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LETTER TO THE EDITOR

Melting of an antiferromagnetic Heisenberg spin chain by external magnetic fields

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Abstract. We study the magnetic-field-induced insulator–metal transition in the t–J' chain model at quarter filling. In this model the nearest-neighbour hopping energy t competes with the next-nearest-neighbour exchange energy J', and for a small t/J' the system is an insulator accompanied by a charge ordering. Response to external magnetic fields is investigated numerically by the density-matrix renormalization-group method. We have found that a transition from the charge ordered insulating phase to a metallic phase occurs at a finite strength of the magnetic field for small t/J'. The transition is an example of magnetic-field-induced melting transition of a quantum antiferromagnetic Heisenberg spin chain system.

The metal–insulator transition controlled by the magnetic field has considerable practical and scientific interest. For example, in some pseudo-perovskite manganite materials, the magnetic-field-induced transition from the antiferromagnetic (AF) insulating phase with the charge ordering to the ferromagnetic metallic phase was observed [1]. In these manganite materials, multi-3d orbitals of Mn play an important role. It is possible, however, that such a transition occurs in simpler systems. In this letter, we propose a simple single band electronic system in which the insulator–metal transition is induced by the magnetic field. The system is described by the one-dimensional (1D) t–J' model. The Hamiltonian of the model is defined as

$$\mathcal{H} = -t \sum_{i\sigma} (\tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{i+1\sigma} + \text{H.c.}) + J' \sum_{i} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2} \tag{1}$$

where the operator $\tilde{c}^{\dagger}_{i\sigma}$ ($\tilde{c}_{i\sigma}$) creates (annihilates) a particle with spin σ at the ith site. These operators are defined in the subspace where double occupancy is excluded. $\boldsymbol{S}_i$ denotes the spin operator at the ith site (figure 1). In this model, the nearest-neighbour hopping energy t competes with the next-nearest-neighbour exchange energy J'. In a previous paper [2], we have shown that the transition from the AF charge-ordered insulator to the metal occurs at a finite value of t/J' ($(t/J')_{\mathrm{C}} \simeq 0.18$) in the 1D t–J' model at quarter filling. For $t/J' \leqslant (t/J')_{\mathrm{C}}$ the system behaves as a 1D antiferromagnetic (AF) Heisenberg spin system. On the other hand, for $t/J' > (t/J')_{\mathrm{C}}$, the system belongs to the class of Tomonaga–Luttinger liquids.

Since the charge ordering is caused by the AF Heisenberg coupling between spins, it is expected that the charge ordering is broken by the magnetic field. Here we investigate whether or not the insulator–metal transition occurs under finite strength of the magnetic field for the region $t/J' < (t/J')_{\mathrm{C}}$ in the 1D t–J' model. We restrict ourselves to quarter

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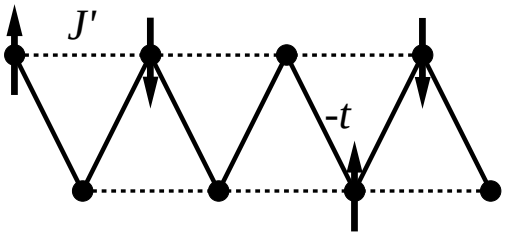

Figure 1. The t–J' chain model. Each dot denotes a site and arrows represent carriers with spins specified by arrows. The solid and broken lines denote the nearest-neighbour hoppings t and the next-nearest-neighbour exchange interactions J', respectively.

