

Magnetic-field induced quantum phase transition and critical behavior in a gapped spin system TiCuCl_3

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Abstract

Magnetization measurements were performed on TiCuCl_3 with gapped ground state. The critical density and the magnetic phase diagram were obtained. The interacting constant was obtained as $U/k_B = 313$ K. The experimental phase boundary for $T < 5$ K agrees perfectly with the magnon BEC theory based on the Hartree–Fock approximation with realistic dispersion relations and $U/k_B = 320$ K. The exponent ϕ obtained with all the data points for $T < 5$ K is $\phi = 1.99$, which is somewhat larger than theoretical exponent $\phi_{\text{BEC}} = \frac{3}{2}$. However, it was found that the exponent converges at $\phi_{\text{BEC}} = \frac{3}{2}$ with decreasing fitting window.

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1. Introduction

TiCuCl_3 is an $S = \frac{1}{2}$ interacting dimer system, which has an excitation gap $\Delta = 7.5$ K [1]. In an external magnetic field, the gap closes and the system undergoes magnetic phase transition for $H > 5.4$ T. This phase transition is a magnetic quantum phase transition and is described as the Bose–Einstein condensation (BEC) of spin triplets called magnons or triplons [2]. The BEC theory based on the Hartree–Fock (HF) approximation with a parabolic isotropic dispersion relation $\hbar^2 \mathbf{k}^2 / 2m$ gives the phase boundary described by the power law $(g/2)[H_N(T) - H_c] \propto T^\phi$ with exponent $\phi_{\text{BEC}} = \frac{3}{2}$ [2], where $H_c = \Delta / g\mu_B$ is the gap field. A point given by $T = 0$ and $H = H_c$ on the temperature vs field diagram denotes the quantum critical point. In the previous study [3,4], it was shown that the experimental phase boundary is expressed by the power law with exponent $\phi = 2.0$ – 2.2 . This exponent is somewhat larger than $\phi_{\text{BEC}} = \frac{3}{2}$. Recently, the deviation of the exponent ϕ toward larger value from $\phi_{\text{BEC}} = \frac{3}{2}$ was theoretically discussed [5–7]. Misguich and Oshikawa [7]

extended the HF calculation by Nikuni et al. [2] by using a realistic dispersion relation and achieved remarkable quantitative agreement with the experimental phase diagram. They also calculated the critical density of triplons $n_{\text{cr}}(T)$ and estimated the interacting constant $U/k_B = 340$ K. We carried out magnetization measurements on TiCuCl_3 to reevaluate $n_{\text{cr}}(T)$, U and critical exponent ϕ .

2. Experimental details

Single crystals of TiCuCl_3 were grown by the vertical Bridgman method. The details of preparation were reported in Ref. [3]. The magnetization measurements were performed using SQUID magnetometer (Quantum Design MPMS XL) in the temperature region $1.8 \text{ K} \leq T \leq 100 \text{ K}$ in magnetic fields of up to 7 T. The magnetic fields were applied parallel to the b -axis and $[2, 0, 1]$ direction and perpendicular to the $(1, 0, \bar{2})$ plane. The magnetization measurements were also performed using Faraday Force Magnetometer [8] at Institute of Solid State Physics in the temperature region $30 \text{ mK} \leq T \leq 4 \text{ K}$ in

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magnetic fields up to 8 T. The magnetic fields were applied perpendicular to the $(1, 0, \bar{2})$ plane.

3. Results and discussion

The critical density n_{cr} of triplons corresponds to the absolute values of the magnetization at T_N or H_N . Fig. 1 shows the critical density n_{cr} as a function of temperature obtained from the magnetization measurement. The solid line in Fig. 1 is the critical density calculated with the realistic dispersion by Misguich and Oshikawa with $U/k_B = 320$ K [7]. The experimental and theoretical critical density agree well in the low temperature region for $T \leq 3$ K. From the relation $(g/2)[H_N(T) - H_c] = 2Un_{\text{cr}}(T)$, the interacting constant U is estimated as $U/k_B = 312$, 311 and 315 K for $H \parallel b$, $H \perp (1, 0, \bar{2})$ and $H \parallel [2, 0, 1]$, respectively. Their average is $U/k_B = 313$ K.

Transition temperatures $T_N(T)$ and transition field $H_N(T)$ measured by temperature ($M-T$) and field ($M-H$) scans are summarized in Fig. 2. Phase boundaries for $H \parallel b$, $H \parallel [2, 0, 1]$ and $H \perp (1, 0, \bar{2})$ coincide when normalized by the g -factor and can be expressed by the power law. The solid line in Fig. 2 is the result of the BEC theory based on the HF approximation with the realistic dispersion relations and $U/k_B = 320$ K [7]. Both results agree perfectly for $T < 5$ K.

We analyze the phase boundary for the magnetic field perpendicular to the $(1, 0, \bar{2})$ plane using the power law. In the present analysis, we set the lowest temperature at $T_{\text{min}} = 30$ mK and varying temperature range for fitting.

