Low-temperature thermodynamics of one class of flat-band models

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Abstract. We consider the antiferromagnetic Heisenberg model and the repulsive Hubbard model for a class of frustrated lattices with a completely dispersionless (flat) lowest one-particle (either one-magnon or one-electron) band. We construct exact many-particle ground states for a wide range of particle densities, calculate their degeneracy, and, as a result, obtain closed-form expressions for the low-temperature thermodynamic quantities around a particular value of the magnetic field \(h_{\text{sat}}\) or the chemical potential \(\mu_0\). We confirm our analytic findings by numerical data for finite lattices.

1. Introduction

Strongly correlated systems on geometrically frustrated lattices represent a playground to study many collective quantum phenomena. In this paper, we consider a particular class of geometrically frustrated lattices, namely lattices which support flat (i.e. completely dispersionless) one-particle bands. The antiferromagnetic Heisenberg model on such lattices was examined in Refs. [1–4], although in the context of flat-band ferromagnetism some of these lattices were discussed even earlier [5, 6], see also Ref. [7]. The flat one-particle band leads to the possibility to localize the corresponding one-particle states within a finite region of a lattice. Considering further many-particle states one may expect that the states with localized particles which are spatially separated from each other are also the eigenstates of the Hamiltonian with interaction. Under certain conditions a manifold of localized states may constitute a highly degenerate ground state of the interacting many-particle system and as a result the localized states may dominate the low-temperature thermodynamics.

In the present paper we compare and contrast the consideration of the localized-states effect for the low-temperature thermodynamics for two models, the spin-1/2 antiferromagnetic Heisenberg model and the one-orbital repulsive Hubbard model. For concreteness we focus on the sawtooth-chain (\(\Delta\)-chain) lattice shown in Fig. 1 (for other lattices see Ref. [4]). More specifically, we deal with the antiferromagnetic Heisenberg Hamiltonian

\[
H_{\text{Heis}} = \sum_{\langle i,j \rangle} J_{i,j} \left[ \frac{1}{2} (s_i^+ s_j^- + s_i^- s_j^+) + s_i^z s_j^z \right] - h \sum_i s_i^z \tag{1}
\]

with the nearest-neighbor exchange integrals \(J_{i,j} > 0\), and the Hubbard Hamiltonian
with the on-site repulsion $U > 0$. We have chosen the sign of hopping terms $t_{i,j} > 0$ in the Hubbard model (2) in order to emphasize the correspondence with the Heisenberg model (1). Note that the magnetic field $h$ in the Heisenberg model (1) plays the same role as the chemical potential $\mu$ in the Hubbard model (2). Below we consider the spin model (1) in strong magnetic fields around the saturation field $h_{\text{sat}}$ and the Hubbard model (2) at values of the chemical potential around a characteristic value $\mu_0$, see below. Although both models represent different physics, we will demonstrate that the mathematical consideration exhibits many common features. The physical properties for the spin system for $h \approx h_{\text{sat}}$ and for the electron system for $\mu \approx \mu_0$ will be governed exclusively by either localized magnon or electron states which exist due to lattice geometry.

We begin with the spin model (1) [1–4]. The lowest excitations in strong magnetic fields $h > h_{\text{sat}}$ are one-magnon states above the fully polarized ferromagnetic state $|\text{FM}\rangle$. The lower of the two branches of the one-magnon dispersion for the sawtooth chain becomes flat for $J_2 = 2J_1$.

For this case one can construct magnon states located in one of the valleys of the sawtooth chain $|2j\rangle = (s_{2j-1}+2s_{2j}+s_{2j+1})|\text{FM}\rangle$ with the energy $E_{\text{FM}} - \epsilon_1 - h(N/2 - 1)$, $E_{\text{FM}}$ is the energy of the state $|\text{FM}\rangle$ of the spin system (1), $\epsilon_1 = 4J_1$. Next, we consider the electron model (2) [5–7]. The lower one-electron band becomes completely flat for $t_2 = \sqrt{2}t_1$. The localized one-electron states can be written as $|2j, \sigma\rangle = (c_{2j-1,\sigma} \pm \sqrt{2}c_{2j,\sigma} \pm c_{2j+1,\sigma})|0\rangle$ and their energy is $\epsilon_1 = -2t_1 + \mu$. Although the one-particle problem for both Hamiltonians is quite similar, the many-particle problem will obviously be different. For the Heisenberg system we deal with magnons which are hard-core bosons with nearest-neighbor repulsion (see Eq. (1)), whereas for the Hubbard system we deal with interacting spinful electrons which represent a two-component fermionic mixture with one-site repulsion (see Eq. (2)).