filling and we fix the value of t/J' as $t/J' = 0.1$. It has been confirmed that the system is in an insulating phase for $t/J' = 0.1$ [2]. In order to investigate the transition, we calculate the charge density order parameter $n_{\rm cd} = n_{\rm odd} - n_{\rm even}$, where $n_{\rm odd}(n_{\rm even})$ is the mean value of the number density n_i at odd (even) sites. The order parameter is defined by

$$n_{\rm cd} \equiv \frac{1}{L/2} \sum_{i\ {\rm odd}} (n_i - n_{i+1}) \tag{2}$$

where L denotes the system size. While $n_{\rm cd}$ should be zero in the metallic phase, it should be finite in the insulating phase. In the insulating phase, clearly there is two-fold degeneracy for the charge ordering. We calculate $n_{\rm cd}$ with a small external field ϵ at the end of the system in order to break the symmetry. This external field is added to the model Hamiltonian (1) as $\mathcal{H} - \epsilon \sum_\sigma \tilde{c}^\dagger_{1\sigma} \tilde{c}_{1\sigma}$ at the first site ($\epsilon > 0$). We study the response of the system against the small symmetry breaking field. For the numerical calculation, we use the density-matrix renormalization-group (DMRG) method [3], which is one of the standard numerical methods for studying 1D quantum systems. We study systems of various sizes ($L = 16, 24, 32$ and 48) by using the finite-system algorithm of the DMRG method [3]. The technical details of the numerical calculation are given in the previous paper.

The effect of the magnetic field in the system is described by the Zeeman term as

$$\tilde{\mathcal{H}} = \mathcal{H} - g\mu_{\rm B} H \sum_i S^z_i \tag{3}$$

where S^z_i denotes the z-component of the ith site spin operator. Hereafter, the g-factor g, Bohr magneton $\mu_{\rm B}$, and the magnetic field H are expressed by h as $h = g\mu_{\rm B} H$. In practical calculations, we obtain the ground state of the system in subspace with a certain value of $S^z_{\rm tot} \equiv \sum_i S^z_i$. The value of $S^z_{\rm tot}$ varies from $S^z_{\rm tot} = 0$ to $S^z_{\rm tot} = S^z_{\rm max} \equiv L/4$.

Figure 2 shows examples of the local number density n_i for various values of $S^z_{\rm tot}$ with an external field $\epsilon/J' = 1.0 \times 10^{-3}$ ($L = 32$). Shown here are the central 28 sites excluding four sites at both ends of the system. Without the magnetic field, the system clearly shows the charge ordering behaviour. Increasing the value of $S^z_{\rm tot}$, the difference between $n_{\rm odd}$ and $n_{\rm even}$ decreases.

Charge density order parameters $n_{\rm cd}$ are shown in figure 3 for various system sizes ($L = 24, 32$ and 48). The value of $n_{\rm cd}$ obtained by the simple linear extrapolation with no magnetic field is equal to 0.915. Error bars represent the standard deviation. While the region of the charge ordered phase spreads out for larger-size systems, it is clear that $n_{\rm cd}$ vanishes in the region $S^z_{\rm tot}/S^z_{\rm max} \geqslant 0.5$ for all system sizes.

Since we cannot carry out the simple extrapolation for system sizes because of a limited set of data for each value of $S^z_{\rm tot}$, we cannot determine the transition point with

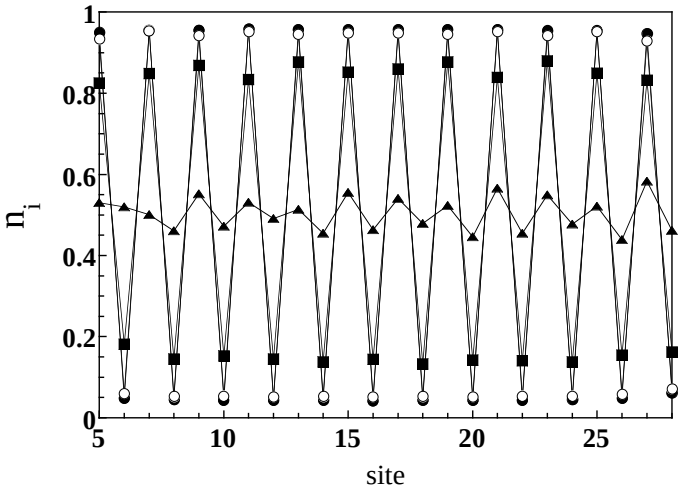

Figure 2. Local number density n_i at each site for various values of $S^z_{\rm tot}$; $S^z_{\rm tot}/S^z_{\rm max} = 0$ (closed circles), $1/8$ (open circles), $1/4$ (closed squares) and $3/8$ (closed triangles). The system size L of this example is 32 ($\epsilon/J' = 1.0 \times 10^{-3}$).

