Thermodynamic Properties of the S=1/2 Heisenberg Chain with Staggered Dzyaloshinsky-Moriya Interaction

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Thermodynamic properties of the S=1/2 Heisenberg chain in transverse staggered magnetic field $H_y^s$ and uniform magnetic field $H_z^s$ perpendicular to the staggered field is studied by the finite-temperature density-matrix renormalization-group method. The uniform and staggered magnetization and specific heat are calculated from zero temperature to high temperatures up to $T/J = 4$ under various strength of magnetic fields from $H_y^s/J, H_z^s/J = 0$ to 2.4. The specific heat and magnetization of the effective Hamiltonian of the Yb$_4$As$_3$ are also presented, and field induced gap formation and diverging magnetic susceptibility at low temperature are shown.

I. INTRODUCTION

The one-dimensional spin systems exhibit many interesting physical phenomena. Although these systems have only spin degrees of freedom, their ground state and thermodynamic behavior have diversity with various types of magnetic interactions. Recently, microscopic analysis on Yb$_4$As$_3$, a typical system showing field induced gap opening at low temperature, confirmed that its effective Hamiltonian is a S=1/2 Heisenberg model with Dzyaloshinsky-Moriya (DM) interaction. This microscopic analysis supports previous scenario for the field induced gap opening due to the DM interaction, and stimulates more precise and detailed comparison between experiment and theory.

The Yb$_4$As$_3$ is a 4f electron system, which undergoes charge ordering at 290K [9]. Below this temperature one of the four Yb ions becomes trivalent and forms one-dimensional (1D) chain along [111] direction [10]. The Yb$^{3+}$ ion has one hole in the 4f closed shell. The $J = 7/2$ ground multiplet splits into four doublets by the crystal-field effect. Thus the low temperature dynamics is described by an effective S=1/2 spin chain. The neutron scattering experiments on Yb$_4$As$_3$ actually confirmed that the excitation spectrum is well described by the 1D S=1/2 isotropic Heisenberg model [11].

Unusual features which can not be understood from the 1D isotropic Heisenberg model are observed under applied magnetic fields. One is the upturn of the magnetic susceptibility at low temperature, and the other is the formation of the excitation gap [10,11].

Recently, it was shown that these unusual features are caused by the staggered DM interaction, which generates effective staggered field under applied magnetic fields [12]. Since the staggered spin correlation length $\xi(q=\pi)$ of the Heisenberg model diverges at $T = 0$, drastic change occurs in the ground state. By using a mapping on to the sine-Gordon model, it has been shown that the excitation gap is formed by any finite staggered field [13]. The analytic expressions of the gap, magnetic susceptibility, and specific heat of Yb$_4$As$_3$ are calculated within the sine-Gordon theory, and they are consistent with the experiments at low temperatures [14].

However the sine-Gordon model describes only the low energy physics of the effective one-dimensional S=1/2 model. In the present paper, we directly calculate thermodynamic quantities of the effective Hamiltonian of Yb$_4$As$_3$ over a wide range of temperatures and magnetic fields.

II. MODEL AND METHOD

The microscopic study on the Yb$_4$As$_3$ shows that its low temperature effective Hamiltonian is the S=1/2 anisotropic Heisenberg model with the DM interaction:

$$\mathcal{H} = J \sum_i \{ S_i^x S_{i+1}^x + \cos 2\theta (S_i^y S_{i+1}^y + S_i^z S_{i+1}^z) \} + J \sin 2\theta \sum_i (-1)^i (S_i \times S_{i+1})^z + g H \sum_i S_i^z. \quad (1)$$

Here, $H$ is the uniform external magnetic field perpendicular to the 1D spin-chain. The DM interaction is eliminated by rotating the spins in the staggered way in the x-y plane:

$$\begin{align*}
S_i^x &= \cos \theta \hat{S}_i^x + (-1)^i \sin \theta \hat{S}_i^y, \\
S_i^y &= -(-1)^i \sin \theta \hat{S}_i^x + \cos \theta \hat{S}_i^y, \\
S_i^z &= \hat{S}_i^z.
\end{align*} \quad (2)$$

After this transformation, the Hamiltonian is mapped on to

$$\mathcal{H} = J \sum_i \hat{S}_i \cdot \hat{S}_{i+1} + g H^x \sum_i \hat{S}_i^x + g H^y \sum_i (-1)^i \hat{S}_i^y, \quad (3)$$

where $H^x = H \cos \theta$ and $H^y = H \sin \theta$. This is equivalent to the isotropic Heisenberg model when external magnetic field is absent. Under finite external magnetic field $H$, both the effective uniform field $H^x$ and transverse staggered field $H_y^s$ are applied to the Heisenberg spin-chain.