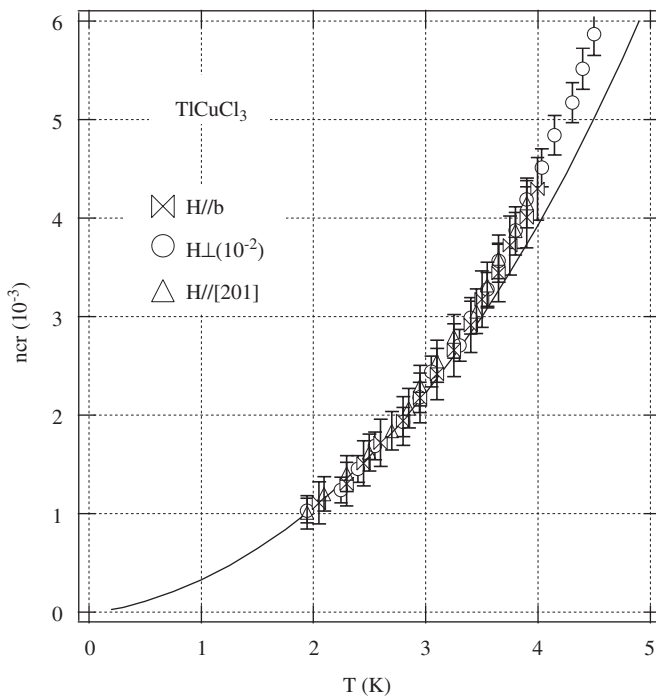


Fig. 1. Temperature dependence of the critical density of triplons in TiCuCl_3 for $H \parallel b$, $H \parallel [2, 0, 1]$ and $H \perp (1, 0, \bar{2})$. The solid line is the theoretical calculation by Misguich and Oshikawa [7].

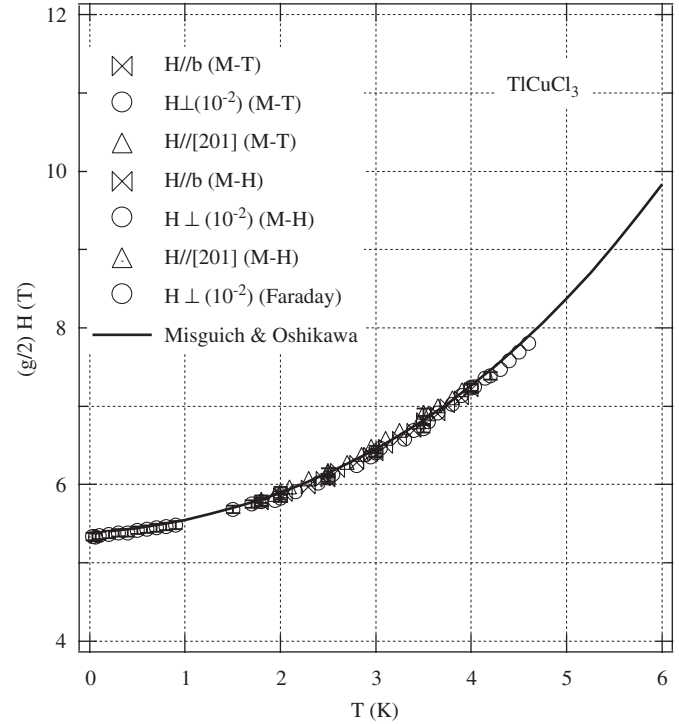


Fig. 2. Phase diagram normalized by the g -factors in TiCuCl_3 . The solid line is the result of calculation by Misguich and Oshikawa [7].

Using all the data points, we obtained $\phi = 1.99$, which is somewhat larger than $\phi_{\text{BEC}} = \frac{3}{2}$ derived by the triplon BEC theory based on HF approximation [2] as obtained in the previous measurements $\phi = 2.0-2.2$ [3,4]. However, the critical exponent ϕ decreases with decreasing fitting window, and converges at $\phi_{\text{BEC}} = \frac{3}{2}$, as predicted by Nohadani et al. [6]. For $T \leq 1.80$ K, we obtain $\phi = 1.52 \pm 0.06$, which is nearly equal to $\phi_{\text{BEC}} = \frac{3}{2}$ derived from the triplon BEC theory [2].

4. Conclusion

We have presented the critical density of triplons and the magnetic phase diagram of TiCuCl_3 . The interacting constant was estimated as $U/k_B = 313$ K. The phase boundary is expressed by the power law and agrees perfectly with the triplon BEC theory based on the HF approximation with realistic dispersion relations and $U/k_B = 320$ K [7]. The critical exponent ϕ decreases with decreasing fitting range. We obtained $\phi = 1.52 \pm 0.06$ for $T \leq 1.80$ K, which is nearly equal to $\phi_{\text{BEC}} = \frac{3}{2}$ derived from the triplon BEC theory [2]. These results strongly support the BEC description of field-induced magnetic ordering in TiCuCl_3 .

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