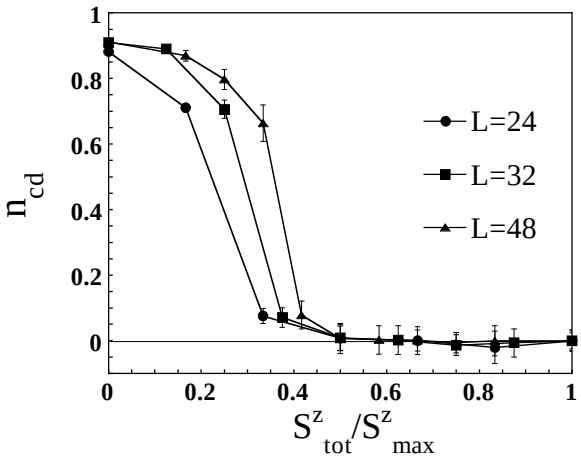

Figure 3. Results of $n_{\rm cd}$ versus $S^z_{\rm tot}/S^z_{\rm max}$ for various system sizes: $L = 24$ (circles), 32 (squares) and 48 (triangles).

high accuracy. However, one can clearly see from the size dependence of $n_{\rm cd}$ that the charge ordering is completely broken for $S^z_{\rm tot}/S^z_{\rm max} \geqslant 0.5$. In order to obtain the strength of the magnetic field h corresponding to the value of $S^z_{\rm tot}$ such as $S^z_{\rm tot}/S^z_{\rm max} = 0.5$, we calculate the total ground state energy $\tilde{E}_{\rm g}(S^z_{\rm tot}; L; h) = E_{\rm g}(S^z_{\rm tot}; L) - hS^z_{\rm tot}$. For a given value of $S^z_{\rm tot}$, the strength of the magnetic field h is given by $\tilde{E}_{\rm g}(S^z_{\rm tot} + 1; L; h) = \tilde{E}_{\rm g}(S^z_{\rm tot}; L; h)$, i.e. $h = E_{\rm g}(S^z_{\rm tot} + 1; L) - E_{\rm g}(S^z_{\rm tot}; L)$. For $S^z_{\rm tot}/S^z_{\rm max} = 0.5$, the corresponding magnitude of h is $h \simeq 0.97J'$, which is obtained by the infinite system size extrapolation. Thus the charge ordering expressed by $n_{\rm cd}$ completely vanishes for the magnetic field strength $h \sim J'$.

We can obtain information on the order of the transition from the system-size dependence shown in figure 3. One can see that all values of $n_{\rm cd}$ in the region $S^z_{\rm tot}/S^z_{\rm max} < 0.5$ increases

as the system size increases, and the values of n_{cd} for $S^z_{tot}/S^z_{max} = 0.5$ are fixed to zero. If the transition is of second order, the system-size dependence should be different from the present result; there exists a point above which values decrease as the system size increases. Besides, the system-size dependence is similar to the result of the system-size dependence of n_{cd} versus t/J' in the previous study [2]. In the previous study we could conclude that the phase transition is of first order. These facts therefore suggest that the magnetic-field-induced transition discussed in the present paper is of first order.

