Kikuchi *et al.* Reply: In the preceding Comment [1], Gu and Su (GS) reported the finite temperature transfer matrix renormalization group (TMRG) method results for the distorted diamond chain (DDC) model. They pointed out that the double-peak behavior of $\chi(T)$ found in experiment cannot be reproduced by our parameter set $J_1{:}J_2{:}J_3 = 1{:}1.25{:}0.45$ [2], but well fitted by $J_1{:}J_2{:}J_{3z} = 1{:}1.9{:}-0.3$ with $J_{3x}/J_{3z} = J_{3y}/J_{3z} = 1.7$.

In response to GS's Comment, we have performed the additional density matrix renormalization group (DMRG) and the exact diagonalization calculations for the magnetization curve $M(H)$ at $T = 0$ of the DDC model with GS's parameter set. As can be seen from Fig. 1, the DMRG $M(H)$ curve with GS's parameter set does not well explain the experimental results.

The positional relations between Cu^{2+} ions corresponding to J_1 and J_3 are very similar to each other as can be seen in the schematic view of the crystal structure of $Cu_3(CO_3)_2(OH)_2$ in Fig. (1b) of our previous Letter [2]. The distance of two Cu^{2+} ions corresponding to J_1 is 327.5 pm with bond angle 113.7° and that to J_3 is 329.0 pm with bond angle 113.5°. Thus it is unlikely that J_1 is antiferromagnetic without the XXZ anisotropy while J_3 is ferromagnetic with strong XXZ anisotropy. Further, as far as we know, such a strong XXZ anisotropy has not been observed at all in the $S = 1/2$ spin systems of Cu^{2+} ions.

The double-peak behaviors of $\chi(T)$ and $C(T)$ are not necessarily attributed to the frustration effect. The mechanism for the double-peak behaviors will be as follows. In the case of $J_2 \gg J_1, |J_3|$ as lowering the temperature, spins coupled by J_2 are going to form singlet dimers at first. The remaining spins are nearly free because they are separated by singlet dimers located between remaining spins. However, there exist weak interactions between nearly free spins mediated by the singlet dimers, which may expressed as an effective coupling J_{eff} as calculated by Honecker and Läuchli [3]. Thus the degree of freedom of the original system can be approximately decomposed into two parts: one is the independent J_2 dimer part and the other is the weakly interacting remaining spin chain part with coupling constant J_{eff}. If $J_2 \gg J_{\text{eff}}$, the Schottky peaks of $\chi(T)$ and $C(T)$ by J_2 will be clearly separated from the Bonner-Fisher peaks by J_{eff}. Otherwise, we will observe the so-called shoulder-type behaviors or the single-peak behaviors. This scenario is not dependent on whether J_3 is antiferromagnetic or ferromagnetic. We think that the decomposition of the degree of freedom might be incomplete for our parameters set, because the condition $J_2 \gg J_1, J_3$ is not well satisfied as already stated in our previous Letter [2]. Thus the double-peak behavior in $\chi(T)$ was not observed in GS's TMRG results for our parameters.

Thus we do not think that GS's parameter set hits the point. Of course, it is also a serious problem that the double-peak behavior of $\chi(T)$ cannot be reproduced by our parameter set. We think that more detailed studies will be needed for the full understanding of $Cu_3(CO_3)_2(OH)_2$ [4].

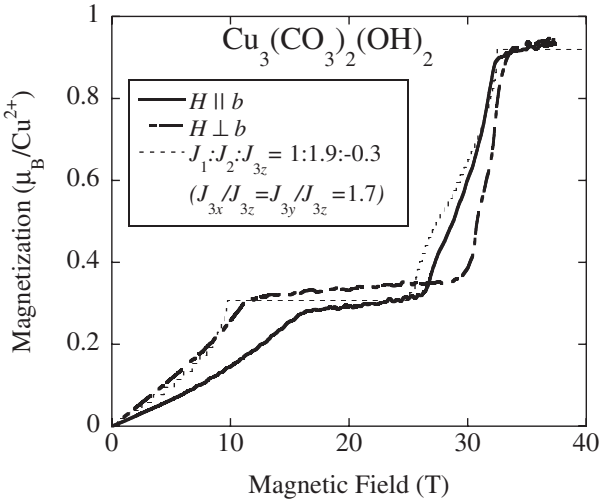

FIG. 1. A comparison between the observed magnetization curve $M(H)$ of $Cu_3(CO_3)_2(OH)_2$ and the calculated one (dotted line) for $H \parallel z$ with GS's parameter set. The solid and dash-dot curves are $M(H)$ for $H \parallel b$ and for $H \perp b$ measured at 1.5 K, respectively.

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