSs and compute their contribution to thermodynamic quantities for any model of this type [20]. Furthermore, the average over the localized-electron GSs does not yield any macroscopic magnetic moment in this case [20].

In the case where trapping cells overlap, two electrons with different spin projection generally feel the repulsive interaction if they are localized in overlapping regimes. This favors parallel spin alignment in the GS for larger electron fillings. If all trapping cells are connected and each of them is occupied by one electron, these arguments give rise to a fully saturated ferromagnetic GS (flat-band ferromagnetism) [1-3]. In order to count all localized-electron

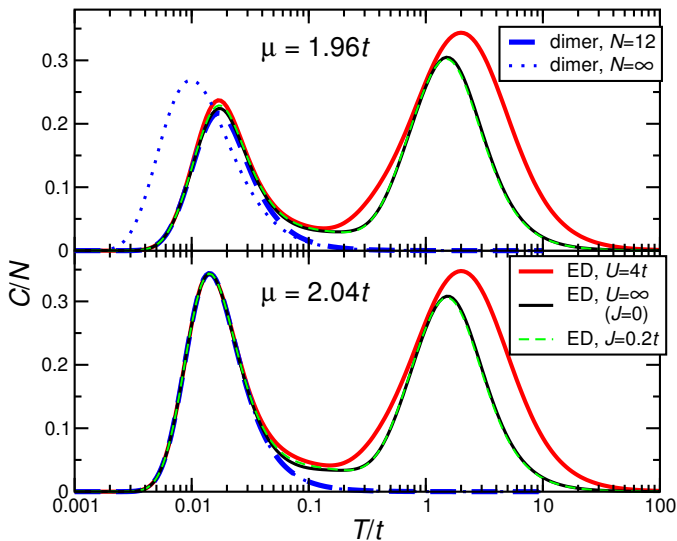


Fig. 2. Specific heat C per site N in the grand canonical ensemble for the sawtooth chain with $t' = \sqrt{2}t$ for two values of the chemical potential μ . Exact diagonalization (ED) results are for $N = 12$ sites.

GSs, we decompose the system into n -electron clusters, each of which has a $n + 1$ -fold spin degeneracy [19]. In one dimension, a suitable labeling yields a mapping to a dimer-type model which can be solved with a transfer matrix method [19]. For the sawtooth chain with $t' = \sqrt{2}t$ we find a GS entropy per site $S/N = \ln((1 + \sqrt{5})/2) = 0.48121 \dots$ [19], which should be compared to the above lower bound $S/N \geq \ln 3/4 = 0.27465 \dots$ and the lower bound of [17]: $S/N \geq \ln 2/2 = 0.34657 \dots$. Note that the dimer mapping can be applied to other one-dimensional models like a model originally due to Watanabe [4] or two kagome-like chains [7].

We emphasize that the localized-electron states should form a basis of the GS manifold for $U = 0$ in order to ensure completeness also for $U > 0$. This completeness condition can be satisfied if the flat band is separated by a finite gap from the next dispersive band, as is the case for the sawtooth chain. However, if a dispersive band touches the flat band, this gives rise to additional GSs.

3. Numerical results for the sawtooth chain

Now we illustrate and extend some of the above general considerations by presenting a comparison with exact diagonalization (ED) for the sawtooth chain.

Fig. 2 shows the specific heat C in the *grand canonical ensemble* for $t' = \sqrt{2}t$ and two values of μ . Firstly, we observe a low-temperature maximum around $T = \mathcal{O}(10^{-2}t)$ in the ED results for both values of the chemical potential. This low-temperature maximum is (almost) the same for a finite- U Hubbard model, the $U = \infty$ Hubbard model (which is equivalent to the $J = 0$ case of the $t - J$ model), and even the $t - J$ model with $J = 0.2t$. This maximum is well described by the effective dimer model [19], *i.e.*, it arises from the GS manifold which is split due to the de-