In order to calculate thermodynamic quantities, we employ the finite-temperature density-matrix renormalization-group (finite-T DMRG) method [15,16]. Since the finite-$T$ DMRG method iteratively expands the quantum transfer matrix in $\beta$-direction restricting the number of basis states, the thermodynamic quantities are obtained for desired temperature. Thermodynamic quantities are obtained from the maximum eigenvalue and its eigenvector of the quantum transfer matrix, and the extrapolation on the system size is not needed [12]. The numerical error is estimated from the eigenvalues of the density matrix which are truncated off, and thus the accuracy is systematically improved by increasing the number of basis states.
with the periodic boundary conditions. The thermodynamic limit is taken by using finite size scaling.

\[ \Delta(H_y) \sim H_y^{0.62} \]

FIG. 1. Excitation gap of the 1D Heisenberg model in the staggered field \( H_y \). The uniform field \( H_x \) is set to be zero. \( J = 1 \), \( g_\perp = 1 \).

\[ \Delta = 1.78(H_y^{0.62}-\ln H_y^{0.62})^{1/6} \]

III. EXCITATION GAP AND MAGNETIZATION

In Fig. 1 we show the excitation gap \( \Delta \) as a function of staggered field \( H_y \). The gap follows power law in the weak staggered field, and is well fitted by the exponent 0.62 between \( H_y \sim 0.002J \) and 2\( J \). The power law dependence is also obtained in the field theory, which predicts \( \Delta = 1.78(H_y^{0.62}-\ln H_y^{0.62})^{1/6} \) including logarithmic correction. This result is plotted in the figure by the dashed line. We find good agreement below \( H_y \sim 0.1J \).

In the region of intermediate strength of the staggered field \( H_y \sim J \), the gap slightly deviate from the predicted power law, but still is quite close to the value \( \Delta = 1.9(H_y^{0.62})^{0.62} \). For strong field \( H_y > 2J \), the spins are almost completely aligned to the staggered field and the gap is given by \( \Delta = H_y + J \) as shown in the dotted line.

The magnetization induced by the magnetic field is shown in Fig. 2. The transverse staggered magnetization \( M_y \) at \( T = 0 \) is shown in Fig. 2 (a), and the uniform magnetization \( M_x \) is shown in Fig. 2 (b). For small staggered fields, the staggered magnetization monotonically increases with increasing uniform field until \( H_x \sim 2J \). This result shows that the uniform field enhances the transverse staggered susceptibility. At \( H_x \sim 2J \), however, the staggered magnetization sharply decreases. The decrease in \( M_y \) is related to the sharp increase in uniform magnetization \( M_x \) as shown in Fig. 2 (b). The substantial change in the ground state at \( H_x = 2J \) is due to the singular behavior at the saturation of \( M_x \) in the limit of weak \( M_y \). For large \( H_y \), both the staggered magnetization and the uniform magnetization show monotonic change and no singular behavior is observed at \( H_y \sim 2J \).

FIG. 3. Transverse staggered magnetization at \( T = 0 \). \( g_\perp = 1 \).
staggered field. This result shows that $\alpha$ is determined by the slope in the figure, and $\alpha = 0.32$ is obtained at $H^x = 0$. This is almost consistent with the result $1/3$ obtained by the field theory \[39\]. With increasing uniform field up to $H^x \sim 1.8J$, the power law exponent $\alpha$ decreases down to 0.24. The field theory also predicts the lowering of the power law exponent \[40\].

The temperature dependence of the staggered magnetization at $H^y = 0.01J$ is shown in Fig. 4. At high temperature, $M^y$ is almost the same for $H^x \lesssim 1.6J$. With decreasing temperature, $M^y$ increases monotonically and becomes almost constant below $T/J \sim 0.2\Delta$. For $H^x = 2J$, the staggered magnetization is small compared with that for small uniform fields $H^x \lesssim 1.6J$, but it continues to increase even at low temperatures below $T/J \sim 0.01$ due to the strongly reduced gap at $H^x = 2J$. For $H^x > 2J$, the spins are almost completely aligned to the uniform magnetic field and the temperature dependence is small.

