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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 $h_{\rm sat}$ or the chemical potential μ_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 (Δ-chain) lattice shown in Fig. 1 (for other lattices see Ref. [4]). More specifically, we deal with the antiferromagnetic Heisenberg Hamiltonian

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

with the nearest-neighbor exchange integrals $J_{i,j} > 0$, and the Hubbard Hamiltonian

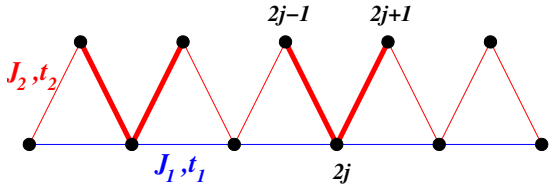

Figure 1. The sawtooth chain. The exchange (hopping) integrals are J_1 (t_1) along the base line and J_2 (t_2) along the zigzag line. The bold valleys show the area occupied by localized magnons (electrons).

$$H_{\rm Hub} = \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} t_{i,j} \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + c^{\dagger}_{j,\sigma} c_{i,\sigma} \right) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \mu \sum_{\sigma=\uparrow,\downarrow} \sum_{i} n_{i,\sigma} \tag{2}$$

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 μ in the Hubbard model (2). Below we consider the spin model (1) in strong magnetic fields around the saturation field $h_{\rm sat}$ and the Hubbard model (2) at values of the chemical potential around a characteristic value μ_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 $h \approx h_{\rm sat}$ 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 $h > h_{\rm sat}$ are one-magnon states above the fully polarized ferromagnetic state $|{\rm FM}\rangle$. 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 $|2j\rangle = (s^{-}_{2j-1} - 2s^{-}_{j} + s^{-}_{2j+1})|{\rm FM}\rangle$ with the energy $E_{\rm FM} - \epsilon_1 - h(N/2-1)$, $E_{\rm FM}$ is the energy of the state $|{\rm FM}\rangle$ 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 $|2j,\sigma\rangle = (c^{\dagger}_{2j-1,\sigma} - \sqrt{2}c^{\dagger}_{2j,\sigma} + c^{\dagger}_{2j+1,\sigma})|0\rangle$ and their energy is $\varepsilon_1 = -2t_1 + \mu$. 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 $S^{-} = \sum_i c^{\dagger}_{i,\downarrow} c_{i,\uparrow}$ or $S^{+} = \sum_i c^{\dagger}_{i,\uparrow} c_{i,\downarrow}$ 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 sawtooh-chain lattice is $n_{\rm max} = N/4$ for magnons but $n_{\rm max} = N/2$ (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 the localized n-particle states is $E_n^{\rm lm} = E_{\rm FM} - hN/2 + n(h - 4J_1)$ for the Heisenberg model and $E_n^{\rm le} = n(\mu - 2t_1)$ for the electron model. Obviously, the localized-magnon states (localized-electron states) are degenerate at the saturation field $h = h_{\rm sat} = 4J_1$ (at a characteristic value of the chemical potential $\mu = \mu_0 = 2t_1$).

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

$$Z(T,h,N) = \sum_{n=0}^{n_{\rm max}} g_N^{\rm mag}(n) \exp\left(-\frac{E_n^{\rm lm}}{T}\right) \propto \sum_{n=0}^{n_{\rm max}} g_N^{\rm mag}(n) \exp\left(\frac{h_{\rm sat}-h}{T} n\right). \tag{3}$$

Here $g_N^{\rm mag}(n)$ 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 μ_0. Using the (grand-canonical) ensemble with fixed (μ, N) we find the following contribution of the localized-electron states to the partition function

$$\Xi(T,\mu,N) = \sum_{n=0}^{n_{\rm max}} g_N^{\rm el}(n) \exp\left(-\frac{E_n^{\rm le}}{T}\right) = \sum_{n=0}^{n_{\rm max}} g_N^{\rm el}(n) \exp\left(\frac{\mu_0-\mu}{T} n\right). \tag{4}$$

Here $g_N^{\rm el}(n)$ 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 $g_N^{\rm mag}(n) = Z(n, N/2)$, $n = 0, 1, \ldots, N/4$, where $Z(n,\mathcal{N})$ is the number of spatial configurations of n hard dimers on a chain of $\mathcal{N}$ sites [2–4]. For the electron system it can be shown that $g_N^{\rm el}(n) = Z(n,N)$, $n = 0, 1, \ldots, N/2-1$, but $g_N^{\rm el}(N/2) = N/2+1$ [7]. Substituting $g_N^{\rm mag}(n)$ and $g_N^{\rm el}(n)$ 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 $h_{\rm sat}$ or μ_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.

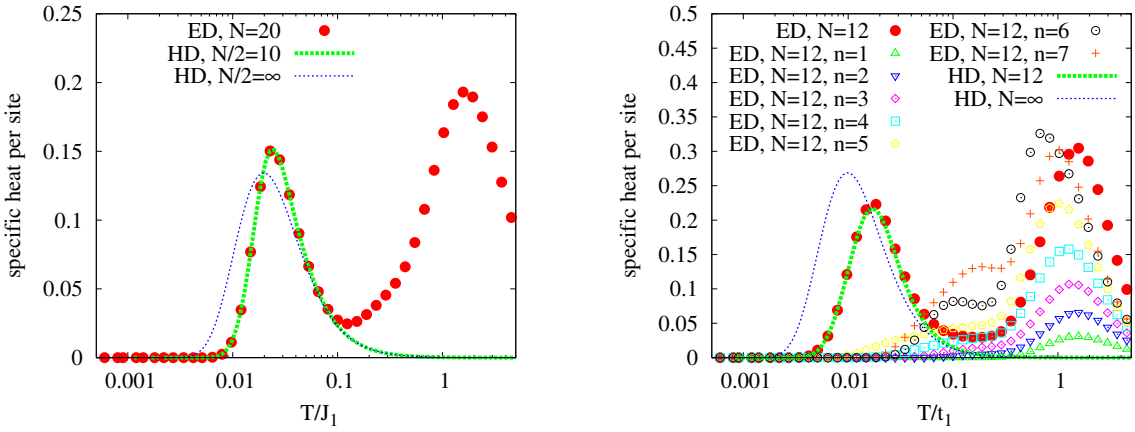

Figure 2. Specific heat for the spin model (1) ($J_1 = 1$, $J_2 = 2$) at $h = 0.98h_{\rm sat} = 3.92J_1$ (left) and the electron model (2) ($t_1 = 1$, $t_2 = \sqrt{2}$) around $\mu_0 = 2t_1$ (right). Left: exact diagonalization data for $N = 20$ (filled circles); hard-dimer data for $N/2 = 10$ (thick 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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