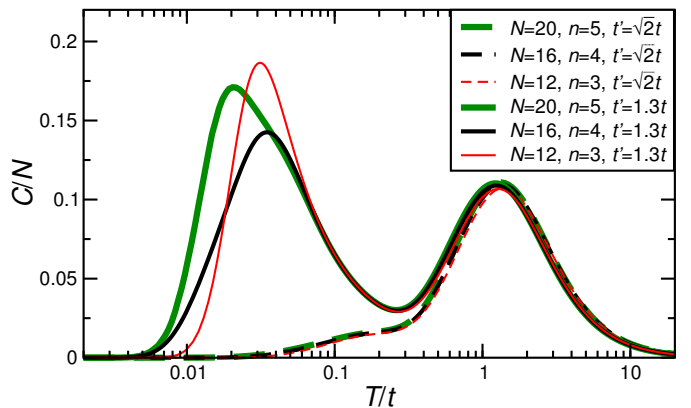


Fig. 3. Specific heat C per site N in the canonical ensemble for the sawtooth chain with $n = N/4$ electrons. All results are for the $U = \infty$ Hubbard model, or equivalently the $t - J$ model with $J = 0$.

viation $\mu \neq \mu_0 = 2t$. Comparison with other system sizes than the $N = 12$ results of Fig. 2 reveals some finite-size effects for $\mu < \mu_0$ while they are negligible for $\mu > \mu_0$ [19]. Note that the limit $N \rightarrow \infty$ can be carried out in the effective dimer model (dotted line in Fig. 2) [19]. The remaining states give rise to another maximum in C at a higher temperature $T = \mathcal{O}(t)$. The area under this second maximum is clearly smaller in the $t - J$ model than in the Hubbard model, reflecting the reduced Hilbert space. Finite-size effects are negligible in the high-temperature region [19].

We use the $t - J$ model with $J = 0$ to discuss some complementary aspects. The specific heat C of the effective dimer model vanishes identically in the *canonical ensemble* since the energy of a localized electron state depends only on the electron number n . Accordingly, the low-temperature maximum in C disappears for $t' = \sqrt{2}t$, as illustrated by the ED results for $n = N/4$ shown in Fig. 3. However, a detuning $t' \neq \sqrt{2}t$ leads to a splitting of the GS manifold such that the low-temperature maximum reappears, as demonstrated in Fig. 3 for $t' = 1.3t$ (note that finite-size effects tend to be bigger in the canonical ensemble than in the grand canonical ensemble). This shows that the low-temperature maximum in C is not only robust under a small violation of the flat-band condition, but that such a detuning actually helps to stabilize this feature.

The separation of the GS manifold at $t' = \sqrt{2}t$ from states with $n > N/2$ is controlled by the charge gap $\Delta\mu$ which in the Hubbard model opens linearly as $\Delta\mu \approx 0.46U$ for small $U \ll t$ [19] and saturates at $\Delta\mu \approx 2t$ for large $U \gg t$ [16, 19]. We quantify the excitations in the sectors with $n \leq N/2$ using the integrated number of states with an energy of at most ΔE above the degenerate GS manifold. This quantity is shown in Fig. 4 for the $N = 12$ Hubbard model with different values of U . The case $n = N/4 = 3$ is representative of the generic situation while the energy of the lowest excited state is smallest in the sector $n = N/2 - 1 = 5$. We observe that an appreciable density of states appears at rather low energies above the highly degenerate GSs. The fact that the curves in Fig. 4 are very similar for small U when ΔE is scaled by U indicates that

