Magnetic excitations in the high-temperature phase of α'-NaV_2O_5

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Abstract

We measured the ^{51}V nuclear spin relaxation rate in the high-temperature phase of the quarter-filled ladder compound α'-NaV_2O_5. We compare the results with theories for the spin-$\frac{1}{2}$ Heisenberg chain and find no serious discrepancies between them.

Key words: α'-NaV_2O_5; NMR; charge ordering; spin excitation

α'-NaV_2O_5 is known to show a charge ordering at $T_C \sim 34$ K which involves valence change of V ions as $2V^{4.5+} \rightarrow V^{4+} + V^{5+}$ [1]. This charge ordering is an insulator-insulator transition [2]; the insulating behavior in the high-temperature phase was explained by the anisotropic electronic hopping amplitude ($t_\perp \gg t_\parallel$) in a quarter-filled ladder [3,4]. In the anisotropic limit, one electron occupies a V-O-V molecular orbital on a rung, and the system becomes equivalent to one-dimensional chains. Indeed, the magnetic susceptibility has temperature dependence similar to that of the spin-$\frac{1}{2}$ Heisenberg chain with $J \sim 560$K [5].

In α'-NaV_2O_5, the anisotropy of the hopping amplitude is not very large, and the inter-site Coulomb repulsion, which is responsible for the charge ordering, is important for the optical properties even in the high-temperature phase [6,7]. Thus the charge fluctuations on the rungs are not small, and it is an open question why the magnetic properties is similar to the spin-$\frac{1}{2}$ Heisenberg chain. In this paper, we report the ^{51}V nuclear spin relaxation rate ($1/T_1$) in the high-temperature phase. We compare the experimental result with the theoretical calculation for the spin-$\frac{1}{2}$ Heisenberg chain, and discuss the difference in the magnetic excitations between α'-NaV_2O_5 and the spin-$\frac{1}{2}$ Heisenberg chain.

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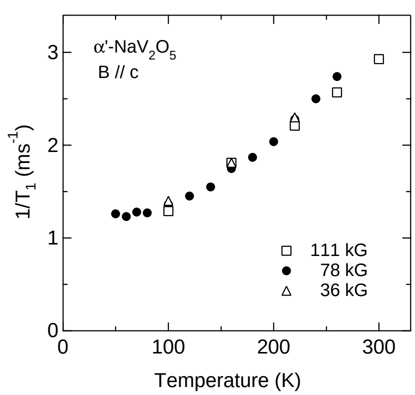

Fig. 1. Temperature dependence of the anisotropy of $1/T_1$ for B = 36, 78, 111 kG along a axis.

The relaxation rate was measured with a magnetically-aligned powder sample for $B\|c$ and a single-crystalline sample for the magnetic field $B\|a$. We show the temperature dependence of $1/T_1$ for $B\|c$ and the anisotropy of $1/T_1$ in Fig. 1 and 2, respectively.

As shown in Fig. 2, the ratio of $1/T_1$ for $B\|a$ to that for $B\|c$ is almost temperature-independent (~ 5.0). If the off-diagonal elements of the hyperfine coupling tensor $A_{\alpha\beta}$ and the supertransferred hyperfine coupling from the nearest neighbor V sites are negligible, this ratio is given by

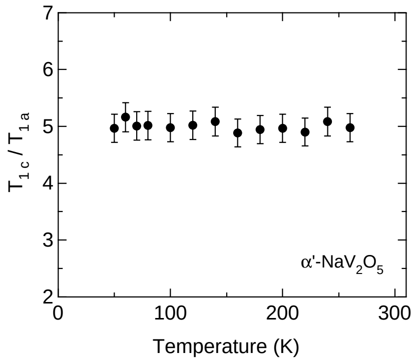

Fig. 2. Temperature dependence of the anisotropy of $1/\mathrm{T}_1$.

$$\left(\frac{1}{T_1}\right)_{\mathrm{a}} \Big/ \left(\frac{1}{T_1}\right)_{\mathrm{c}} = \frac{A_b^2 + A_c^2}{A_a^2 + A_b^2}. \quad (1)$$

The experimental result of the hyperfine coupling, $A_a = -4.4 \times 10^{-19}$, $A_b = -2.9 \times 10^{-19}$, and $A_c = -14.8 \times 10^{-19}$ erg [1,8], gives the ratio 8.2. This disagreement may indicate that the assumption on the hyperfine coupling is wrong. Since A_c is much larger than A_a and A_b, and is dominated by the diagonal contact interaction, it is reasonable to assume that $(1/T_1)_a \propto (A_b^2 + A_c^2)$ in the comparison with the theories.