In Fig. 3 we show the staggered field dependence of the staggered magnetization at fixed uniform field. We plot

$$\frac{d \log M^y}{d \log H^x} \log H^y$$

to eliminate logarithmic dependence on the staggered field. In this figure we find linear dependence for weak staggered field. This result shows that $M^y$ depends on $H^y$ as $M^y \propto (H^y)^\alpha (\log H^y)^\beta$. The power law exponent $\alpha$ is determined by the slope in the figure, and $\alpha = 0.32$ is obtained at $H^x = 0$. This is almost consistent with the result $1/3$ obtained by the field theory \[39\]. With increasing uniform field up to $H^x \sim 1.8J$, the power law exponent $\alpha$ decreases down to 0.24. The field theory also predicts the lowering of the power law exponent \[40\].

In Fig. 5 we show the staggered field dependence of the staggered magnetization at fixed uniform field. We plot $C/T$ and the uniform field $H^x$. $g_\perp = 1$.

IV. SPECIFIC HEAT

Fig. 5 shows the specific heat at several strength of the staggered field $H^y$ under zero uniform field $H^x = 0$. Since the excitation gap exists for finite $H^y$, deviation occurs from the $T$-linear dependence at $T \sim \Delta$. The specific heat has a broad peak below $T \sim \Delta$, and then exponentially decreases down to zero. As shown In Fig. 5 (b), which show the specific heat divided by temperature, the sharp decrease occurs around the temperature $T \sim 0.2\Delta$ with a broad peak at higher temperature $T \sim 0.4\Delta$. The exponential dependence due to the gap is observed only below $T \sim 0.2\Delta$.

The effects of uniform field $H^x$ under a finite staggered field $H^y = 0.01J$ is shown in Fig. 6. The low temperature behavior below $T \sim 0.2\Delta$ is almost the same for $H^x \lesssim 1.6J$. Since the low temperature behavior is characterized by the gap, this result shows almost constant gap for $H^x \lesssim 1.6J$. In contrast to the behavior below
$T \sim 0.2\Delta$, the broad peak at intermediate temperature strongly depend on the uniform field. The maximum of the specific heat around $T/J \sim 0.4$ at $H^z = 0$ becomes smaller and shifts to lower temperature with increasing $H^z$. At $H^z = 1.6$ the small dip appears at $T/J \sim 0.2$, and the main peak is divided into two peaks. With increasing $H^z$, the peak at lower temperature shifts toward $T = 0$. The low temperature behavior is strongly modified at $H^z = 2J$, and the peak at low temperature disappears for $H^z > 2J$. With further increasing $H^z$, the gap turns to increase with clear exponential temperature dependence at low temperature.

V. APPLICATION TO Yb$_4$As$_3$

The magnetization of Yb$_4$As$_3$ is calculated from the effective Hamiltonian Eq. (3) with rotating the spins back to the original coordinates. Thus the magnetization perpendicular to the 1D chain of Yb$_4$As$_3$ is given by $M = M^x \cos \theta + M^y \sin \theta$. The calculated $M$ are shown in Fig. 7 for various tan $\theta$, which is related to the ratio between the DM interaction ($D_{DM}$) and $J$ as $\sin \theta = D_{DM}/J$. The magnetization sharply increases near $H = 0$, and the exponent is 0.32 in the limit of $H = 0$. The magnetization curves gradually change its shape with decreasing tan $\theta$. By fitting the present results with the experimentally obtained magnetization using the experimentally estimated value of $g_\perp = 1.3$, tan $\theta$ is estimated to be 0.19 [17].

Temperature dependence of the magnetization divided by the magnetic field $H$ is presented in Fig. 8. In this calculation we use the parameters tan $\theta = 0.19$, $J = 26K$, and $g_\perp = 1.3$ which reasonably reproduce susceptibility data [17]. We also plot the susceptibility of 1D Heisenberg antiferromagnet (1D-HAF) for comparison. At high temperatures $T > J$ the susceptibility is almost the same to that of 1D-HAF. With decreasing temperature, however, the susceptibility of Yb$_4$As$_3$ largely increases especially for small magnetic field due to the component of the transverse staggered susceptibility of the effective Heisenberg model [17]. The susceptibility diverges at $T = 0$ in the limit of $H = 0$. This is caused by the fact that the staggered correlation length of the Heisenberg model $\xi(g=\pi)$ diverges at $T = 0$.

The specific heat of Yb$_4$As$_3$ under the magnetic field perpendicular to the 1D chain is presented in Fig. 9. The temperature dependence is similar to the results in Fig. 5, but in the present case, uniform field about four times larger than the effective staggered field induced by the DM interaction is present. Similarly to the results in Fig. 5 the specific heat $C/T$ has a maximum around $T = 0.4\Delta \sim 0.6\Delta$ and exponentially decreases down to zero.

It is highly desired that the theoretical results presented in this paper will be compared with experimental results for a monodomain sample under magnetic fields perpendicular to the chain direction.
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