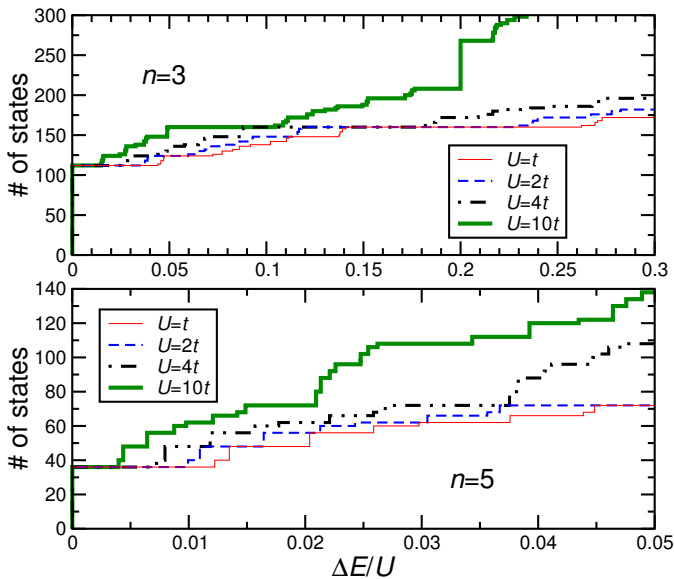


Fig. 4. Integrated number of states with an excitation energy below ΔE for the sawtooth Hubbard model with $t' = \sqrt{2}t$, $N = 12$ sites, and different values of U . The upper and lower panels show the sectors with $n = 3$ and 5 electrons, respectively.

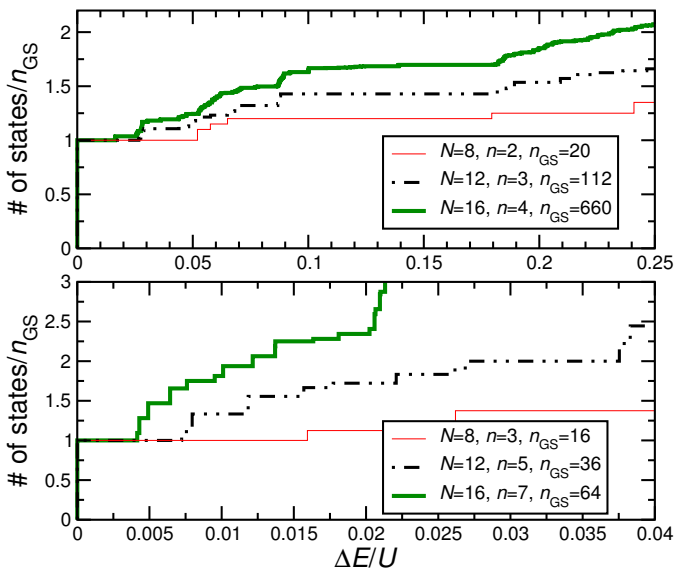


Fig. 5. Integrated number of states normalized by the number of ground states n_{GS} for the sawtooth Hubbard model with $t' = \sqrt{2}t$ and $U = 4t$. The upper and lower panels show the sectors with $n = N/4$ and $n = N/2 - 1$ electrons, respectively.

these low-lying excitations originate from states which used to be GSs for $U = 0$. The finite-size dependence at $n = N/4$ and $n = N/2 - 1$ is analyzed in Fig. 5 for the example $U = 4t$. In order to be able to compare different values of N , we divide the integrated number of states by the number of GSs n_{GS} (see legends of Fig. 5 for the values). We observe that the density of low-energy excitations increases with N , even when compared to n_{GS} . It is not completely clear at present whether this indicates the absence of a thermodynamic excitation gap for $N \rightarrow \infty$, which would imply quantitative corrections to the dimer model for all temper-

atures $T > 0$. In any case, this large density of low-lying excitations is probably the origin of the small deviations for $\mu = 1.96t$ in Fig. 2 between the effective dimer model and the Hubbard model with $U = 4t$.

4. Conclusions

We have argued that in highly frustrated Hubbard and $t - J$ models one finds a macroscopic GS degeneracy for a certain value of the chemical potential μ_0 or, equivalently, in a certain range of electron fillings. A splitting of this GS manifold, e.g., by a small deviation $\mu \neq \mu_0$ or deviation from the ideal flat-band geometry leads to a characteristic low-temperature peak in the specific heat. These general considerations have been illustrated with ED results for the sawtooth chain. We have also exhibited a large number of low-lying excited states in the sawtooth chain.

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