2. Localized states in the presence of interactions

Since the localized states are located in a restricted area of the whole lattice, it is clear that many-particle states consisting of several isolated (no common sites) occupied valleys are exact eigenstates of both Hamiltonians [1–7]. However, for the Hubbard model, by contrast to the Heisenberg model, the localized states with the same spin polarization may also have common sites. By direct computation one shows that, e.g., $|2j, \sigma\rangle|2j+2, \sigma\rangle$ is indeed an eigenstate of the Hamiltonian (2) in the two-electron subspace. Further localized two-electron states with one common site can be obtained owing to SU(2) symmetry of the Hubbard model (2) by applying operators $S^- = \sum_i c_{i,\sigma}^\dagger c_{i,\downarrow}$ or $S^+ = \sum_i c_{i,\sigma}^\dagger c_{i,\uparrow}$ on $|2j, \sigma\rangle|2j+2, \sigma\rangle$. This example clearly shows a difference between magnons and electrons conditioned by different particle statistics and interaction. Finally, we notice that a maximal number of localized magnons/electrons which can be put on the sawtooth-chain lattice is $n_{\text{max}} = N/4$ for magnons but $n_{\text{max}} = N/2$ (corresponding to quarter filling) for electrons; here $N$ is the (even) number of sites of the sawtooth-chain lattice.

Since the localized states are the lowest-energy states in the one-particle subspace, one may also expect that the states with $n$ isolated (independent) localized particles are the lowest-energy
states in the \( n \)-particle subspace (for rigorous proofs see Ref. [8]). We can also confirm this by exact diagonalizations of finite systems \([1, 3, 4, 7]\). Moreover, numerics gives evidence that for many lattices these ground states are separated from the higher-energy states by a gap. Another important property of the localized states is their linear independence \([9]\). The energy of many lattices these ground states are separated from the higher-energy states by a gap. Another exact diagonalizations of finite systems \([1, 3, 4, 7]\). Moreover, numerics gives evidence that for low-temperature thermodynamics.

In Fig. 2 we illustrate the localized-state predictions (3) and (4) for the temperature dependence of the specific heat. The low-temperature maximum in Fig. 2 is due to the manifold of localized states. Obviously, the localized-state picture excellently reproduces exact diagonalization data for finite systems in the low-temperature regime for small deviation from the values \( h_{\text{sat}} \) or \( \mu_0 \). Moreover, we note that localized-state thermodynamics implies an enhanced magnetocaloric effect \([10, 11]\).

### 3. Summary
To summarize, we have studied the localized-state effects for two strongly interacting models (antiferromagnetically interacting Heisenberg spins and standard Hubbard electrons) on the sawtooth-chain lattice which supports a flat one-particle band. Under certain conditions (values of external magnetic field or chemical potential) the localized states in both models govern the low-temperature thermodynamics.
Figure 2. Specific heat for the spin model (1) \((J_1 = 1, J_2 = 2)\) at \(h = 0.98h_{\text{sat}} = 3.92J_1\) (left) and the electron model (2) \((t_1 = 1, t_2 = \sqrt{2})\) around \(\mu_0 = 2t_1\) (right). Left: exact diagonalization data for \(N = 20\) (filled circles); hard-dimer data for \(N/2 = 10\) (thick curve) and \(N/2 \to \infty\) (thin curve). Right: exact diagonalization data for \(U \to \infty\), \(N = 12\) for \(C(T, n, N)/N\), \(n = 1, 2, 3, 4, 5, 6, 7\) electrons (up-triangles, down-triangles, diamonds, squares, pentagons, circles, and crosses, respectively) and \(C(T, \mu = 0.98\mu_0, N)/N\) (filled circles); hard-dimer data for \(N = 12\) (thick curve) and \(N \to \infty\) (thin curve) for \(C(T, \mu = 0.98\mu_0, N)/N\).

Several remarks are in order here. The large-\(U\) limit of the Hubbard Hamiltonian (2) yields the \(t-J\) model. Therefore, it is not astonishing that the localized-electron states are also eigenstates of the \(t-J\) Hamiltonian and they are the ground states for \(n = 1, \ldots, N/2\) electrons for small exchange couplings \(J_{i,j}\) [12]. Some prominent peculiarities of low-temperature thermodynamic quantities conditioned by localized states remain stable to small deviations from the ideal lattice geometry, increasing chances to observe the examined properties in solid-state systems [3]. Although we focus here on one representative example, the sawtooth-chain lattice, the elaborated scheme can also be applied to spin and electron models on other lattices [4, 13].

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