The dynamics of the spin-$\frac{1}{2}$ Heisenberg chain has been well understood recently with field theory and numerical calculation. At high temperatures, the dynamical structure factor grows sharply as $k \to 0$ and $\omega \to 0$. At low temperatures, on the other hand, spectral weight around $k \sim \pi$ is dominant [9]. To compare the experimental results with the theories, we define the normalized dimensionless relaxation rate as

$$\left(\frac{1}{T_1}\right)_{\mathrm{norm}} = \frac{2\hbar J}{A_b^2 + A_c^2}\left(\frac{1}{T_1}\right)_a \quad (2)$$

with $J \sim 560$K. The $k \sim \pi$ contribution to $1/T_1$, which is dominant at low temperatures, is given by

$$\left(\frac{1}{T_1}\right)_{\mathrm{norm}} \cong 2D\sqrt{\ln\frac{\Lambda}{T} + \frac{1}{2}\ln\left(\ln\frac{\Lambda}{T}\right)}, \quad (3)$$

where $D = (2\pi)^{-3/2}$, $\Lambda = 2\sqrt{2\pi}\mathrm{e}^{\mathrm{C}+1}J$, and C is Euler's constant [10]. This result contains no adjustable parameters.

In Fig. 3, the experimental result is shown with the theoretical one. Below $T \sim 0.2J$, $1/T_1$ is almost temperature independent and near the theoretical value. At higher temperatures, $1/T_1$ increases noticeably, although the theoretical $1/T_1$ decreases slowly. This discrepancy can be due to the $k \sim 0$ contribution to $1/T_1$. This ferromagnetic mode often has diffusive behavior, which leads to strong magnetic field dependence of $1/T_1$. However, as shown in Fig. 1, at high temperatures above 150K, where $1/T_1$ increases remarkably,

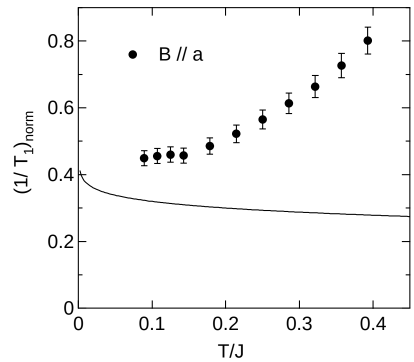

Fig. 3. Normalized relaxation rates. Closed circle shows experimental results for $B\|a$, and solid line does theoretical results.

it depends only weakly on the magnetic field. If the supertransferred coupling is significant, the couplings for the $k \sim 0$ and $\sim \pi$ modes become different. Then the anisotropy of $1/T_1$ should change, when the $k \sim 0$ mode grows with temperature. But this is not the case. Quantum Monte Carlo calculations of $1/T_1$ show only weak temperature dependence below $T \sim 0.5J$ [9]. Only from the present results, it is unclear that the observed dynamics is understood as that of the spin-$\frac{1}{2}$ Heisenberg chain.

Another possible origin of the discrepancy at high temperatures is the effect of charge fluctuation. Recently, a theoretical study on quarter-filled ladders suggests that strong charge fluctuation modifies the magnetic excitaions from those of the Heisenberg chain [11], but it is unknown how it does in detail.

In summary, we measured $1/T_1$ in high-temperature phase of α'-NaV_2O_5 and compared the results with theories for the spin-$\frac{1}{2}$ Heisenberg chain. We found no serious discrepancy between them, but further experimental and theoretical studies are desirable to obtain clear conclusions.

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