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

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

with the nearest-neighbor exchange integrals $J_{i,j} > 0$, and the Hubbard Hamiltonian
applying operators \( S^+ = \sum_i c_{i,\uparrow} \) or \( S^- = \sum_i c_{i,\uparrow} c_{i,\downarrow} \) 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

\[
H_{\text{Hub}} = \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} t_{i,j} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \mu \sum_{\sigma=\uparrow,\downarrow} \sum_i n_{i,\sigma} \quad (2)
\]

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 \( |2j\rangle = (s_{2j-1}^- - 2s_j^- + s_{2j+1}^-)|\text{FM}\rangle \) 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 \( |2j,\sigma\rangle = (c_{2j-1,\sigma}^\dagger - \sqrt{2}c_{2j,\sigma}^\dagger + c_{2j+1,\sigma}^\dagger)|0\rangle \) 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 \( S^- = \sum_i c_{i,\uparrow} c_{i,\downarrow} \) or \( S^+ = \sum_i c_{i,\downarrow}^\dagger c_{i,\uparrow}^\dagger \) 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.
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 the localized $n$-particle states is $E_n^{lm} = E_{FM} - hN/2 + n(h - 4J)$ for the Heisenberg model and $E_n^{le} = n(\mu/2 + 2\ell)$ for the electron model. Obviously, the localized-magnon states (localized-electron states) are degenerate at the saturation field $h = h_{sat} = 4J_1$ (at a characteristic value of the chemical potential $\mu = \mu_0 = 2\ell$).

Consider now the spin model in a strong magnetic field $h$ around the saturation field $h_{sat}$. Using the ensemble with fixed $(h, N)$ we find the following contribution of the localized-magnon states to the partition function

$$Z(T, h, N) = \sum_{n=0}^{n_{\text{max}}} g_{N}^{\text{mag}}(n) \exp\left(-\frac{E_n^{lm}}{T}\right) \propto \sum_{n=0}^{n_{\text{max}}} g_{N}^{\text{mag}}(n) \exp\left(h_{sat} - \frac{h}{T}\right)$$

Here $g_{N}^{\text{mag}}(n)$ is the degeneracy of the states with $n$ independent localized magnons. Thermodynamic quantities follow by the standard relations: $F(T, h, N) = -T\ln Z(T, h, N)$, $S(T, h, N) = -\partial F(T, h, N)/\partial T$ (entropy), $C(T, h, N) = T\partial S(T, h, N)/\partial T$ (specific heat) etc. Similarly, we consider the electron model at a value of the chemical potential around $\mu_0$. Using the (grand-canonical) ensemble with fixed $(\mu, N)$ we find the following contribution of the localized-electron states to the partition function

$$\Xi(T, \mu, N) = \sum_{n=0}^{n_{\text{max}}} g_{N}^{\text{el}}(n) \exp\left(-\frac{E_n^{le}}{T}\right) \propto \sum_{n=0}^{n_{\text{max}}} g_{N}^{\text{el}}(n) \exp\left(\frac{\mu_0 - \mu}{T}\right)$$

Here $g_{N}^{\text{el}}(n)$ is the degeneracy of states with $n$ independent localized electrons. Thermodynamic quantities follow by the standard relations: $\Omega(T, \mu, N) = -T\ln \Xi(T, \mu, N)$, $S(T, \mu, N) = -\partial \Omega(T, \mu, N)/\partial T$ (entropy), $\bar{n}(T, \mu, N) = \partial \Omega(T, \mu, N)/\partial \mu$ (average number of electrons) etc. We note that the specific heat $C(T, n, N)$ at constant $n$ equals zero for $n = 1, \ldots, N/2$.

The central problem now is the calculation of the degeneracy $g_{N}(n)$ for localized magnon and electron states. This can be done using a mapping of localized states onto spatial configurations of hard dimers on a simple chain. For the spin system it can be shown that $g_{N}^{\text{mag}}(n) = Z(n, N/2)$, $n = 0, 1, \ldots, N/4$, where $Z(n, N)$ is the number of spatial configurations of $n$ hard dimers on a chain of $N$ sites [2–4]. For the electron system it can be shown that $g_{N}^{\text{el}}(n) = Z(n, N)$, $n = 0, 1, \ldots, N/2 - 1$, but $g_{N}^{\text{el}}(N/2) = N/2 + 1$ [7]. Substituting $g_{N}^{\text{mag}}(n)$ and $g_{N}^{\text{el}}(n)$ into Eqs. (3) and (4) we obtain a grand-canonical partition function of one-dimensional hard dimers, which can be calculated using the transfer-matrix method. As a result, we obtain the low-temperature thermodynamics for both models.

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 $h_{sat}$ 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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