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 \( \kappa^{(th)}(T, N) \), 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 \( \kappa^{(th)} \) 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 \( \lim_{T \to \infty} [T^2 C^{(th)}(T, N)] = C(N) \), 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 \( \kappa^{(th)}(T, N) \) 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 \( T^*(N^*) \) where the monotonic decrease of \( \kappa^{(th)}(T, N) \) with increasing system size observed at high temperatures changes to a monotonic increase of \( \kappa^{(th)}(T, N) \) 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 \( \kappa^{(th)}(T) \) in the thermodynamic limit.

Summarizing our numerical analysis of gapped, frustrated chains, both in the high- and 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 \( \kappa^{(th)}(T, N) \) at low temperatures to conjecture a finite \( \kappa^{(th)}(N \to \infty) \). 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 La2Cu9Cu24O41 [5].

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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 \( \kappa^{(th)} \) in Refs. [1, 2] differ by a trivial factor of \( \pi \).
[4] We define \( T^*(N^*) \) by \( \kappa^{(th)}(T^*, N + 2) = \kappa^{(th)}(T^*, N) \) with \( N^* = (N + 1) \) and even \( N \).
[5] C. Hess et al., Phys. Rev. B 64, 184305 (2001).