We need to comment on the fully polarized case. When S^z_{tot} is equal to S^z_{max}, the next-nearest-neighbour AF exchange interaction J' works as the repulsive interaction between the two spins on the next-nearest-neighbour sites. Therefore the system behaves as the spinless fermion system interacting with the next-nearest-neighbour repulsion. In this case, the particles avoid each other so as not to be on next-nearest-neighbour sites and another type of charge ordering occurs. In this charge ordering, there are two empty sites between every two neighbouring occupied sites: this type of charge ordering may be called 'ooee' ordering. In order to confirm this type of the 'ooee' ordering, we calculate the local number density n_i for the fully polarized system, $S^z_{tot} = S^z_{max}$. To obtain the unique ground state we calculate n_i with an external potential δ at the first and end sites of the system as $\mathcal{H} + \delta \sum_\sigma (n_{1\sigma} + n_{L\sigma})$ (we set $\delta = J'$). Figure 4 shows the local number density for the case of $S^z_{tot} = S^z_{max}$. One can see that the 'ooee' charge ordering actually takes place. Note that the charge ordering state at $S^z_{tot} = S^z_{max}$ is singular and for any value of $S^z_{tot} < S^z_{max}$ this charge ordering disappears while fluctuations towards the 'ooee' ordering remain for large values of S^z_{tot}. For an infinite-size system, the number of the down spins is proportional to the system size for any incomplete ferromagnetic state. Since the down spins destroy the phase coherence of the 'ooee' ordering, it is expected that the charge ordering disappears for any value of $S^z_{tot} < S^z_{max}$ in the thermodynamic limit.

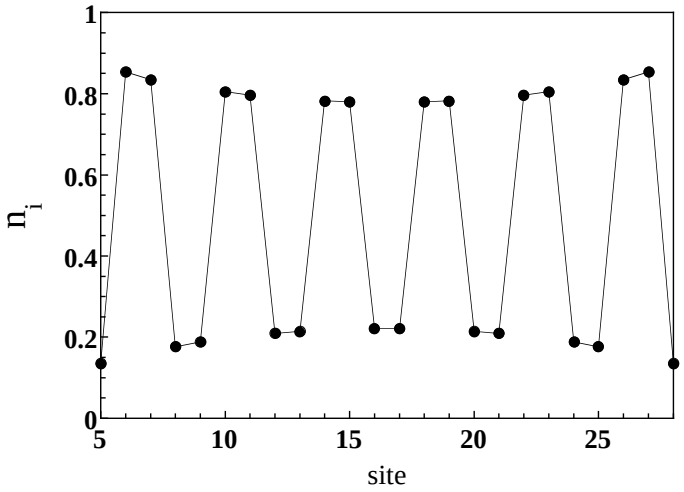

Figure 4. Local number density n_i for the fully polarized case $S^z_{tot}/S^z_{max} = 1$. The system size L of this example is 32. In the calculation we apply the local potential δ at both ends of the system: $\delta/J' = 1.0$ (see the text).

In conclusion, we have calculated by the DMRG method the charge density order parameter n_{cd} in the t–J' chain model ($t/J' = 0.1$) in the quarter-filled case. We have found that the charge ordering defined by n_{cd} completely disappears for $S^z_{tot}/S^z_{max} \geqslant 0.5$.

The charge ordering disappears, not for the infinitesimal strength of the magnetic field, but beyond a certain finite strength. The value of $S^z_{\rm tot}$ of the transition corresponds to the magnetic field strength $h \sim J'$. It is consistent with the fact that the energy scale of the AF Heisenberg spin chain system is dominated by J'. In [2] we calculated the charge gap $\Delta_{\rm c}$ of the system, and obtained the result that the infinite-system-size extrapolation value of $\Delta_{\rm c}(L)$ is comparable to the hopping energy t for $t/J' = 0.1$ in the paramagnetic phase. It means that the charge gap is reduced by the magnetic field from $\Delta_{\rm c} \sim t$ at $h = 0$ to $\Delta_{\rm c} = 0$ at $h \sim J'$. The transition discussed in the present paper is an example of melting of the 1D quantum Heisenberg antiferromagnet induced by the magnetic field.

This type of transition is expected to occur in some insulating materials. For instance, in the chain part of $Sr_{14}Cu_{24}O_{41}$, the system is insulating [4] instead of the partially filled Cu 3d band [5, 6, 7]. If the insulating state is caused by the AF interaction between next-nearest-neighbouring electrons, it is possible that the insulator–metal transition which is discussed here occurs under a strong magnetic field. However, it should be noted that the typical magnitude of the magnetic field of the transition must be large, since the energy scale corresponding to the AF interaction should be bigger than the spin gap $\Delta_{\rm s} \sim 140$ K of the system [8].

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