Comment on "Anomalous Thermal Conductivity of Frustrated Heisenberg Spin Chains and Ladders"

In a recent Letter [1], Alvarez and Gros have presented a numerical study of the thermal conductivity of frustrated chains and spin ladders with spin 1/2. Using exact diagonalization of finite systems with $N \leq 14$ sites, they have computed the zero-frequency weight $\kappa^{(\mathrm{th})}(T, N)$, i.e., the Drude weight, of the thermal conductivity where T is the temperature and N the number of sites. One of their main conclusions is that the numerical data indicate a *finite* value of $\kappa^{(\mathrm{th})}$ in the thermodynamic limit ($N \to \infty$) for spin ladders and frustrated chains. In the latter case, this conclusion is based on a finite-size analysis of the high-temperature residue $C(N)$, given by $\lim_{T\to\infty}[T^2\kappa^{(\mathrm{th})}(T, N)] = C(N)$, for $\alpha = 0.1, 0.24, 0.35$ (see Refs. [1, 2] for definitions; also note [3]).

In this Comment, we argue that, from the systems investigated in [1], *no* conclusions of a finite thermal Drude weight in the gapped regime of frustrated chains for $N \to \infty$ can be drawn. This will be corroborated by supplementary data for systems up to $N = 18$ sites. In Figs. 1(a) and 1(b), we show the size dependence of $C(N)$ for $8 \leq N \leq 18$ and $\alpha = 0.35, 0.5, 1$ where $C(N)/C(N = 8)$ is plotted versus $1/N$. Figure 1(b) is a log-log display of Fig. 1(a). An overall and monotonic decrease of $C(N)$ is evident, consistent with a *vanishing* thermal Drude weight for $T \gg J$ and $N \to \infty$. Indeed, the curvature of the curves in the log-log plot of $C(N)/C(N = 8)$ versus $1/N$ suggests that $C(N)$ vanishes more rapidly than any power of $1/N$ as $N \to \infty$. Most important, for the case of $\alpha = 0.35$ and $8 \leq N \leq 14$ studied in [1], the overall decrease of $C(N)$ remains clearly observable, except for minor finite-size oscillations, which, however, justify no extrapolation to a finite value for $N \to \infty$.

In their Letter, Alvarez and Gros have also argued that the behavior of $\kappa^{(\mathrm{th})}(T, N)$ for $\alpha = 0.35$ at *low* temperatures supports the conclusion of a finite thermal Drude weight in the thermodynamic limit. Indeed, there is a crossover temperature $T^*(N^*)$ [4] where the monotonic decrease of $\kappa^{(\mathrm{th})}(T, N)$ with increasing system size observed at high temperatures changes to a monotonic increase of $\kappa^{(\mathrm{th})}(T, N)$ with system size (see Fig. 3 in Ref. [2]). However, as shown in Fig. 1(c), $T^*(N^*)$ decreases with increasing system size already for $N^* \geq 11$, i.e., *including* systems studied in [1], and could well extrapolate to zero for $N^* \to \infty$. In any case, finite-size effects for $T \lesssim 0.1J$ are far too large even at $N = 18$ to allow for any reliable predictions regarding $\kappa^{(\mathrm{th})}(T)$ in the thermodynamic limit.

Summarizing our numerical analysis of gapped, frustrated chains, both in the high- and the low-temperature regime we find no evidence in favor of a finite thermal Drude weight in the thermodynamic limit in contrast to Ref. [1].

Finally, for spin ladders Alvarez and Gros have used only the size dependence of $\kappa^{(\mathrm{th})}(T, N)$ at low temperatures to conjecture a finite $\kappa^{(\mathrm{th})}(N \to \infty)$. In view of the results for the frustrated chain presented in this Comment, we suggest to perform a finite-size analysis of the high-temperature residue $C(N)$ to substantiate this conjecture. We believe that this is important for the analysis of the thermal conductivity in the spin ladder material $La_5Ca_9Cu_{24}O_{41}$[5].

We acknowledge financial support by the DFG and a DAAD-ANTORCHAS exchange program.

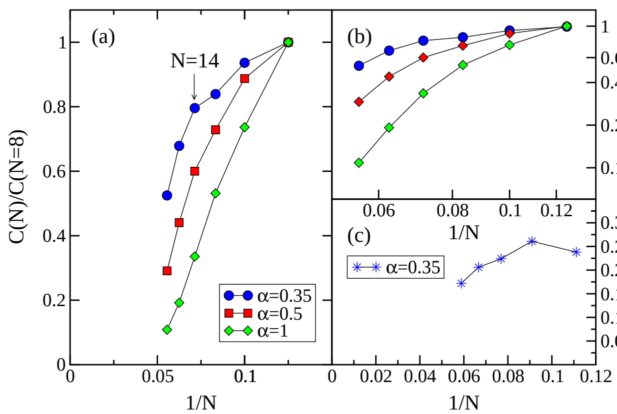

FIG. 1: (a), (b) Size-dependence ($N = 8, 10, 12, 14, 16, 18$) of the high-temperature residue $C(N)$ for different values of the frustration α in the gapped regime. (b) Both axes are scaled logarithmically. (c) Size dependence of $T^*(N^*)$ (see text for details) for $\alpha = 0.35$. Solid lines are guides to the eye.

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[1] J. V. Alvarez and C. Gros, Phys. Rev. Lett. **89**, 156603 (2002).
[2] F. Heidrich-Meisner et al., Phys. Rev. B **66**, 140406(R) (2002).
[3] For $N \leq 14$ and $\alpha = 0.35$ the data in Ref. [1] are identical to that published in [2] which, however, includes systems up to $N = 18$. The definitions of $\kappa^{(\mathrm{th})}$ in Refs. [1, 2] differ by a trivial factor of π.
[4] We define $T^*(N^*)$ by $\kappa^{(\mathrm{th})}(T^*, N+2) = \kappa^{(\mathrm{th})}(T^*, N)$ with $N^* = (N + 1)$ and even N.
[5] C. Hess et al., Phys. Rev. B **64**, 184305 (2001).